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Predicting the thermal conductivity of composites based on high density polyethylene-cold plasma modified graphite by application of several analytical micromechanical models

Predicción de la conductividad térmica de materiales compuestos basados en polietileno de alta densidad y grafito modificado con plasma frío mediante la aplicación de varios modelos analíticos micromecánicos

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Abstract

The experimental data of the thermal conductivity of high-density polyethylene composites filled with as-received and modified graphite particles by ethylene plasma polymerization were compared with the theoretical values obtained after applying the following micromechanical analytical models: the series model, the Maxwell model, as well as the Nielsen and the Agari's models. The experimental thermal conductivity of the composites was determined by modulated differential scanning calorimetry. The theoretical results of each model adjusted to a greater or lesser extent to the experimentally obtained data. However, the Agari's model was the one that most closely approximates the experimental values while the series model is the one with the least precision.

Keywords: Thermal conductivity composites, plasma polymerization, Agari's predictive model.

Resumen

En este trabajo, se realiza una comparación de los datos experimentales de conductividad térmica de compuestos de polietileno de alta densidad rellenos con partículas de grafito sin modificar y modificadas mediante polimerización por plasma de etileno con los valores teóricos obtenidos después de aplicar los siguientes modelos analíticos micromecánicos: modelo en serie, modelo de Maxwell, así como los modelos de Nielsen y Agari. La conductividad térmica experimental de los compuestos se determinó por calorimetría diferencial de barrido modulada. Los resultados teóricos de cada modelo se ajustaron en mayor o menor medida a los datos obtenidos experimentalmente. Sin embargo, el modelo de Agari fue el que más se aproxima a los valores experimentales, mientras que el modelo en serie es el que menos precisión tiene.

Palabras clave: Compósitos con conductividad térmica, polimerización por plasma, modelo predictivo de Agari.

1 Introduction

Considering that the number of possible polymer-filler combinations is unlimited, the use of prediction models has become an indispensable tool to theoretically predict the thermal conductivity of the composites for each study, limiting the number of experiments. There are several models that allow with a certain precision, the determination of the thermal conductivity of polymeric composites, such is the case of the Maxwell model, which considers the thermal conductivities of the filler and the polymeric matrix to calculate the thermal conductivity of the compound final (Guo *et al*., 2018), (Guo, Yang, *et al*., 2019). The results obtained with some models are quite close to the experimentally obtained thermal conductivity values (Bigg, 1986), (Lin, Bhatia, & Ford, 1993), (Progelhof, Throne, & Ruetsch, 1976), (Guo, Ruan, *et al*., 2019). These models are classified as: micromechanical analytical models and finite element simulations (H. Chen *et al*., 2016). In this document, reference will be focused on the micromechanical analytical models, which propose the existence of an ideal interface in which the polymer-particle interaction is total, and therefore the interfacial resistance is null, in addition it assumes that the filler is perfectly distributed within the polymer matrix.

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Two of the simplest models to calculate the thermal conductivity of polymeric composites are: the parallel model and the series model, both giving the upper and lower limits, respectively (Cernuschi *et al*., 2004). Almost all experimental results fall between these two models, however, the series model approximates more closely the experimental values (Bigg, 1995). Other models have successfully applied their own theoretical approaches based on various parameters, but these are fundamentally based on the parallel or the series models. Agari, for example, proposes a semi-theoretical model based on the series model, which considers important factors such as the formation of networks or thermal conduction paths as well as the effect of possible changes in the crystallinity of the polymeric resin by the addition of the filler (Agari *et al*., 1993; Agari & Uno, 1986).

On the other hand, the Nielsen model, which is derived from the model proposed by Halpin and Tsai (Abdel Ghafaar *et al*., 2006), conforms quite precisely to the thermal conductivity values of several polymeric compounds (Terao *et al*., 2010), (Weber *et al*., 2003). In this model, the concentration, aspect ratio, and orientation of the filling, as well as the maximum filling fraction of the particles, are considered relevant (Pietrak & Wiśniewski, 2015).

As just mentioned, Agari, Maxwell, Nielsen and series models only consider aspects such as: load content, the thermal conductivity of the load and resin, the formation of thermal conduction networks or paths and changes in crystallinity of the resin by the presence of the load (Agari), aspect ratio and maximum packing fraction of the filling (Nielsen). Because of this, they are quite appropriate to predict in a simple and precise way the thermal conductivity of polymeric composites. Precisely, in this study, the experimentally obtained values were compared with the theoretical values given after applying these models. As will be seen below, the main contribution of the applied models is that the experimental results are quite close to the theoretical results, with the Agari's model being the closest to the experimental values at all load levels because this model considers the effect of the load on the formation of thermal conduction networks or paths and on the crystallinity of the polymeric resin. A brief description of these models is presented below.

1.1 The series model

For polymer composites with homogeneously distributed fillers throughout the polymer matrix, the series model is ideal. In this model, the filler is dispersed in such a way that there is no percolation at any filler level. In addition, it assumes that there is no contact between the filler particles; consequently, the contribution of the particles is restricted to the part of the matrix immediately around the particles. In this model, the thermal conductivity is expressed as:

$$k_c = \left[\frac{1-\phi_f}{k_m} + \frac{\phi_f}{k_f}\right]^{-1} \tag{1}$$

where; k_c, k_m and k_f corresponds to the thermal conductivities of the composite, polymer and filler, respectively, while ϕ_f corresponds to the filler volume fraction (H. Chen *et al*., 2016). As already mentioned, the series model is closer to the experimental results than the parallel model. Due to this, there are some models based on its mathematical approach, although these consider more complex aspects such as weighted averages of thermal conductivities, parameters of semi-theoretical adjustments based on approximations of effective means, etc. Some models derived from the series model are: the Maxwell-Garnett, Rayleigh and the Bruggeman models (L. Chen *et al*., 2016), (Voshchinnikov et al, 2007).

1.2 The Maxwell model

In his work on magnetism and electricity, Maxwell developed analytical expressions to determine the effective conductivity of the heterogeneous medium (Maxwell, 2010). Using the theory of potentials, he established that the conductivity of a mixture of two phases could be expressed as:

$$k_c = k_m\left[1 + \frac{3\phi_f}{\left(\frac{k_f+2k_m}{k_f-k_m}\right)\phi_f}\right] \tag{2}$$

In this model, one of the phases consists of randomly and homogeneously distributed spheres which do not interact with each other. Nevertheless, this expression would only be valid for filler contents below 0.25 volume fraction.

1.3 The Nielsen model

The equation to determine the thermal conductivity (k_c) from this model is the following:

$$k_c = k_m\left(\frac{1+AB\phi_f}{1-B\psi\phi_f}\right) \tag{3}$$

where:

$$A = k_E - 1 \tag{4}$$

$$B = \frac{\frac{k_f}{k_m} - 1}{\frac{k_f}{k_m} + A} \tag{5}$$

$$\psi = 1 + \phi_f \left(\frac{1 - \phi}{\phi^2} \right) \tag{6}$$

A is a constant related to the generalized Einstein coefficient (k_E), which is a function of the aspect ratio and orientation of the filler (Robert F. Landel, 1993). B is a factor that considers the conductivities of the components and ψ is a factor related to the maximum packing fraction of filler. Finally, ϕ is the maximum packing fraction of filler. Table 1 shows some maximum packing fraction values for particles of various shapes.

1.4 Agari's model

Among the several models that consider the ability of the filler to form effective thermal conduction paths or networks (Agari *et al*., 1993; Wunderlich Bernhard, 1976), the Agari's model has been used in the study of several polymer matrices filled with graphite (Agari & Uno, 1986; Bigg, 1995; Wunderlich Bernhard, 1976). In this model, the thermal conductivity of the polymer composite is obtained using the following equation:

$$\log k_c = \phi_f C_2 \log k_f + (q - \phi_f) \log(C_1 k_m) \tag{7}$$

C_1 is a coefficient that considers the effect of the filler on the crystallinity of the polymer and hence, thermal conductivity of the polymer matrix. C_2 is a coefficient related to the ease of forming thermal conduction paths in the composite. Agari's model states that when the parameter $C_1 \geq 1$ the load does not have any significant effect on the crystallinity of the composite and if $C_2 \geq 1$ the formation of thermal conduction networks is feasible, k_c, k_f, k_m, and ϕ_f were previously described.

2 Materials and methods

2.1 Materials

Materials used included: ethylene 99.9% pure from INFRA, México. Graphite (NG) from GrafTech, USA, with particle size $\leq$ 105 μm and density of 2.217 g/cm^3. High Density Polyethylene (HDPE) from PEMEX, México, with crystallinity around 80-85%, melt flow index (MFI) of 5.0 g/10 min, and density of 0.966 g/cm^3.

2.2 Modification via cold ethylene plasma of the NG particles

Cold plasma polymerization has been a technique used to compatibilized materials that require high interfacial interaction (Fabela-Sánchez *et al*., 2019). For the surface treatment of the graphite particles, an Advanced Energy RFX600 13.56 MHz radiofrequency plasma generator, similar to the one described elsewhere (Ramos-de Valle *et al*., 2019; Zendejo-Covarrubias *et al*., 2018) was used. For each treatment, 6 g of NG are placed inside the reactor. Before starting the plasma treatment, the system was stabilized for 15 minutes at 1 $\times 10^{-1}$ mbar.

Table 1. Maximum packing fraction values for several particle types (Weber *et al*., 2003).

Particle Shapes	**Type of Packing**	ϕ
Spheres	Hexagonal close	0.7405
Spheres	Face centered cubic	0.7405
Spheres	Body centered cubic	0.6
Spheres	Simple cubic	0.524
Spheres	Random close	0.601
Spheres	Random close	0.637
Irregular particles	Random close	~0.637
Fibers	Three dimensional random	0.52
Fibers	Uniaxial hexagonal close	0.907
Fibers	Uniaxial simple cubic	0.785
Fibers	Uniaxial random	0.82

Subsequently, the ethylene is introduced until the system reaches a pressure of 4.5 $\times 10^{-1}$ mbar, the system is allowed to stabilize for another 15 minutes. The NG particles are treated at 100 W for 5 minutes (NG 100W-5min) and 60 minutes (100W-60min).

2.3 Preparation of HDPE-NG composites via melt mixing

Polymer composites of HDPE filled with pure NG (HDPE/NG), NG treated at 100W-5min (HDPE/NG 100W-5min), and NG treated at 100W-60min (HDPE/NG 100W-60min) were prepared at five different filler contents: 0.0044, 0.0133, 0.0365, 0.0714 and 0.1574 (volume fraction). For this, a Micro Compounder Xplore 15CC was used. The mixing conditions were: time = 5 min, speed = 60 rpm, isothermal temperature = 170 °C. The injection temperature of the mixture in the molten state was 170 °C. The composites were obtained in the form of specimens with the following dimensions: length = 75 mm, width = 12.7 mm, thickness = 3.25 mm.

2.4 Characterization techniques

2.4.1 Characterization of the NG

Morphological aspects of pure and ethylene plasma treated NG particles were studied in a JOEL JMS-7401F microscope (Field Emission Scanning Electron Microscope) operated at 5 kV, with secondary electron detector (SEI) and a working distance of 8mm between the objective lens and the sample.

2.4.2 Determination of the thermal conductivity of HDPE-NG composites

The thermal conductivity was determined according to the criteria of the ASTM E1952-11 standard (E1952-11., 2017). For this, two cylinders were prepared, the first with a length of 0.4 ± 0.1 mm (thin specimen) and the second with a length of 3.5 ± 0.3 mm (thick specimen), both with a diameter of 6.3 ± 0.2 mm. In this determination, a Differential Scanning Calorimeter in Modulated Mode (MDSC) model Q100 TA Instruments was used. The measurements were made in quasi-isothermal mode. The parameters used in the MDSC were the following: amplitude of sinusoidal temperature oscillation = ± 0.5 °C, oscillation period = 40 s, temperature = 25 ºC, equilibrium time = 15 min.

3 Results and discussion

In the theoretical thermal conductivities of the HDPE-NG compounds calculated using each of the four models described, the thermal conductivity of the graphite (k_f) was considered to be 208 W/mK (Agari & Uno, 1986), while for the HDPE resin (k_m) at 0.436 W/mK. The theoretical thermal conductivities, according to the model of the series and Maxwell (eq. 1 and 2) are presented in Table 2. It is important to clarify that both models considered only the level of load (ϕ_f) and the thermal conductivities of the resin (k_m) and the load (k_f). Because of this, the theoretical thermal conductivity values of HDPE-NG composites are the same for each load level.

In order to use the Nielsen model, it is necessary to choose two suitable parameters for the filler used. Nielsen suggests that for particles with an irregular shape, A=3 and ϕ=0.637 are appropriate (Robert F. Landel, 1993).

As shown in the SEM micrograph presented in Fig. 1, the pure and treated NG particles have irregular size and shape, due to this, the aforementioned values for A and ϕ are considered in this study.

Table 2. Thermal conductivity values obtained using the series and the Maxwell models for HDPE-NG based composites.

Material	ϕ_f vol fraction	k_c (series) W/mK	k_c (Maxwell) W/mK
HDPE/NG	0	0.436	0.436
	0.00438	0.438	0.442
HDPE/NG 100W-5min	0.0133	0.442	0.454
	0.03651	0.452	0.485
HDPE/NG 100W-60min	0.0714	0.469	0.536
	0.15735	0.517	0.678

Table 3. Values of ψ, for different filler vol. fractions (ϕ_f), considering ϕ= 0.637.

Material	ϕ_f	ψ
HDPE/NG	0	1
	0.00438	1.004
HDPE/NG 100W-5min	0.0133	1.012
	0.03651	1.033
HDPE/NG 100W-60min	0.0714	1.064
	0.15735	1.141

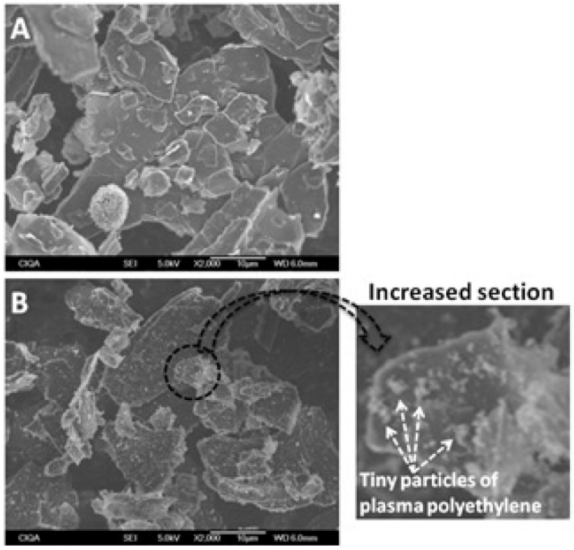

Fig. 1. SEM micrograph of pure (A) and plasma treated (B) NG particles.

Another important aspect that can be appreciated in these images is the many particles of plasma polymerized polyethylene (Ramos-de Valle *et al.*, 2019) deposited on the NG plasma treated particles (Fig. 1B), which are absent in the untreated NG particles (Fig. 1A).

Knowing that: k_f= 208 W/mK [7] and k_m = 0.436 W/mK, and following equations 5 and 6, we proceed to determine the values of B and ψ. Solving these two equations we found that B is equal to 0.992.

Table 3 shows the values of ψ that would correspond to the different values of ϕ_f. After all the parameters required to solve the Nielsen model have been obtained, the theoretical thermal conductivity is determined using eq. 3.

Table 4 shows the results obtained using this model. Although the Nielsen model considers some aspects of the particle, its approach excludes the contribution of plasma treatment in the properties of NG and the thermal conductivity of composites.

Table 4. Theoretical thermal conductivity values obtained for different filler volume fraction (ϕ_f) using the Nielsen model for HDPE-NG based composites.

Material	ϕ_f	k_c (Nielsen) [W/mk]
HDPE/NG	0	0.436
	0.00438	0.444
HDPE/NG 100W-5min	0.0133	0.459
	0.03651	0.502
HDPE/NG 100W-60min	0.0714	0.572
	0.15735	0.779

For this reason, as in the models of the series and Maxwell, the theoretical values of thermal conductivity obtained by the Nielsen model will be the same in all the HDPE-NG composites for each load level.

In order to apply the Agari's model, we first have to obtain the parameters C_1 and C_2. The parameter C_1 is associated with the polymer crystallinity and expresses how it is affected due to the filler presence C_2 is associated with the capacity of the filler to form thermal conduction paths or networks within the polymeric matrix.
Taking eq. 7 of Agari's model:

$$\log k_c = \phi_f C_2 \log k_f + (1-\phi)\log(C_1 k_m) \quad (8)$$

k_c, k_m and k_f correspond to the thermal conductivities of the composite, polymer and filler, respectively, while ϕ_f corresponds to the filler volume fraction. After expanding the second term on the right:

$$\log k_c = \phi_f[C_2 \log k_f - \log(C_1 k_m)] + \log(C_1 k_m) \quad (9)$$

After re-arranging the above, we obtain:

$$\log k_c = \phi_f[C_2 \log k_f - \log(C_1 k_m)] + \log(C_1 k_m) \quad (10)$$

which represents a straight line $y = mx + b$, where:

$$y = \log k_c$$

$$x = \phi_f$$

$$m = C_2 \log k_f - \log(C_1 k_m)$$

$$b = \log(C_1 k_m)$$

This suggests that the difference of the logarithms of the filler and polymer thermal conductivities are linearly related to the filler volume fraction. Thus, after determining the slope and the intercept on the y axis, C_1 and C_2 can be easily calculated (Agari & Uno, 1986). Table 5 shows the experimental thermal conductivities that correspond to the different filler contents.

As already mentioned, the values of C_1 and C_2 are obtained by plotting the logarithms of experimental thermal conductivity vs volume fraction.

Table VI shows the values of C_1 and C_2 in each of the cases. According to the results obtained in parameter C_1, the addition of NG had no effect on the crystallinity of the HDPE, while the results obtained in parameter C_2 indicate that the formation of thermal conduction networks is feasible.

As already mentioned, the values of C_1 and C_2 are obtained by plotting the logarithms of experimental thermal conductivity vs volume fraction.

Table 6 shows the values of C_1 and C_2 in each of the cases. According to the results obtained in parameter C_1, the addition of NG had no effect on the crystallinity of the HDPE, while the results obtained in parameter C_2 indicate that the formation of thermal conduction networks is feasible.

Following the Agari's model, once the parameters C_1 and C_2 have been determined, and knowing that k_f= 208 W/mK (Agari & Uno, 1986) and k_m= 0.436 W/mK, the theoretical thermal conductivities are obtained according to eq. 7. Table 7 presents the experimental and theoretical thermal conductivities obtained via the Agari's model for the untreated and two differently treated graphite particles, each at different contents ϕ_f.The theoretical thermal conductivities obtained using the series, the Maxwell, the Nielsen and the Agari's models are compared with the experimentally obtained data for the studied HDPE-NG composites. The theoretical data were taken from Tables II, IV and VII. These comparisons are presented in Figs. 2, 3 and 4.

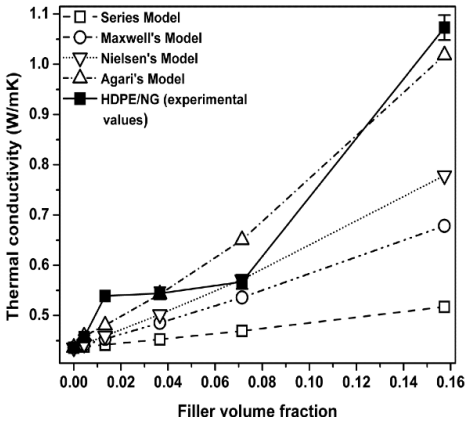

Fig. 2. Theoretical and experimental thermal conductivities vs filler content for the HDPE/NG untreated composite.

Table 5. Experimental thermal conductivities at different filler levels and their logarithms.

Material	ϕ_f [vol. fraction]	k_c [W/mK]	$\log k_c$
HDPE	—-	0.436	-0.36051
HDPE/NG	0.00438	0.457	-0.34011
	0.0133	0.539	-0.26788
	0.03651	0.544	-0.26494
	0.0714	0.567	-0.24643
	0.15735	1.073	0.03059
HDPE/NG 100W-5min	0.00438	0.539	-0.26815
	0.0133	0.597	-0.22407
	0.03651	0.624	-0.20505
	0.0714	0.714	-0.14632
	0.15735	1.115	0.04671
HDPE/NG 100W-60min	0.00438	0.483	-0.31576
	0.0133	0.54	-0.26768
	0.03651	0.557	-0.2547
	0.0714	0.636	-0.19657
	0.15735	1.033	0.01394

Table 6. Values obtained for C_1 and C_2 for each of the studied composites.

Material	C_1	C_2
HDPE/NG	1.029	0.826
HDPE/NG 100W-5min	1.158	0.824
HDPE/NG 100W-60min	1.067	0.790

The graph presented in Figure 2 corresponds to the theoretical and experimental thermal conductivity values as a function of the filler content for the HDPE/NG compound. For loads from 0 to 0.071, the models of Maxwell, Nielsen and Agari approximate the experimental results with greater precision about the model of the series, however, for loads of 0.157 models of the series, Maxwell and Nielsen are clearly below of the value obtained experimentally.

The Maxwell model assumes that the filler particles are spherical (Maxwell, 2010), and the particles are limited to a certain degree of dispersion. However, the formation of thermal conduction roads had a favorable effect when there are the laminar structures of the NG and proper distribution of the fill during the mixing process of the elaboration of the composites. Hence, the experimental values are higher than those predicted by this model since their approach is not considered these variables.

Regarding the Nielsen model, it can be seen that as the load level increases, the theoretical values move away from the experimental ones, it is known that this model becomes unstable to increase the load level (Pietrak & Wiśniewski, 2015). The Agari's model fits more accurately with most of the experimental results because in its approach it considers the effect of the load on the crystallinity of the polymer matrix (C_1) and the ease of forming thermal conduction paths C_2 (Agari *et al*., 1993; Agari & Uno, 1986).

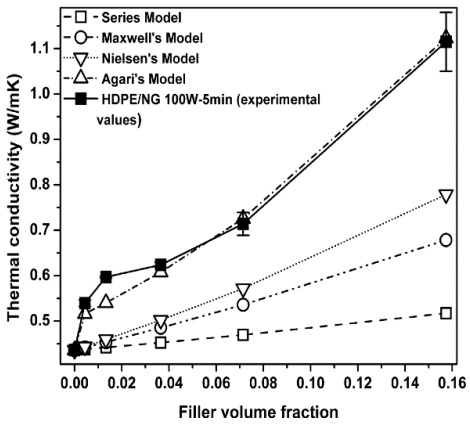

Fig. 3. Theoretical and experimental thermal conductivities vs filler content for the HDPE/NG 100 W-5 min composite.

Table 7. Thermal experimental and theoretical (Agari) conductivities as a function of ϕ_f.

Material	ϕ_f [vol. fraction]	k_c [W/mK]	k_c Agari [W/mK]
HDPE	—-	0.436	0.436
HDPE/NG	0.00438	0.457	0.459
	0.0133	0.539	0.481
	0.03651	0.544	0.542
	0.0714	0.567	0.651
	0.15735	1.073	1.018
HDPE/NG 100W-5min	0.00438	0.539	0.516
	0.0133	0.597	0.54
	0.03651	0.624	0.608
	0.0714	0.714	0.726
	0.15735	1.115	1.123
HDPE/NG 100W-60min	0.00438	0.483	0.476
	0.0133	0.54	0.497
	0.03651	0.557	0.558
	0.0714	0.636	0.664
	0.15735	1.033	1.019

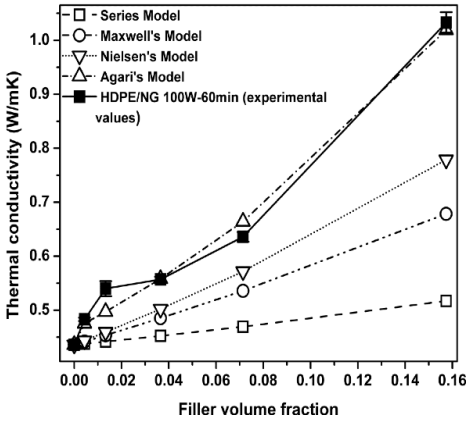

Fig. 4. Theoretical and experimental thermal conductivities vs filler content for the HDPE/NG 100 W-60 min composite.

Figs. 3 and 4 that correspond to the polymeric composites with plasma treated NG particles, show fairly similar behavior. Again, the thermal conductivity values predicted by the series, the Maxwell and the Nielsen models fall below the experimental data curve. The series and the Maxwell falling far below. Again, the Agari's model seems to be quite consistent with the experimental results at all studied filler contents. The parameters C_1 and C_2 (Table 6) have an important role in the theoretical estimation of the thermal conductivity of polymer composites (Agari *et al*., 1993; Agari & Uno, 1986).

In addition, it is observed that polymeric composites with plasma treated NG particles consistently show a higher thermal conductivity than those with untreated NG particles. It is assumed that the plasma polyethylene deposited on the treated NG particles surface (Figure 1B) acts as interphase (Aguilar-Madera *et al*., 2011), (Martín del Campo *et al*., 2019), promoting the interaction with the polyethylene and preventing the phonons dispersion during the thermal conduction process (Krupa & Chodák, 2001), (Ramos-de Valle *et al*., 2019). On the other hand, by increasing the interaction of the fill whit the polymer through this interface, the modified NG particles are distributed homogeneously in the polymer matrix, which favors the formation of thermal conduction networks (C_2) (Ramos-de Valle *et al*., 2019).

Conclusions

Composites loaded with plasma-treated NG have higher conductivity values than those loaded with untreated NG. This fact is attributed to that the plasma polyethylene deposited on the NG promotes thermal conduction between the limits of the particle and the polymer, thus avoiding the dissipation of phonons during the thermal conduction process.

Of the four models studied, Agari's model adjusts more precisely to the experimental results. It is assumed that this is because it considers two phenomena that have a significant impact on thermal conductivity, the effect of the load on the formation of thermal conduction trajectories (C_2), as well as on the crystallinity of the polymer matrix (C_1). The thermal conductivities predicted by the Agari's model coincide with high precision with the experimental values. This occurs more so with the composites filled with ethylene plasma treated NG composites.

The thermal conductivities predicted by the series, the Maxwell and the Nielsen models, tended to give lower values than the experimental results. Additionally, in these three cases, the predicted values of thermal conductivity moved away from the experimental data, as the filler content increases. In all cases, the series model was the one with the most significant disparity.

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