RECyT
Year 24 / Nº 37 / 2022 / 64–72
DOI: https://doi.org/10.36995/j.recyt.2022.37.008

Simulation of the electrical percolation of carbon nanotube composites in polymethylmethacrylate matrix: two-dimensional and three-dimensional analyses using a tortuosity effect of nanofillers

Simulación de la percolación eléctrica de nanotubos de carbono a través de una matriz de polimetilmetacrilato: análisis bidimensional y tridimensional usando el efecto de la tortuosidad de los nanoaditivos

Jessica P. Silva[1], Lailson Sousa[1], Harvey A. Villa-Vélez[1], Paulo H. S. L. Coelho[1, *]

1- Departamento de Ingeniería Química, Universidade Federal do Maranhão, São Luís, Maranhão, Brasil.
*E-mail: coelho.paulo@ufma.br

Received: 11/03/2021; Accepted: 14/12/2021

Abstract

The present work aims to study the simulation of the electrical percolation of carbon nanotubes (CNTs) in polymethylmethacrylate matrix (PMMA). In order to do this, simulations were employed in two-dimensional and three-dimensional analyses through a program developed by the Monte Carlo method, supported by the excluded volume model in order to analyze the geometric tortuosity in the polymeric matrix. The percolation threshold was analyzed by different aspect ratios, volumetric fractions and conductive load geometries. In the simulations, a decrease in the percolation threshold was observed when the aspect ratio increased and the particles became more tortuous, being these characteristics the parameters to evaluate both two-dimensional and three-dimensional systems. The results show percolation threshold values of 0.625% vol and aspect ratio of 1000 for two-dimensional analyses and, 0.08% vol and aspect ratio of 250 for three-dimensional analyses, being the adequacy to the main models for electrical percolation with tortuosity effect of the nanocarriers proposed by literature.

Keywords: Carbon nanotubes; Cubic-matrix approach, Monte Carlo method; Polymethylmethacrylate; Tortuosity.

Resumen

El presente trabajo tiene como objetivo estudiar la simulación de la percolación eléctrica de nanotubos de carbono (CNT) en matriz de polimetilmetacrilato (PMMA). Para ello, se utilizaron simulaciones en análisis bidimensionales y tridimensionales a través de un programa desarrollado utilizando el método Monte Carlo, apoyado en el modelo de volumen excluido para analizar la tortuosidad geométrica en la matriz polimérica. El umbral de percolación se analizó mediante diferentes relaciones de aspecto, fracciones volumétricas y geometrías de carga conductiva. En las simulaciones, se observó una disminución en el umbral de percolación cuando aumentaba la relación de aspecto y las partículas se volvían más tortuosas, siendo estas características los parámetros para evaluar sistemas tanto bidimensionales como tridimensionales. Los resultados muestran valores de umbral de percolación de 0.625% vol y relación de aspecto de 1000 para análisis bidimensionales y 0.08% vol y relación de aspecto de 250 para análisis tridimensionales, siendo la adecuación a los principales modelos de percolación eléctrica con efecto de tortuosidad los nanoaditivos propuestos por la literatura.

Palabras clave: Nanotubos de carbono; Enfoque de matriz cúbica, Método de Monte Carlo; Polimetilmetacrilato; Tortuosidad.

Introduction

Currently, the application of polymeric materials has been intensified in areas of material science, engineering and technology industries due to its large scale production, simple processing and higher capacity to be combined with others materials (Birman & Kardomateas, 2018; Formela, Zedler, Hejna, & Tercjak, 2018). These materials offer a versatile alternative to metallic and ceramic biomaterials which suffer from stress shielding and effects that are a

result of their high elastic modulus (Ramesh, Moratti, & Dias, 2018). In contrast, polymers have high malleability and lightness. Also, when compared with metals, they show low resistivity, tenacity and conductivity (Huang & Cheng, 2017; Ondreas et al., 2019).

Amongst all polymers, the polymethylmethacrylate or PMMA is a promising polymer for applications in electro-diffusion or electro-osmotic flow, sensors, analytical separation, and conductive devices (Ali, Karim, & Buang, 2015). Due to its compatibility and easy processing as a polymer moiety, PMMA can be incorporated with inorganic materials such as carbon black (CB), carbon nanotubes (CNT), graphite (G) and carbon fiber (CF), playing an important role in nanotechnology development (Sun, Bao, Guo, & Yu, 2009). PMMA is a polymer that enhances the behavior at the interface between the carbon nanotube and the copolymer (Khun Nay, Loong Poh, Liu, & Li, 2016).

Since its discovery in 1991, carbon nanotubes, as a single material, have shown excellent mechanical, electrical and thermal properties (Liu & Kumar, 2014). By dispersing the nanotubes in the polymeric matrix, they form a network of percolation with paths that allow the transportation of electrical current, at a certain concentration of composite named percolation threshold (p_c). Its high aspect ratio makes the p_c lower when compared with conventional fillers (Kim, Chae, Choi, Yoon, & Jin, 2008). Thus, when added in polymers such as PMMA, a stability improvement was found on the electrical, mechanical and thermal properties of the composite (Ali et al., 2015; Moaseri et al., 2020). The main issue of the polymeric composite conductors is related with the conductivity variation as function of the concentration of conductive particles, where there is a critical concentration, occurs a conductivity increase in the system, being the phenomenon explained by the theory of percolation (Lux, 1993; Sun et al., 2009).

Percolation in the reinforced composite happens by the alignment and movement of carbon nanotubes in the porous media of the polymeric matrix. Percolation depends on the material loads in the polymeric matrix, since the modeling of the electrical percolation of carbon-filler-filled is very important for the conductive behavior prediction of the materials and its design (Moaseri et al., 2020; J.-E. Park et al., 2018).

Several models have been proposed to describe the value of p_c, and basically consist in determining a set of points distributed in the space, and among them there are some linked pairs. The occurrence of these point connections is governed by a random mechanism. These models can be classified in two groups: the percolation by site and percolation by link (stru¨mpler & Glatz-Reichenbach, 1999). The percolation by site considers the surface as a large square net in which each square is called a site (S), having the same separation distance, with probability (p) to be filled and (1-p) of not being filled, if filled, leaves to the adjacent site forming a conductive network. Percolation by link also considers a square network, with a link between the sites in which the probability is (p) of connecting with neighboring sites and (1-p) of not connecting. Both models form points connected in order to establish a cluster that carries electric current (Lux, 1993; Stauffer & Aharony, 1994).

Although the percolation phenomena in polymeric matrix have been investigated either by numerical, analytical and semi-empirical modeling techniques (Kumar & Rawal, 2016), some of these techniques were compared and combined together to simulate the percolation threshold of nanocomposites. For this, the excluded volume model proposed by Balberg et al., (Balberg, Anderson, Alexander, & Wagner, 1984) is an universally accepted continuum analytical model that has been applied in combination with Monte Carlo simulations for predicting the p_c of a wide variety of nanocomposites fillers (Coelho, Armellini, & Morales, 2017; S.-H. Park et al., 2019). The excluded volume model considers a geometry as cylindrical sticks with high aspect ratio. This model sets an object, in which its center does not overlap the center of another similar object (Kumar & Rawal, 2016). Therefore, it is of paramount importance that the three-dimensional orientation distribution of fillers should be considered for predicting the p_c.

Many studies on the electrical percolation of these systems consider that the conductive loads have the form of cylinders or straight and rigid spherical cylinders (Balberg et al., 1984; Berhan & Sastry, 2007; Konobeeva, 2018; Muñoz-Sandoval et al., 2017). Such approximation, despite being relatively good for most systems, poorly describes the reality of nanocomposites, since the microscopic structural reality of these loads reveals an undulating and tangled behavior (Berhan & Sastry, 2007). Therefore, percolation models that include tortuosity, or the undulation of loads, are necessary for better representation of these systems. Studies carried out in both two and three dimensions have shown that the percolation threshold decreases when the tortuosity of loads is increased (Berhan & Sastry, 2007; Mutiso & Winey, 2015).

In this study, the two-dimensional analyses and three-dimensional analyses of the electrical percolation threshold of CNT particles in PMMA matrix were addressed, simulating the effect of the tortuosity of nanofillers on the critical concentration.

Simulation procedure

Software performance

In the research, all the programing used to assemble the matrices and perform the simulations were developed through the FORTRAN 95 language (Fortran Company, Chandler, USA).

Algorithm description

The developed programs generated two-dimensional square (2D) matrices with 1000 side elements, and three-dimensional cubic (3D) matrices with 750 edge elements, in which matrix points, defined as 0, represented the insulating polymeric material.

The volumetric fraction of particles presented in the matrix was determined at the beginning of the program by the user himself. Starting from the value of the volumetric fraction informed, the programs calculated the number of particles that must be generated to meet the percentage of conductive material supplied. The initial elements, from which these particles were constructed, were chosen randomly by the program (Monte Carlo Method), from the generation of 2 random positions for 2D matrix (x and y coordinates), Fig. 1*a*, with 4 growing possibilities, and 3 random numbers for 3D matrix (x, y and z axis coordinates), with 8 growing possibilities, Fig. 1*b*. These starting points received a new value of 1, representing the conductive material. At each set of initial coordinates, the program checked if the element in the position identified by these coordinates had a value of 0. Otherwise, a new set of coordinates was generated, because two particles cannot originate from the same starting point.

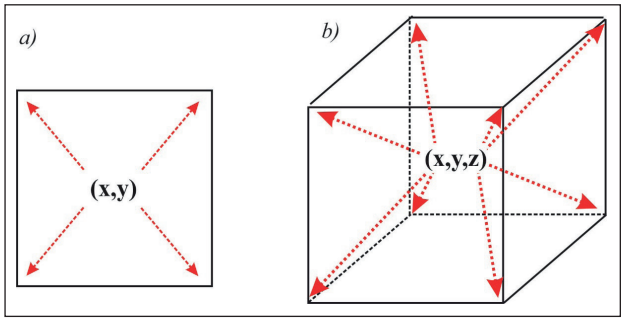


Fig. 1.: Scheme of particles random generation: a) 2D and b) 3D.

From these points, particles were generated according to their respective geometries, the effect of tortuosity of the loads included. As they were constructed, the matrix elements occupied by them received the value of 1, as well as the initial points, identifying them as elements capable of conducting the electric current. Elements that were not occupied by particles continued with the value 0, indicating the absence of conductive material and, therefore, pertinent to the insulating polymer.

As it presented a favorable implementation and reduction of computational effort, the soft-core model (Berhan & Sastry, 2007) was used for the representation of particles, which means that it is possible to superimpose the loads (the same element of the matrix can belong simultaneously to two or more of the generated particles). The growth of the particles is interrupted if the limits of the matrix are reached, generating smaller particles than predicted. Thus, after the end of particle generation, the volumetric fraction value occupied by conductive particles at the end of the program may be lower than the value provided by the user, due to the use of the soft nucleus and the interruption of the growth of particles that would exceed the matrix limits. To solve this problem, the program scans the fraction of elements that was actually filled in the matrix and, if this value was less than 99% of the user-supplied value, new particles were generated in order to reduce this error. This scan was performed until the actual volumetric fraction of particles shows an error of less than 1% in relation to the value imposed by the user.

The number of simulations performed by the program was also defined by the user, and positions of particles in the matrix were modified at each simulation. A system completely independent than the latter was obtained in each simulation. After the generation of conductive particles and the confirmation of the fraction occupied by the conductive material, a new sweep was performed from the upper face of the matrix to the lower face, verifying if there were paths formed between the points, which allow the conduction of electric current along the entire matrix. The sweep was performed as it follows: the values of the entire upper face of the matrix were assigned as 2, which indicates the elements in which there was electrical conduction. Then, the elements that were in the vicinity of these with value 2 were examined (here, the tunneling effect was considered, the elements that are at a distance equal to or less than two matrix elements were considered to the effect). If the evaluated elements have the value of 1, it is assigned the value of 2, which means that until that element, there was passage of current. The sweep was made in all layers of the matrix, from top to bottom, until it reaches the bottom face. If there was a value element of 2 on this side, it means that the current has passed through the entire length of the array and, therefore, the material was conductive. Percolation threshold was defined as the concentration (in terms of occupied volumetric fraction) of conductive particles from which percolation occurs in at least 50 out of every 100 simulations, i.e. 50% connection possibility (CP) (Cheng, Wang, Pan, & Zhang, 2014).

Mathematical modeling

Considering that the deleted volume (V_{ex}) and the percolation threshold (p_c) are inversely proportional quantities [11-13], as shown in Eq. (1):

$$p_c \propto \frac{1}{V_{ex}} \tag{1}$$

From Eq. (1), for a 3D system was possible to define the critical volumetric concentration of percolation through the total excluded volume of particles (V_{ex}), as observed in Eq. (2):

$$p_c = 1 - \exp^{\left(-\frac{<V_{ex}V>}{<V_e>}\right)} = 1 - \exp^{(-N_c V)} \quad (2)$$

were V is the real volume of particle, V_e is the excluded volume of particle and N_c is the number of particles. According to Balberg et al., (Balberg et al., 1984), this same concept of volume can be applied to 2D systems, considering the excluded area for each particle.

For the insertion of the aspect ratio (*ar*) in the simulator, *t* fiber diameter was defined as unitary, so that the value inserted in the programming was only the length of the tube. Thus, was possible to calculate via CNT number the concentration desired by the user for 2D from Eq. (2), being this number determined by Eq. (3):

$$N_{CNT(2D)} = \frac{10^6 \cdot V_{CNT}}{ar} \quad (3)$$

where V_{CNT} is the CNT volumetric fraction simulated and *ar* is the aspect ratio.

The number of CNT for 3D generated by the program is given by Eq. (4):

$$N_{CNT(3D)} = \frac{750^3 \cdot \frac{V_{CNT}}{100} + 1}{ar} \quad (4)$$

Results and discussion

Two-dimensional simulation

Fig. 2 shows the two-dimensional particles simulation at different geometries and aspect ratio (*ar* = 40).

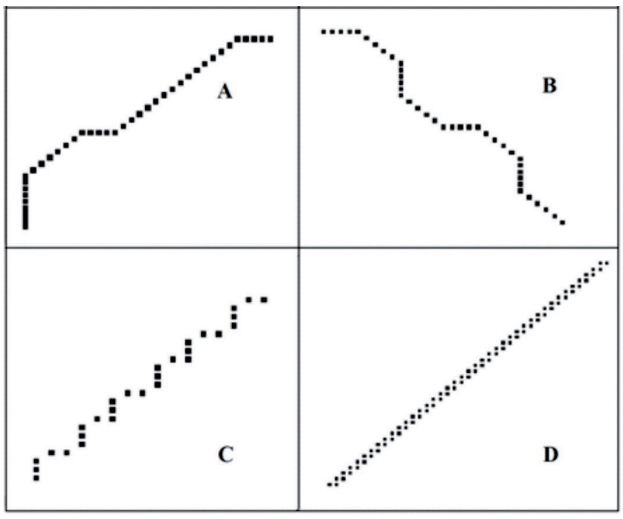


Fig. 2.: Two-dimensional simulation with tortousity effect for the geometries A, B, Cand the discretized linear geometry D.

In Fig. 2, the tortuous geometries simulated were tested at different aspect ratio values (500, 1000, 2000 and 4000) varying the volume fraction of the particles. The polymeric matrix represented by the quadratic form shows an electrical percolation of the CNT with no traditional ways compared with the cylindrical sticks with high aspect ratio from the percolation theory, showed in the geometry D. In this, different ways of the CNT percolated into the PMMA matrix were obtained at different aspect ratios, going from a geometry A with low aspect ratio and linear wavelength between the CNT, followed by a geometry B with a medium aspect ratio and cyclic entangled between the CNT, finishing with geometry C which is entangled at a high aspect ratio with cylindric form between the CNT. Thus, from the simulation with the totuosity, electric percolations of CNT in the PMMA matrix with different ways can be constructed using the excluded volume method. These entangled forms can be compared with an electronic micrography of the CNT (Muñoz-Sandoval et al., 2017; Soleimani et al., 2018), once their structure does not demonstrate an unique geometry between the percolate fillers of the CNT.

Park et al., (S.-H. Park et al., 2019) shows the importance of the agglomerate representation in matrix to reach the percolation threshold. In their results, the number of current paths has a proportional relationship with the average number of CNT that cross a neck formed between two neighboring fillers, this is, as the number of fillers increases, the number of necks subsequently increases. For a fixed number of CNT in the composite system, only a subset of necks that has CNT crossing can contribute to the current paths of the percolating network. Moaseri et al., (Moaseri et al., 2020) shows that the formation of many clusters influences the mechanical properties of nanocomposites, because higher reinforcement loads led to a decrease in the tensile strength of the composites, which can be attributed to the aggregation of the CNT. In higher concentrations, long-range attractive Van der Waals forces can overcome the short-range repulsive depletion forces of the polymer chains and cause aggregation of the CNT.

Fig. 3 and Table 1 reveal the expected trend, where the higher the aspect ratio the lower the percolation threshold. Comparing the discretized geometry D with the authors Coelho et al., (Coelho et al., 2017), who used the same discretization, it can be observed that simulation results, for the same methods and models applied, showed values up to 50% lower, better adapting to the excluded volume model proposed by Balberg et al., (Balberg et al., 1984), however, with values of p_c above, that would be the real condition, 3D, the possibility of contact between the particles would be greater, consequently requiring lower concentrations of loads for percolation. This difficulty of adaptation of the excluded volume model for 2D system was smoothed by the addition of the tortuosity effect. Thus, the geometry A shows the best results with a p_c = 0.15% vol of CNT and aspect ratio of 4000. It is believed that due to its geometry, the probability of contact with neighboring particles was

eased by the greater expansiveness of the particle, obtaining greater geographical reach, as can be seen in Fig. 4, when compared with a linear particle such as the presented by geometry D, having a positive influence on the decrease of the percolation threshold.

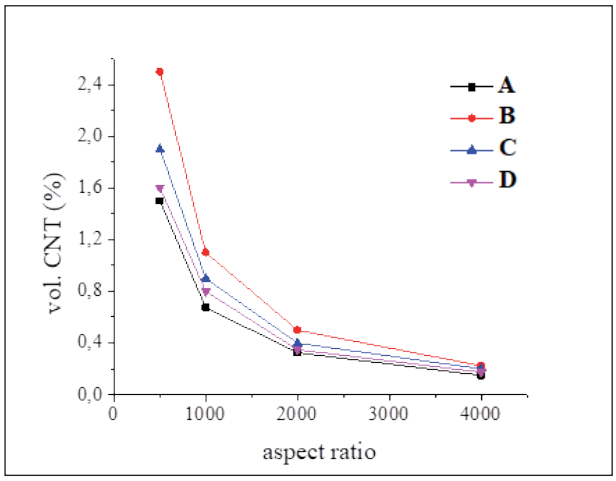


Fig. 3.: Volumetric concentration of the CNT vs. aspect ratio for the different simulated geometries (A, B, C and D).

Table 1: Comparison between percolation thresholds for the simulated geometries A, B, C and D at different aspect ratios.

Simulated geometry	Aspect ratio (ar)			
	500	1000	2000	4000
A	1.500	0.675	0.325	0.150
B	2.500	1.100	0.500	0.225
C	1.900	0.900	0.400	0.200
D	1.600	0.800	0.350	0.175

Comparing the results of the p_c values simulated in 2D with the literature, thresholds belonging to *ar* of 1000 can be observed, ranging from 0.6 to 1.0 % vol, being 0.675 % vol (geometry A) the best value, similar to the one described by Li and Chou (Li & Chou, 2007), with *ra* values around 0.6% vol. For the thresholds simulated at *ar* of 500, Konyushenko et al., (Konyushenko et al., 2006) similar values were presented for carbon nanotubes coated with polyaniline. On the other hand, the results of *ar* of 2000 were higher than those estimated by Ha et al., (Ha, Grady, Lolli, Resasco, & Ford, 2007) for a matrix with carbon nanotubes and styrene-isoprene copolymer latices.

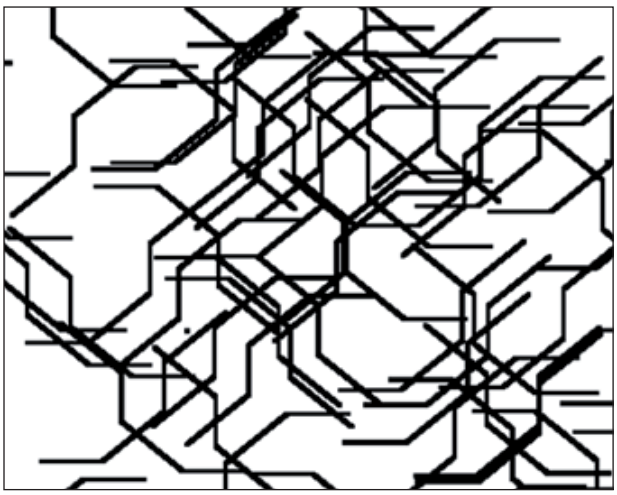


Fig. 4.: 2D Illustration of the percolated system with 0.150% particle geometry A, and ar = 4000.

Three-dimensional simulation

Two geometries with the aspect ratio values of 50, 100, 150, 250 were evaluated, varying the volumetric fraction of the particles. Fig. 5 shows the three-dimensional simulation of the particles with tortuosity effect at different geometries and *ar* = 40.

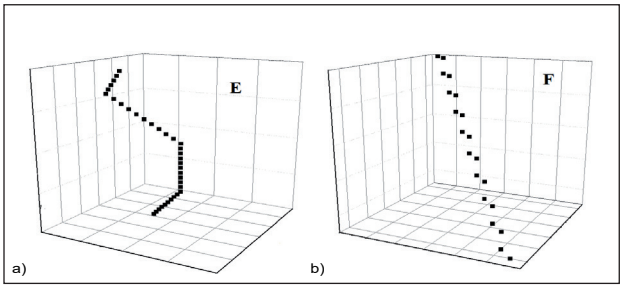


Fig. 5.: Three-dimensional simulated particles with tortuosity effect. Geometry E (Fig. 5a), derived from the geometry A and, geometry F (Fig. 5b), comprises the discretized linear, the geometry D.

In Fig. 5 the 3D simulation of the electrical percolation into de cubic polymeric matrix of PMMA shows a longer wavelength filler of CNT. The tortuosity effect shows free movement of CNT at a low aspect ratio, where, overlapping this geometry simultaneously on the polymeric cubic structure, an entangled behavior (Fig. 6) similar to the one seen in the micrograph content can be observed.

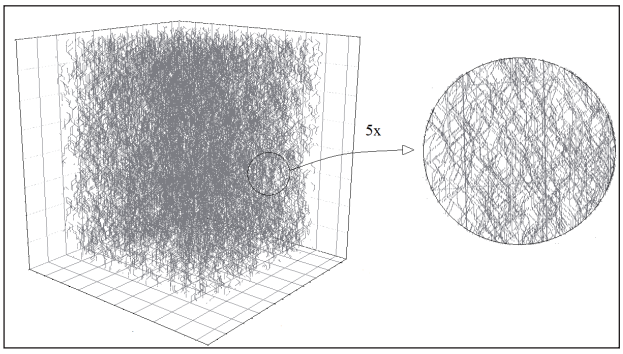
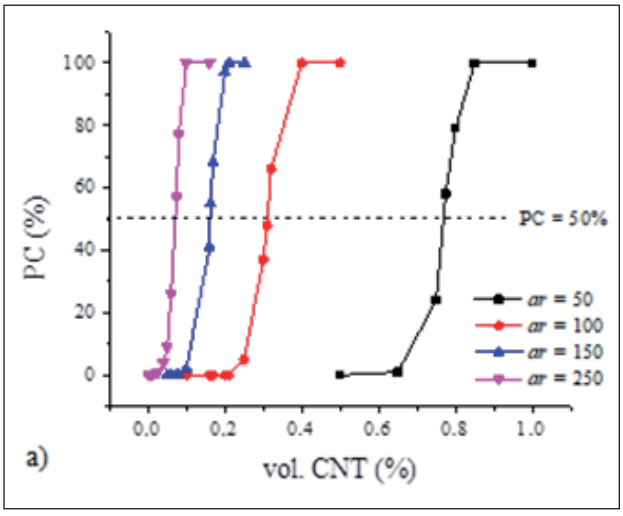


Fig. 6.: Entangled simulation of the electrical percolated system using the geometry E with 0.5 vol. % and ar = 50.

Fig. 7 shows the p_c value simulation, by analyzing the CNT volumetric fraction curve as a function of the possibility of connection (PC), where the black traces show a percolation value of 50% for 100 simulated matrices, a definition derived from literature (Konobeeva, 2018). The analysis shows a consistent result with 2D simulation, where tortuosity led to a decrease in the p_c value related with the linear particle, calculating values of p_c = 0.08% vol for *ar* = 250 and geometry E (Table 2). This decrease can be explained by the possibility expansion of three-dimensional contact of the CNT fillers with surrounding particles, favoring a possible electric current by tunneling, directly influencing the structural formation of the percolative network. It was also possible to notice considerable decrease of p_c related with square matrices, showing a better adaptation to the model by Balberg et al. (Balberg et al., 1984), and in agreement with the values found by Chen et al. (Cheng et al., 2014), who simulated CNT in a 3D system and obtained p_c values between 0.548 and 0.045% for *ar* between 100 and 1000, respectively.



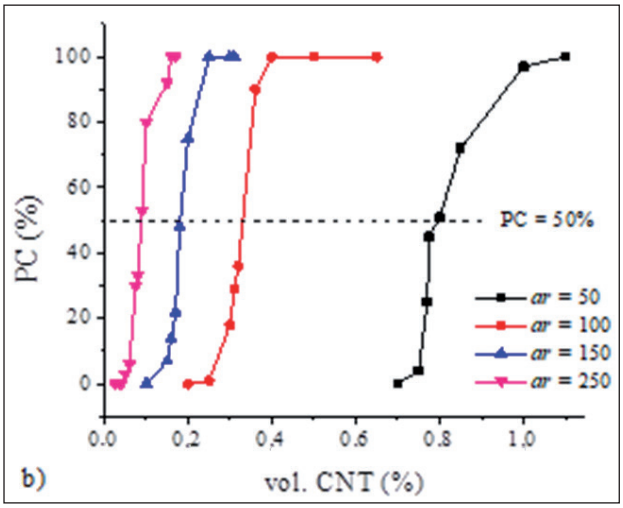


Fig. 7.: Analysis of the 3D percolation threshold simulation by the possibility of connection to: a) geometry E; and b) geometry F.

Table 2: Comparison between the percolation thresholds of the geometries E and F at different aspect ratios.

Geometry	Aspect ratio (ar)			
	50	100	150	200
E	0.764	0.322	0.182	0.080
F	0.788	0.337	0.186	0.091

When comparing the results obtained with experimental values present in literature, it was possible to note a proximity between them. Assuming the effect of load tortuosity, the percolation threshold obtained in the simulations, with *ar* greater than 100, presented values similar to those found in the literature for ultra-high molecular weight polyethylene nanocomposites and CNT (Lisunova, Mamunya, Lebovka, & Melezhyk, 2007), however, for *ar* 50, the results are higher than in other materials such as matrices of polystyrene (Sluzarenko et al., 2006) and epoxy (Pécastaings et al., 2004).

Through the analysis of the *ar* graph as a function of p_c, Fig. 8, a nonlinear exponential regression was performed to provide a mathematical model to calculate the percolation threshold for three-dimensional systems for the E geometry (Fig. 8*a*) and the F geometry (Fig. 8*b*), with a 99% of confidence. Thus, in order to compare the 3D simulation with the 2D, their respective equations were used at *ar* of 1000, obtaining a percolation value of 0.075 % vol. for the tortuous E geometry, and a percolation value of 0.0816 % vol. for the tortuous F geometry. These values were at least one order of magnitude lower than those simulated in 2D, being even more coherent with the results of the precursor model proposed by Balberg et al., (Balberg et al., 1984) who presented the same order of magnitude, values close to 0.05% vol. for 3D systems at the same aspect ratio.

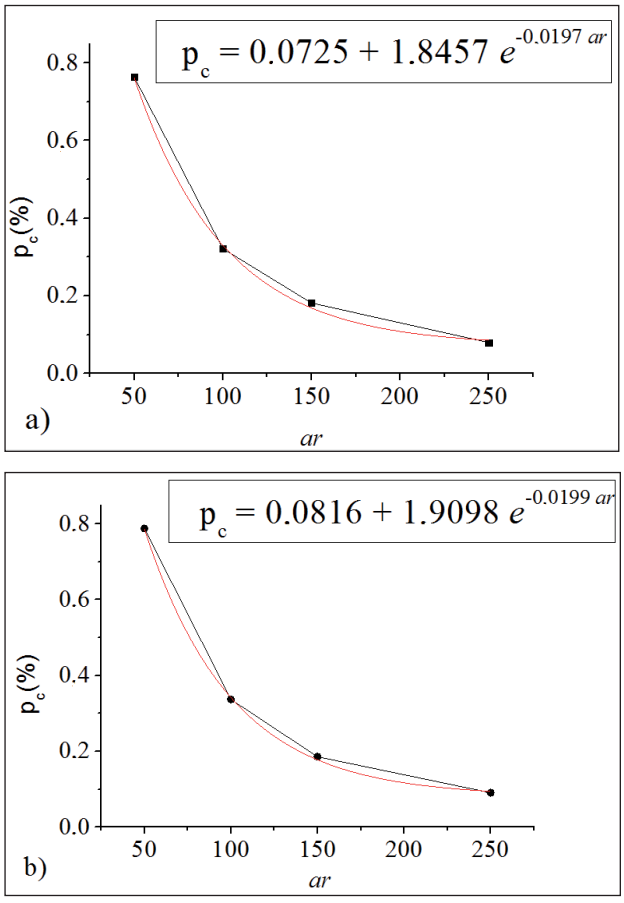


Fig. 8.: Exponential nonlinear regression analysis (R^2 = 0.99) of the percolation threshold of different aspect ratios (ar) and volumetric fractions for: a) geometry E; and b) geometry F.

In general, the results above were similar to the ones observed in Postiglione et al., (Postiglione, Natale, Griffini, Levi, & Turri, 2015) for nanocomposite films, where the percolation threshold values obtained present a good estimative of the actual electrical behavior found in 3D printed filaments. Also, the same author shows the predicted electrical conductivities of MWCNT and SWCNT polymer composites with different rates of work function (r) and tunneling effect. Thus, when CNT deformation effects are included, the work function of CNT decreases, then the tunneling resistance or contact resistance decreases. It is also worth noting that, as volume fraction of CNT increases, the fraction of intrinsic resistances dominates in the increase of total resistance. As a result, the tunneling effects are less significant and the difference in the predicted electrical conductivity with different rates of work functions diminishes (Gong, Zhu, & Haddad, 2013; Postiglione et al., 2015). This study shows that the inclusion of electrical conductivity modeling in the percolation threshold simulation is very important for the semiconductor nanocomposites representation.

Conclusions

Based on the simulation results, the geometry of the conductive load interferes in the percolation threshold, either for two-dimensional or three-dimensional systems, as well as the aspect ratio, based on the series of simulations performed by the Monte Carlo method and supported on the model of the excluded volume. Also, when the aspect ratio of the CNT increased, percolation threshold decreased since the particles present a larger dimension. Due to that, a smaller amount was necessary to form a conductive network, thus being inversely proportional characteristics.

Besides the aspect ratio, the tortuosity of the loads directly influenced the threshold, since the load presented a greater (more tortuous) undulation and the percolation threshold became smaller, as can be seen in the values obtained for two-dimensional and three-dimensional systems. Through the graphical representation of the simulation results in three dimensions, a mathematical model was established to allow the analysis of the percolation threshold in two-dimensional systems for high aspect ratios.

References

1. **Ali, U., Karim, K. J. B. A., & Buang, N. A. (2015).** *A Review of the Properties and Applications of Poly (Methyl Methacrylate) (PMMA)*. Polymer Reviews, 55(4), 678-705. doi:10.1080/15583724.2015.1031377
2. **Balberg, I., Anderson, C. H., Alexander, S., & Wagner, N. (1984).** *Excluded volume and its relation to the onset of percolation.* Physical Review B, 30(7), 3933-3943. doi:10.1103/PhysRevB.30.3933
3. **Berhan, L., & Sastry, A. M. (2007).** *Modeling percolation in high-aspect-ratio fiber systems.* II. The effect of waviness on the percolation onset. Physical Review E, 75(4), 041121. doi:10.1103/PhysRevE.75.041121
4. **Birman, V., & Kardomateas, G. A. (2018).** *Review of current trends in research and applications of sandwich structures.* Composites Part B: Engineering, 142, 221-240. doi:https://doi.org/10.1016/j.compositesb.2018.01.027
5. **Cheng, Y., Wang, S., Pan, F., & Zhang, J. (2014).** *A numerical study on electrical percolation of polymer-matrix composites with hybrid filler of carbon nanotubes and carbon black.* Journal of Nanomaterials, 2014, 1-9. doi:https://doi.org/10.1155/2014/614797
6. **Coelho, P. H. d. S. L., Armellini, V. A. d. D., & Morales, A. R. (2017).** *Assessment of Percolation Threshold Simulation for Individual and Hybrid Nanocomposites of Carbon Nanotubes and Carbon Black*. Materials Research, 20, 1638-1649.
7. **Formela, K., Zedler, L., Hejna, A., & Tercjak, A. (2018).** *Reactive extrusion of bio-based polymer blens and composites - Current trends and future developments*. eXPRESS Polymer Letters, 12(1), 24-57. doi:https://doi.

org/10.3144/expresspolymlett.2018.4

8. **Gong, S., Zhu, Z. H., & Haddad, E. I. (2013).** *Modeling electrical conductivity of nanocomposites by considering carbon nanotube deformation at nanotube junctions*. Journal of Applied Physics, 114(7), 074303. doi:10.1063/1.4818478
9. **Ha, M. L. P., Grady, B. P., Lolli, G., Resasco, D. E., & Ford, W. T. (2007).** *Composites of Single-Walled Carbon Nanotubes and Styrene-Isoprene Copolymer Latices.* Macromolecular Chemistry and Physics, 208(5), 446-456. doi:10.1002/macp.200600521
10. **Huang, C., & Cheng, Q. (2017).** *Learning from nacre: Constructing polymer nanocomposites.* Composites Science and Technology, 150, 141-166. doi:https://doi.org/10.1016/j.compscitech.2017.07.021
11. **Khun Nay, W., Loong Poh, Y., Liu, E., & Li, L. (2016).** *Enhancing electrical and tribological properties of poly(methyl methacrylate) matrix nanocomposite films by co-incorporation of multiwalled carbon nanotubes and silicon dioxide microparticles*. In Journal of Polymer Engineering (Vol. 36, pp. 23).
12. **Kim, H.-S., Chae, Y. S., Choi, J. H., Yoon, J.-S., & Jin, H.-J. (2008).** *Thermal Properties of Poly(ε-Caprolactone)/Multiwalled Carbon Nanotubes Composites*. Advanced Composite Materials, 17(2), 157-166. doi:10.1163/156855108X314788
13. **Konobeeva, N. N. (2018).** *Three-dimensional extremely short optical pulses in the carbon nanotubes medium with polymers*. Optik, 157, 521-524. doi:https://doi.org/10.1016/j.ijleo.2017.11.133
14. **Konyushenko, E. N., Stejskal, J., Trchová, M., Hradil, J., Kovářová, J., Prokeš, J., . . . Sapurina, I. (2006).** *Multi-wall carbon nanotubes coated with polyaniline*. Polymer, 47(16), 5715-5723. doi:https://doi.org/10.1016/j.polymer.2006.05.059
15. **Kumar, V., & Rawal, A. (2016).** *Tuning the electrical percolation threshold of polymer nanocomposites with rod-like nanofillers*. Polymer, 97, 295-299. doi:https://doi.org/10.1016/j.polymer.2016.05.041
16. **Li, C., & Chou, T.-W. (2007).** *Continuum percolation of nanocomposites with fillers of arbitrary shapes*. Applied Physics Letters, 90(17), 174108. doi:10.1063/1.2732201
17. **Lisunova, M. O., Mamunya, Y. P., Lebovka, N. I., & Melezhyk, A. V. (2007).** *Percolation behaviour of ultrahigh molecular weight polyethylene/multi-walled carbon nanotubes composites*. European Polymer Journal, 43(3), 949-958. doi:https://doi.org/10.1016/j.eurpolymj.2006.12.015
18. **Liu, Y., & Kumar, S. (2014).** *Polymer/Carbon Nanotube Nano Composite Fibers–A Review*. ACS Applied Materials & Interfaces, 6(9), 6069-6087. doi:10.1021/am405136s
19. **Lux, F. (1993).** *Models proposed to explain the electrical conductivity of mixtures made of conductive and insulating materials*. Journal of Materials Science, 28(2), 285-301. doi:10.1007/BF00357799
20. **Moaseri, E., Fotouhi, M., Bazubandi, B., Karimi, M., Baniadam, M., & Maghrebi, M. (2020).** *Two-dimensional reinforcement of epoxy composites: alignment of multi-walled carbon nanotubes in two directions*. Advanced Composite Materials, 1-11. doi:10.1080/09243046.2020.1718361
21. **Muñoz-Sandoval, E., Cortes-López, A. J., Flores-Gómez, B., Fajardo-Díaz, J. L., Sánchez-Salas, R., & López-Urías, F. (2017).** *Carbon sponge-type nanostructures based on coaxial nitrogen-doped multiwalled carbon nanotubes grown by CVD using benzylamine as precursor.* Carbon, 115, 409-421. doi:https://doi.org/10.1016/j.carbon.2017.01.010
22. **Mutiso, R. M., & Winey, K. I. (2015).** *Electrical properties of polymer nanocomposites containing rod-like nanofillers.* Progress in Polymer Science, 40, 63-84. doi:https://doi.org/10.1016/j.progpolymsci.2014.06.002
23. **Ondreas, F., Lepcio, P., Zboncak, M., Zarybnicka, K., Govaert, L. E., & Jancar, J. (2019).** *Effect of Nanoparticle Organization on Molecular Mobility and Mechanical Properties of Polymer Nanocomposites.* Macromolecules, 52(16), 6250-6259. doi:10.1021/acs.macromol.9b01197
24. **Park, J.-E., Jang, Y.-S., Park, I.-S., Jeon, J.-G., Bae, T.-S., & Lee, M.-H. (2018).** *The effect of multi-walled carbon nanotubes/hydroxyapatite nanocomposites on biocompatibility.* Advanced Composite Materials, 27(1), 53-65. doi:10.1080/09243046.2017.1374705
25. **Park, S.-H., Hwang, J., Park, G.-S., Ha, J.-H., Zhang, M., Kim, D., . . . Lee, S. H. (2019).** *Modeling the electrical resistivity of polymer composites with segregated structures.* Nature Communications, 10(1), 2537. doi:10.1038/s41467-019-10514-4
26. **Pécastaings, G., Delhaès, P., Derré, A., Saadaoui, H., Carmona, F., & Cui, S. (2004).** *Role of Interfacial Effects in Carbon Nanotube/Epoxy Nanocomposite Behavior.* Journal of Nanoscience and Nanotechnology, 4(7), 838-843. doi:10.1166/jnn.2004.114
27. **Postiglione, G., Natale, G., Griffini, G., Levi, M., & Turri, S. (2015).** *Conductive 3D microstructures by direct 3D printing of polymer/carbon nanotube nanocomposites via liquid deposition modeling.* Composites Part A: Applied Science and Manufacturing, 76, 110-114. doi:https://doi.org/10.1016/j.compositesa.2015.05.014
28. **Ramesh, N., Moratti, S. C., & Dias, G. J. (2018).** *Hydroxyapatite–polymer biocomposites for bone regeneration: A review of current trends.* Journal of Biomedical Materials Research Part B: Applied Biomaterials, 106(5), 2046-2057. doi:10.1002/jbm.b.33950
29. **Sluzarenko, N., Heurtefeu, B., Maugey, M., Zakri, C., Poulin, P., & Lecommandoux, S. (2006).** *Diblock copolymer stabilization of multi-wall carbon nanotubes in organic solvents and their use in composites.* Carbon, 44(15), 3207-3212. doi:https://doi.org/10.1016/j.carbon.2006.06.034
30. **Soleimani, H., Baig, M. K., Yahya, N., Khodapanah, L., Sabet, M.,**

Demiral, B. M. R., & Burda, M. (2018). *Impact of carbon nanotubes based nanofluid on oil recovery efficiency using core flooding.* Results in Physics, 9, 39-48. doi:https://doi.org/10.1016/j.rinp.2018.01.072

31. **Stauffer, D., & Aharony, A. (1994).** *Introduction to percolation theory (2 ed.)*. New York: Taylor & Francis.

32. **stru¨mpler, R., & Glatz-Reichenbach, J. (1999).** *FEATURE ARTICLE Conducting Polymer Composites*. Journal of Electroceramics, 3(4), 329-346. doi:10.1023/A:1009909812823

33. **Sun, Y., Bao, H.-D., Guo, Z.-X., & Yu, J. (2009).** *Modeling of the Electrical Percolation of Mixed Carbon Fillers in Polymer-Based Composites*. Macromolecules, 42(1), 459-463. doi:10.1021/ma8023188