JCAMECH

Vol. 49, No. 1, June 2018, pp 70-85
DOI: 10.22059/jcamech.2017.243530.195

On the Thermal Conductivity of Carbon Nanotube/Polypropylene Nanocomposites by Finite Element Method

R. Ansari[a], S. Rouhi[b,] ∗ *and M. Ahmadi[a]*

[a] *Department of Mechanical Engineering, University of Guilan, P.O. Box 3756, Rasht, Iran*
[b] *Young Researchers and Elite Club, Langroud Branch, Islamic Azad University, Langroud, Guilan, Iran*

ARTICLE INFO

Article history:
Received: 11 October 2017
Accepted: 27 November 2017

Keywords:
Finite element method
Thermal conductivity coefficient
Single-walled carbon nanotube
Polypropylene matrix

ABSTRACT

In this paper, finite element method is used to obtain thermal conductivity coefficients of single-walled carbon nanotube reinforced polypropylene. For this purpose, the two-dimensional representative volume elements are modeled. The effect of different parameters such as nanotube dispersion pattern, nanotube volume percentage in polymer matrix, interphase thickness between nanotube and surrounded matrix and nanotube aspect ratio on the thermal conductivity coefficient of nanotube/polypropylene nanocomposite are investigated. For the dispersion pattern, three different algorithms, including random dispersion, regular dispersion along the temperature difference and regular dispersion perpendicular to the temperature difference are employed. Furthermore, the temperature is considered in the range of 0℃ to 200℃. The nanotube volume percentage in the polymer matrix is selected as 1%, 3% and 5%. It is shown that the polypropylene matrix reinforced by the regular distribution of nanotubes directed parallel to the temperature difference leads to the largest thermal conductivity coefficients. Besides, the nanocomposites with larger volume percentages of carbon nanotubes possess larger thermal conductivity coefficients.

1. Introduction

After publishing the first report on the carbon nanotubes (CNTs) by Iijima [1], due to their exceptionally fantastic physical properties, other nanostructure such as nanoplates [2-8], nanobeams [9-11], nanofilms [12], nanorods [13], nanorings [14] and nanoshells [15] have also been considered by the researchers to evaluate their properties. Based on these great properties, the nanostructures can be selected as good fillers to raise up the mechanical properties of other materials [16-23].

Considering the advantages of the polymers over metals, such as being lighter than metals, more resistant against the corrosion and easier to process, thermal conductive polymer composites can be considered as the possible options to replace the metals in different applications like heat exchangers, generators, power electronics and electric motors. Specially, having high thermal conductivity [24, 25] makes carbon nanotubes (CNTs) as a good candidate to increase the thermal conductivity of polymers. To this end, both experimental [26-35] and theoretical modeling [36-46] approaches have been utilized to investigate the thermal behavior of different materials reinforced by CNTs. Wine et al. [26] investigated the effect of adding CNTs to the polymer matrices on the electrical and thermal conductivities. They showed that the electrical and thermal conductivities of CNT/polymer nanocomposites are strongly influenced by CNT dispersion and alignment.

Adding benzenetricarboxylic acid grafted multi-walled CNTs (BTC-MWCNTs) to the epoxy matrix with the 1–5 volume percent, Yang et al. [27] observed that the thermal conductivity of epoxy composites increases by 684%. A nonlinear trend was observed for denser arrays [28]. For example, 17 volume percent CNTs leads to increasing the thermal conductivity by a factor of 18. Park et al. [29] showed that good adhesion and less voids between nanotubes and polymers leads to increasing the efficiency of CNTs to increase the thermal conductivity of the CNT/polymer nanocomposites.

Gulotty et al. [30] showed that compared to pure CNTs, carboxylic functionalization (COOH groups) of CNTs give better results in increasing the thermal conductivity coefficient of polymer matrices. Besides, it was shown that other fillers such as graphene and boron nitride could also enhance the thermal conductivity of polymer nanocomposites significantly [31]. Kapadia et al. [33] investigated the influence of CNT aspect ratio (length/diameter) on the thermal conductivity enhancement in CNT/polymer composites. It was shown that the thermal

* Corresponding author. Tel.: +98 1342544411; fax: +98 1342544422.; e-mail: s_rouhi@iaul.ac.ir

conductivity of polymer composites experiences a linear increase by incorporating low aspect ratio MWCNTs. They also represented that 15 volume percent oriented graphene platelets (GPLs) in Al_2O_3 can results in ~44% increase in the in-plane thermal conductivity in the in-plane direction at the temperature of 600°C.

Due to difficulty of experiments, some researchers have used theoretical modeling approaches to study the thermal properties of nanocomposites. Clancy and Gates [36] studied the effect of grafting single-walled CNTs (SWCNTs) by hydrocarbon chains with covalent chemical bonds on the thermal conductivity of the nanocomposites. It was shown that using these functionalized SWCNTs increases the thermal conductivity of the nanocomposites significantly. Based on an effective medium theory, a theoretical model was developed by Bagchi and Nomura [37] to compute the thermal conductivity of aligned MWCNT/polymer nanocomposites. Moreover, Guthy et al. [38] used random dispersion for incorporating the SWCNTs into the poly-methylmethacrylate (PMMA) matrix. An increase of 250% was observed at the 9 volume percent.

Modifying the effective continuum micromechanics analysis to obtain the thermal conductivities of nanocomposites, Yu et al. [39] studied the effects of nano-reinforcement morphology, volume fraction, orientation, and nano-reinforcement–resin interphase properties on the effective thermal conductivities of nanocomposites. Mortazavi et al. [40] showed that finite element (FE) method can be more useful to predict the thermal conductivity of nanocomposites with randomly dispersed fillers than Mori–Tanaka and strong contrast modeling approaches. To investigate the effect of interphase on the elastic modulus and thermal conductivity of polymer nanocomposites, they suggested a 3-dimensional (3D) FE modeling, which was used to study the nanocomposites filled by nanoparticles with different orientations and shapes [41]. Mortazavi et al. [42] also used the molecular dynamics (MD) and FE methods to propose a multiscale approach. The suggested approach was used to compute the thermal conductivity of graphene epoxy nanocomposites. Their method was verified by experimental data for effective elastic modulus and thermal conductivity of poly-lactide (PLA)/expanded graphite (EG) nanocomposites [43].

Fiamegkou et al. [44] and Eslami Afrooz and Ochsner [45] also employed FE method to study the effect of filling nanocomposites by CNTs on their thermal conductivity. The influences of covalent and non-covalent functionalization, isotope doping and acetylene linkage in graphene on the thermal properties of graphene-reinforced polymer nanocomposites were investigated by Wang et al. [46] using the MD simulations. It was shown that graphene-epoxy interfacial thermal resistance is not affected by carbon isotope doping in graphene.

In this paper, FE method is employed to examine the thermal behavior of polymer matrix reinforced by SWCNTs. Different volume fractions of SWCNTs with several distribution patterns are dispersed in the polymer matrix. Besides, the effects of interphase thermal properties on the thermal conductivity coefficient of polymer/SWCNT nanocomposite are studied. The nanotubes with different aspect ratios are considered to explore the effect of nanotube geometrical parameters on the thermal behavior of the resulted nanocomposite. This is for the first time that such a comprehensive investigation on the thermal conductivity of the polymer/CNT nanocomposites is performed in which the influences of different parameters including CNT dispersion pattern, CNT volume fraction, temperature and CNT/polymer interphase are considered.

2. Modeling details

FE method is used here to obtain the thermal conductivity coefficient of the SWCNT reinforced polypropylene. The RVEs are modeled as two-dimensional cells. To obtain the thermal conductivity coefficient of the RVEs, a small temperature difference (1°C) is applied to the two opposite vertical edges of the RVEs and the average heat flux (*q*) is calculated. Then, using the Fourier relation, the thermal conductivity coefficient (*K*) is obtained as

$$k = q \frac{dt}{dT} \tag{1}$$

Where *dT* and *dt* are the temperature gradient and distance between two edges on which the temperature difference is applied. Three different patterns are used to disperse the nanotubes in the propylene matrix which are shown in Fig. 1. In the first pattern, the SWCNTs are dispersed randomly over the matrix. The second pattern associates with the nanotubes directed along the temperature difference and in the third pattern, the direction of nanotubes is perpendicular to the temperature difference. The simulations are performed using ABAQUS software. To disperse the CNTs, the Python programming language is utilized. For the first dispersion pattern, the orientation and position of the CNTs are randomly selected. For this purpose, the first CNT is placed in the CNT matrix with the random position and orientation. Then, the second CNT is placed in the polymer matrix with the random position and orientation such that no overlapping happens between the located CNTs. Locating new CNTs are continued until the intended CNT volume fraction is reached. For two other dispersion patterns, only the initial position is randomly selected. Again, no overlapping is allowed. The 8-node plane stress thermally coupled quadrilateral, biquadratic displacement, the bilinear temperature element is used to mesh the matrix and CNTs.

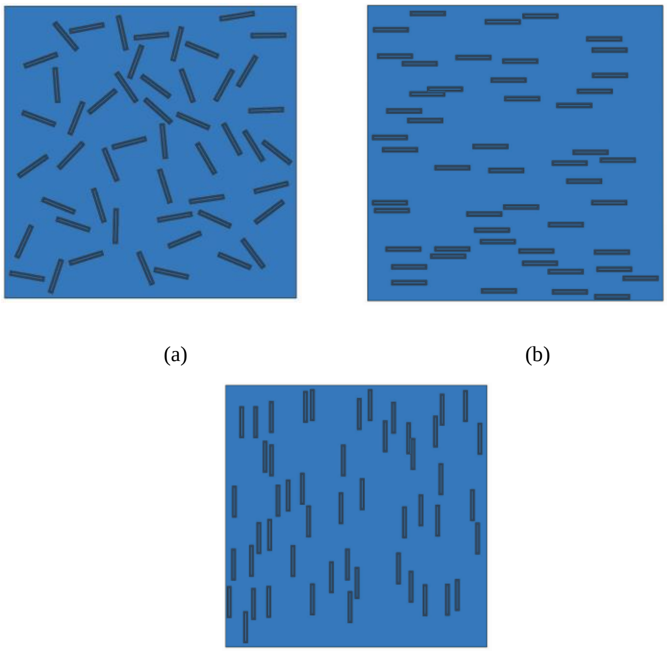
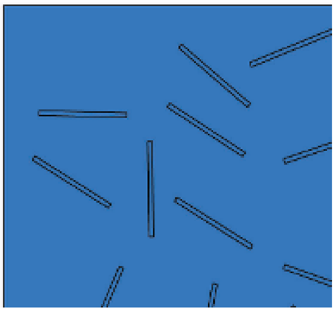


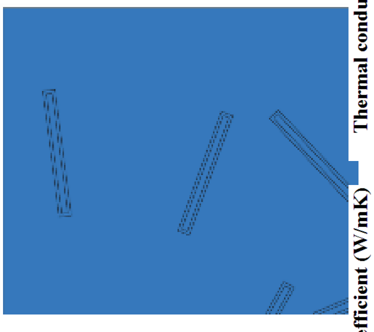
Figure 1. Different dispersion patterns of nanotubes in matrix: (a) random dispersion, (b) nanotubes directed along the temperature difference and (c) nanotubes directed perpendicular to the temperature difference

3. Results and discussion

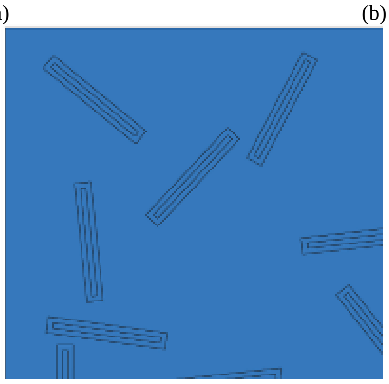
In this section, the thermal conductivities of SWCNT reinforced polypropylene are obtained. The dependence of the thermal conductivity coefficient on the CNT volume fraction, aspect ratio and dispersion pattern is evaluated. Besides, the effect of SWCNT/polypropylene interphase thickness on the thermal behavior of the resulted nanocomposites is explored. As it is seen in Fig. 2, three different interphase thicknesses are considered, including no interphase, interphase thickness equal to the half of the SWCNT diameter and equal to SWCNT diameter. The properties of interphase are considered as twice the properties of the polypropylene. The temperature varies from 0 to 200°C for this study. The thermal properties of SWCNT and polypropylene are extracted from [47] and [48], respectively. To validate the current modeling approaches, the results are compared with the experimental results in Table 1. It can be seen that the employed modeling approach can predict the experimental results with an acceptable accuracy. The precision is better for a larger CNT volume fraction.



(a)



(b)



(c)

Figure 2. Schematics of different interphase thicknesses, (a) 0, (b) half of CNT diameter, and (c) equal to CNT diameter

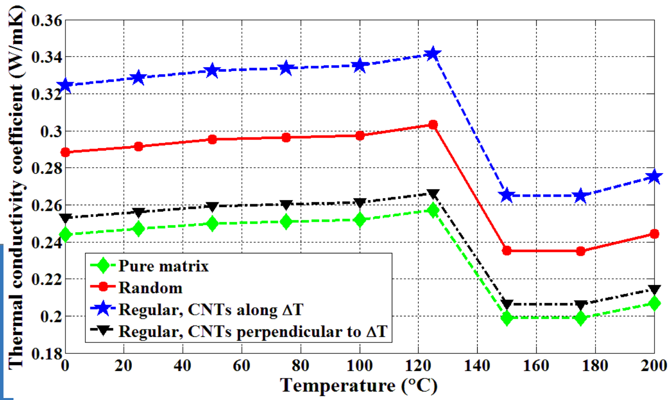
Table 1. Comparing the results of the current modeling approach with the experimental results

Volume fraction	Thermal conductivity coefficient (W/mK)		
	Present work	Experiment [49]	Error (%)
0.3%	0.178	0.2	11.00%
0.6%	0.236	0.24	1.67%

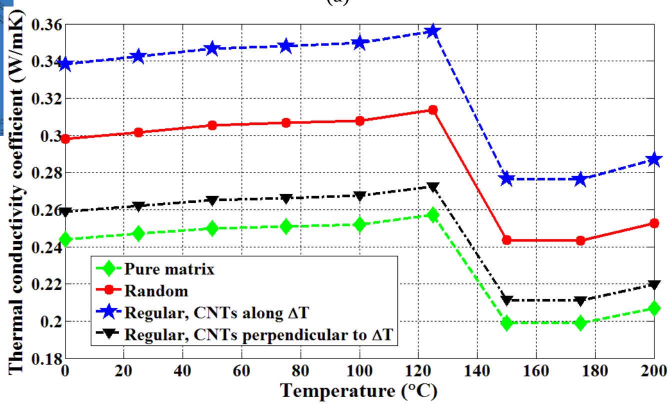
3.1. Effect of CNT distribution pattern

The effect of the distribution pattern of nanotube in polypropylene matrix is given in Fig. 3. The volume percentage of SWCNT in polymer matrix is selected as 3%. Besides, nanotube aspect ratio (length to diameter ratio) is considered as 10.The thickness of interphase is chosen as 0, half of SWCNT diameter and equal to SWCNT diameter. Three different dispersion types are employed.

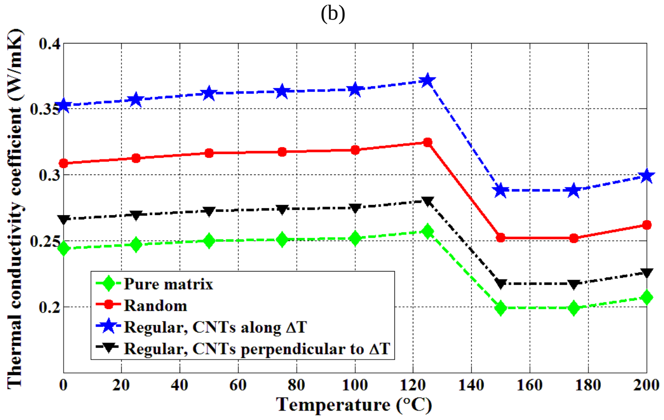
It is observed that the curves of CNT reinforced polypropylene are parallel to that of pure polypropylene. In other words, increasing temperature leads to an increase in the thermal conductivity coefficient of the nanocomposites until 200°C. Then, suddenly the curves drop and again, the thermal conductivity coefficients increase by the temperature. Therefore, it can be concluded that the thermal behavior of the CNT reinforced polypropylene is governed by the thermal behavior of the polymer matrix.



(a)



(b)



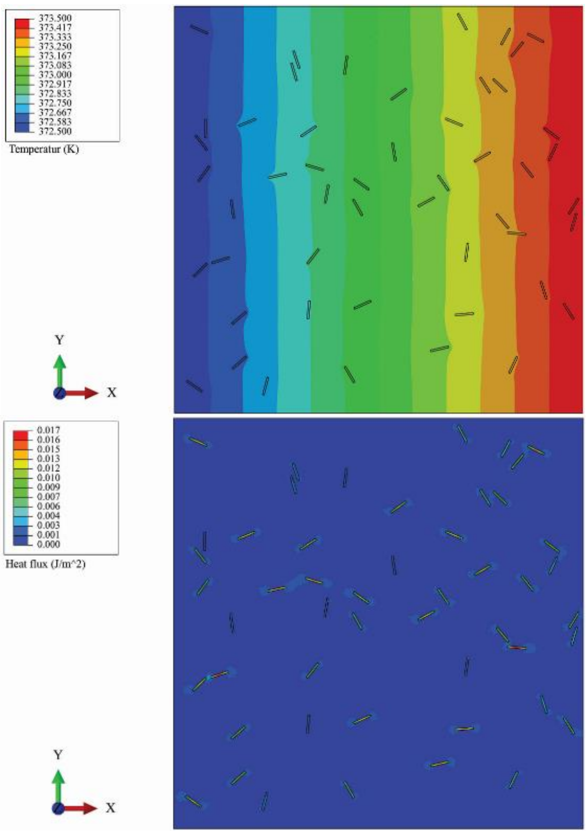
(c)

Figure 3. Thermal conductivity coefficient of polypropylene matrix reinforced by CNTs with different distribution patterns versus temperature (3% volume percent, Thickness of interphase = (a) 0, (b) half of SWCNT diameter and (c) SWCNT diameter)

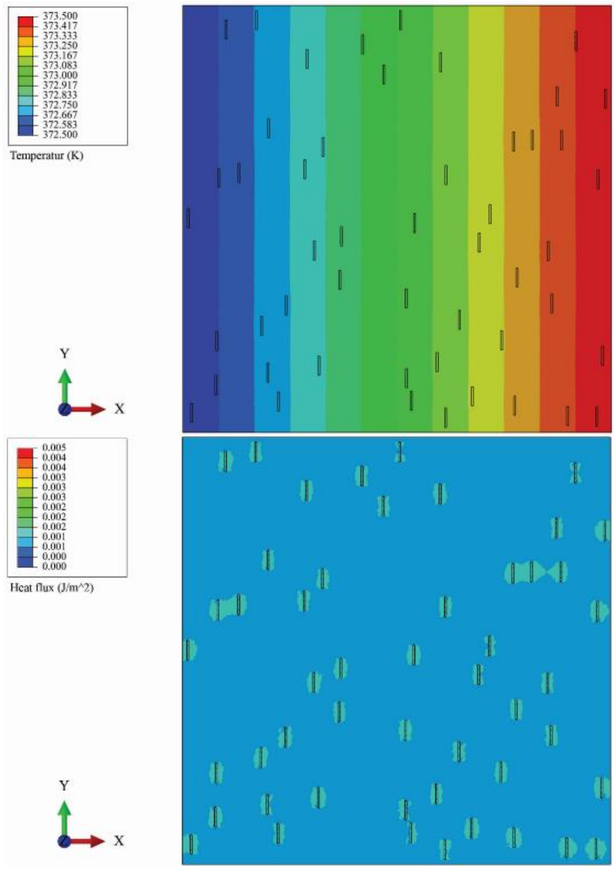
Comparing the curves associated with different dispersion patterns, it is observed that reinforcing polypropylene matrix by regular dispersion of the SWCNTs along the temperature difference gives the largest thermal conductivity coefficients. This is due to the one-dimensional nature of the nanotubes, which leads to strong physical properties in longitudinal direction and weak properties in transverse directions. Therefore, it can be predicted that the lowest thermal conductivities associate with the RVEs with SWCNTs dispersed with the direction perpendicular to the temperature difference.

The effect of dispersion type is more prominent for larger interphase. For example, at the temperature of 75°C, considering the thickness of interphase as 0 leads to 3.67%, 33.02% and 18.09% increase in thermal conductivity coefficient of the polypropylene matrix for regular distribution perpendicular to the temperature difference, regular distribution along the temperature difference and random distribution, respectively. While the corresponding values for the interphase thickness equal to the half of the nanotube diameter are 6.1%, 38.72% and 22.16%, respectively. Besides, considering the interphase thickness as the diameter of CNT, the corresponding values are obtained as 9.12%, 44.6% and 26.51%, respectively.

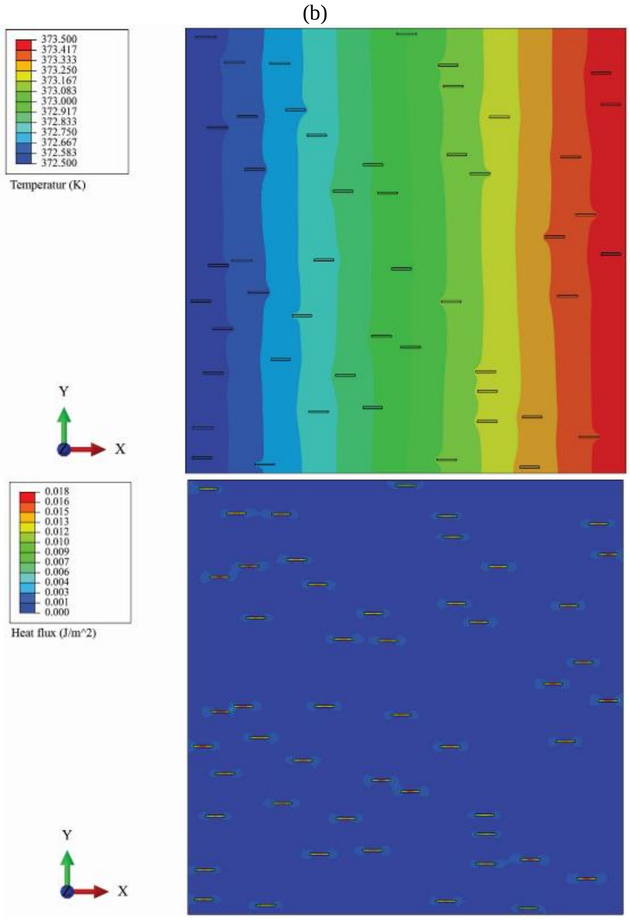
The temperature and heat flux distribution patterns of CNT/polypropylene nanocomposites are given in Fig. 4 for different CNT distribution patterns. The aspect ratio and volume fraction of CNTs are selected as 10 and 1%, respectively. In temperature distribution profiles, it is observed that the tip of CNTs affect the boundaries of the constant temperature areas. Therefore, for regular CNT dispersion perpendicular to the temperature difference in which the nanotubes are parallel to the vertical edges, the boundaries of the constant temperature areas are approximately linear. Furthermore, it is seen that the smallest heat flux associate with the regular CNT dispersion perpendicular to the temperature difference. However, the heat fluxes of two other distributions are approximately similar.



(a)



(b)



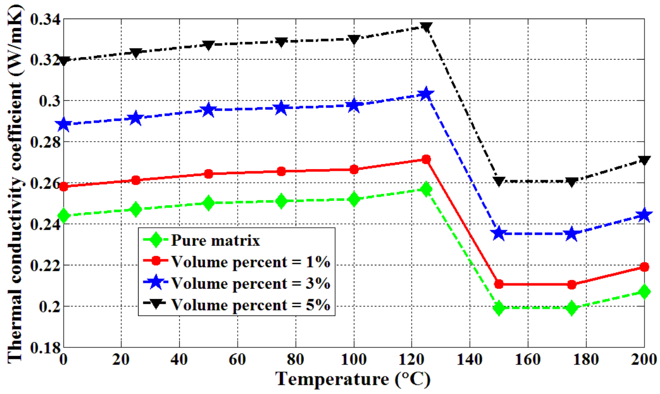
(c)

Figure 4. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution

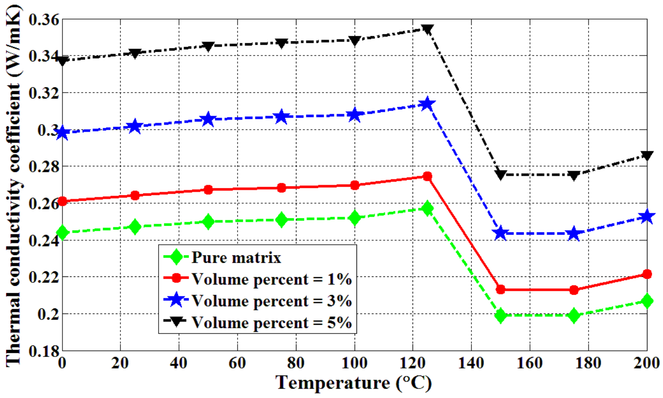
perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 10, CNT volume percent = 1%, temperature = 100°C)

3.2. Effect of CNT volume percent

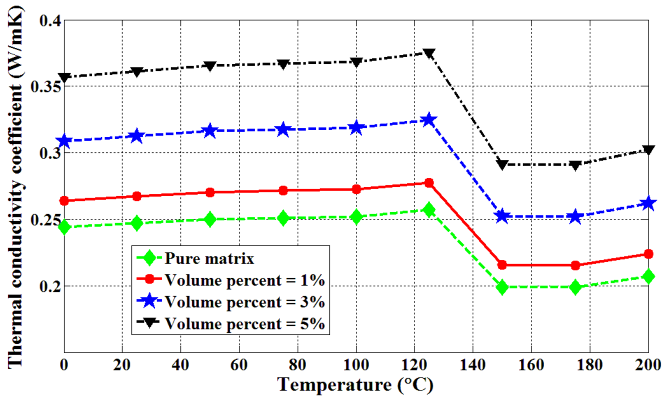
The effect of nanotube volume percent in the polypropylene matrix is investigated in Figs. 5-7. Three volume percentages including 1%, 3% and 5% are considered for CNTs in polypropylene matrix. It is observed that the larger volume fractions, the larger thermal conductivity coefficients. For a same dispersion pattern, the largest effect of the volume percentage on the thermal conductivity coefficient of the polypropylene is observed for the thickness of interphase as the diameter of the nanotube, then considering the thickness as the half of the diameter and last the RVEs without interphase. For example, in Fig. 2, which relates to random distribution of nanotube in polypropylene matrix, the increases of thermal conductivity coefficients at the temperature of 100°C are obtained as 8.16%, 26.53% and 46.23% for the volume percentages of 1%, 3% and 5%, respectively. These values are 6.94%, 22.18% and 38.20% for the thickness of interphase as the half of CNT diameter. The corresponding values of the RVEs without interphase are 5.75%, 18.06% and 30.96. So, it can be concluded that considering the interphase between CNT and polypropylene matrix leads to reinforcing the effect of the volume percentage on the thermal behavior of the CNT reinforced polypropylene matrix.



(a)

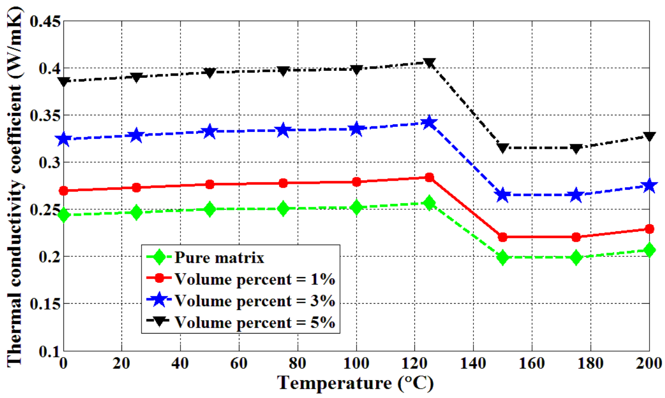


(b)

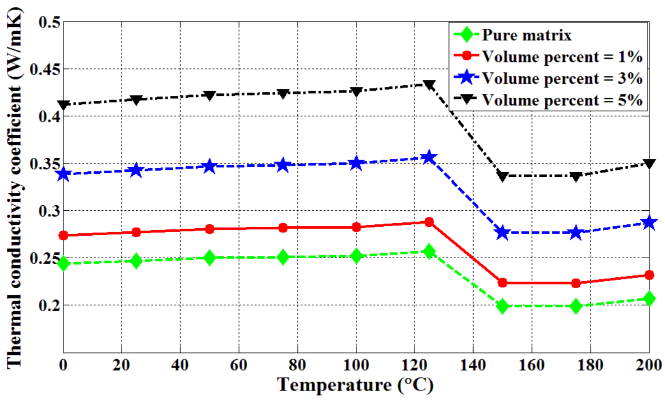


(c)

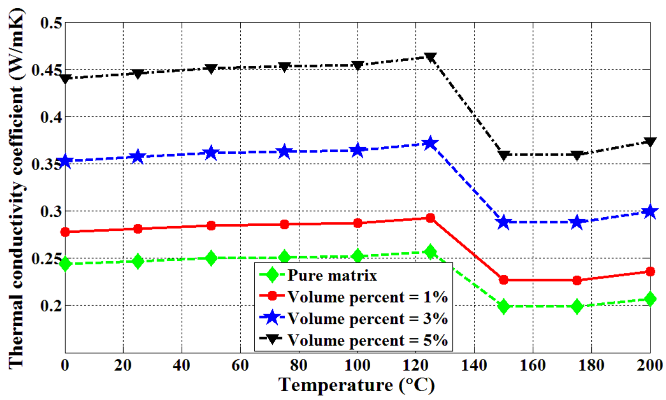
Figure 5. Thermal conductivity coefficient of polypropylene matrix reinforced by CNTs with different volume fractions versus temperature (random distribution, (a) 0 interphase, (b) 0.5 interphase and (c) 1 interphase)



(a)

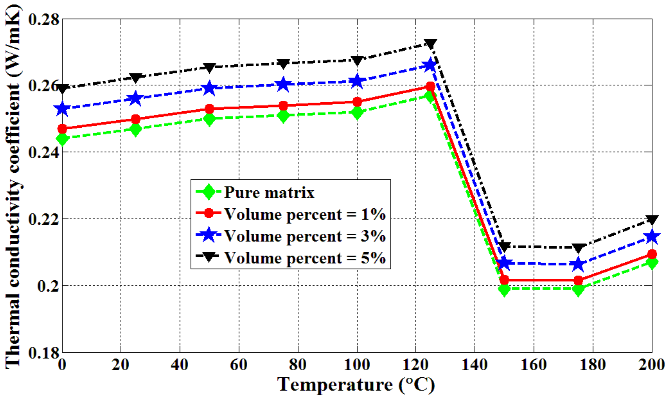


(b)

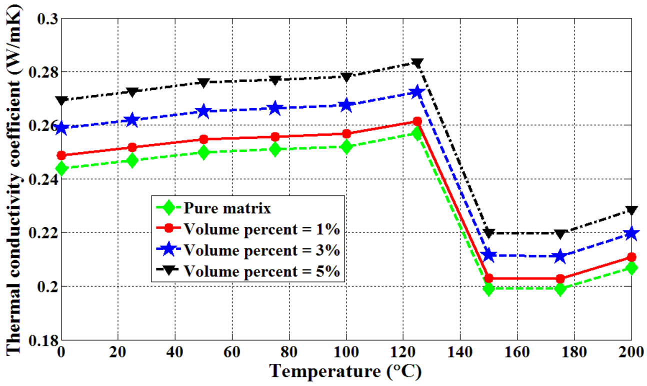


(c)

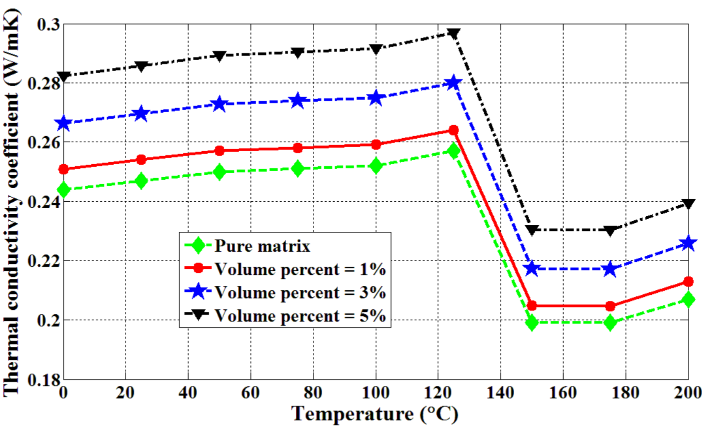
Figure 6. Thermal conductivity coefficient of polypropylene matrix reinforced by CNTs with different volume fractions versus temperature (regular distribution along ΔT, (a) 0 interphase, (b) 0.5 interphase and (c) 1 interphase)



(a)



(b)

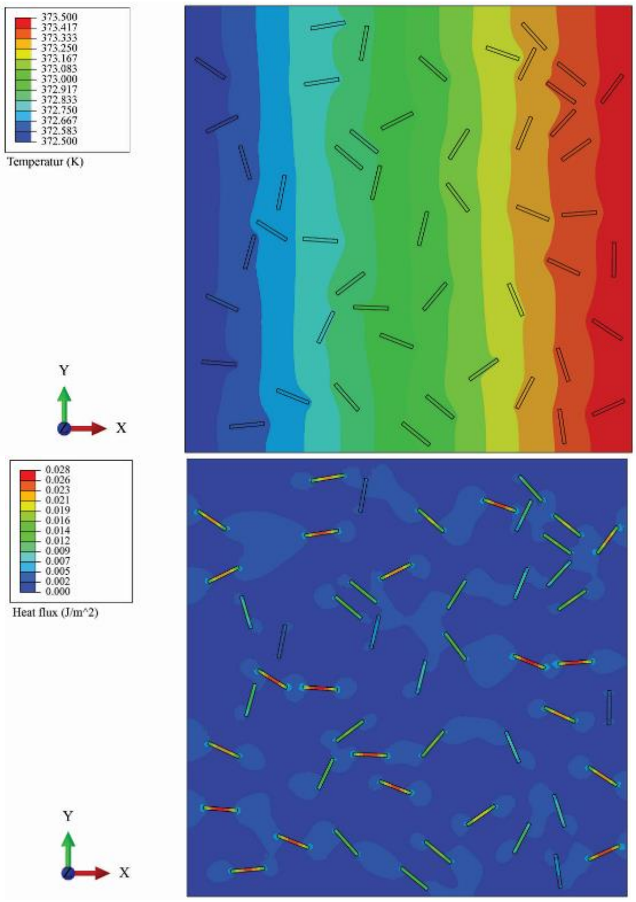


(c)

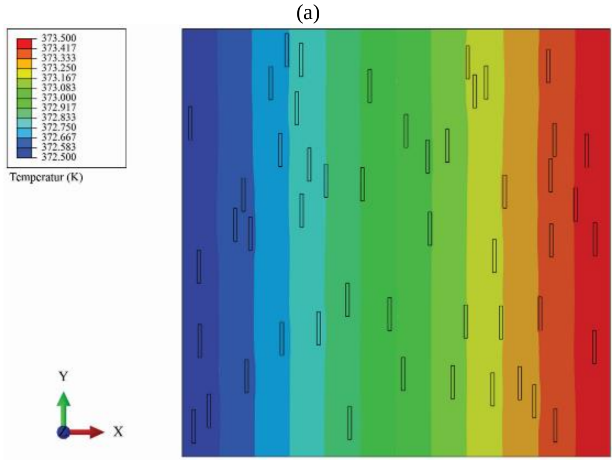
Figure 7. Thermal conductivity coefficient of polypropylene matrix reinforced by CNTs with different volume fractions versus temperature (regular distribution perpendicular to ΔT, (a) 0 interphase, (b) 0.5 interphase and (c) 1 interphase)

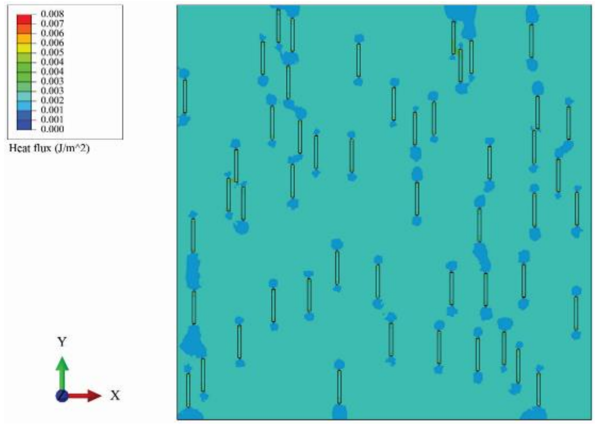
The effect of volume percentage on the thermal conductivity coefficients of the three considered dispersion types are almost similar. For example, the increases of thermal conductivity coefficients at the temperature of 100°C with the interphase as the CNT diameter are equal to 13.95%, 44.62% and 80.47% for the volume percent of 1%, 3% and 5%, respectively. These values are reported for regular dispersion of nanotube along the temperature difference. The corresponding values of random distribution are 8.16%, 26.53% and 46.23% and those of regular distribution perpendicular to the temperature difference are 2.85%, 9.12% and15.96%. It is observed that for all of the considered dispersion types, increasing CNT volume percentage from 1 to 3 and from 3 to 5 leads to 3.2 and 1.75 fold of the thermal conductivity coefficients.

The temperature and heat flux distribution profiles of CNT/polypropylene nanocomposites with the CNT aspect ratios of 3% and 5% are given in Figs. 8 and 9. No interphase has been considered between the nanotubes and matrix. It is seen that for larger volume fractions, the shapes of constant temperature areas deviate more from perfect rectangles. Increasing the volume fraction leads to increasing the heat flux in CNT/polypropylene nanocomposites. Besides, for the larger aspect ratios, the difference between the heat fluxes of polypropylene matrix reinforced by random distributed CNT and regular distributed CNT along the temperature difference is more significant.

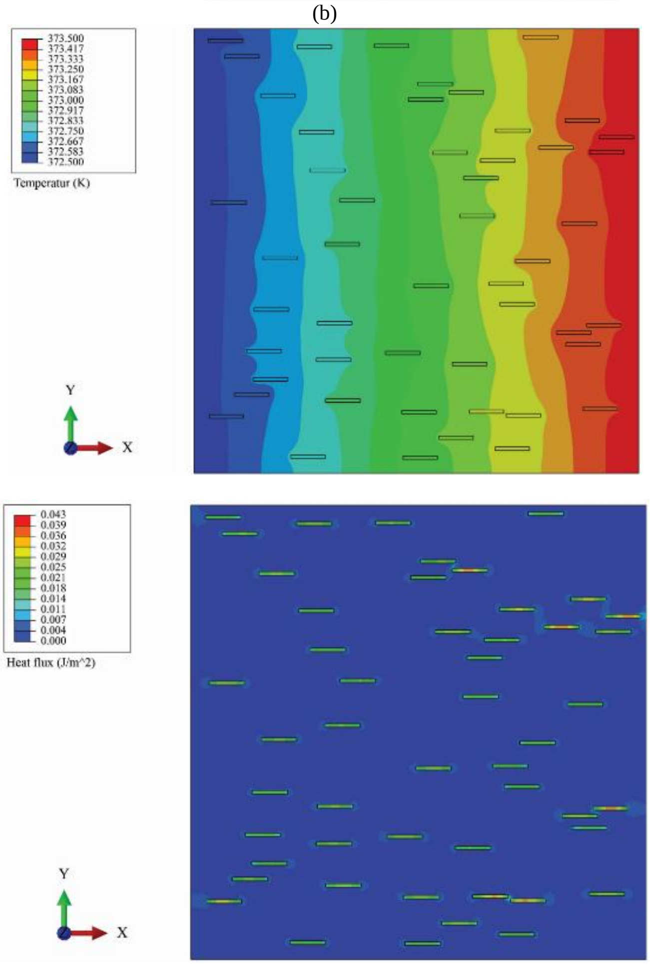


(a)



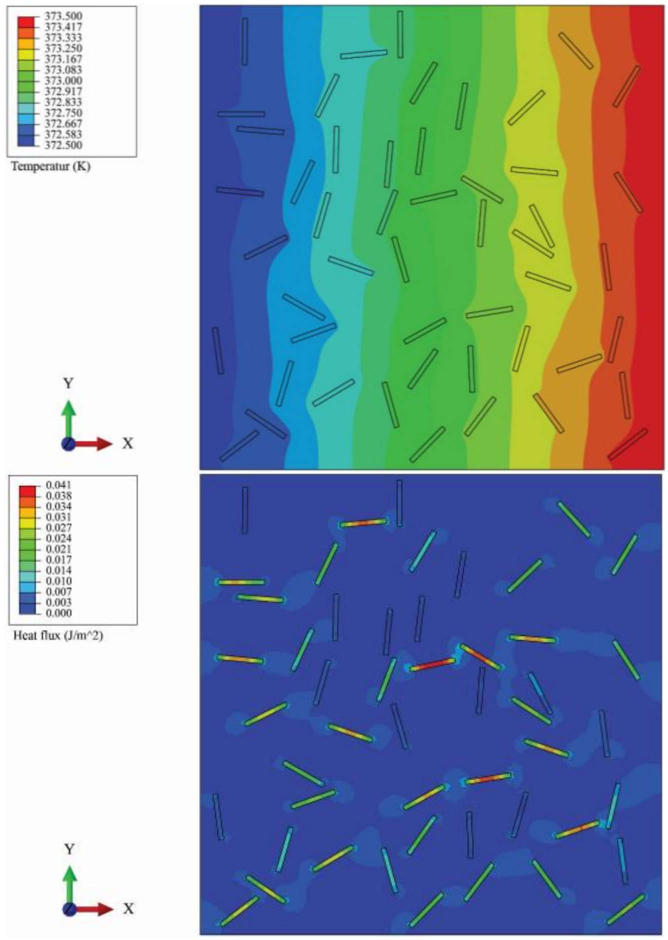


(b)

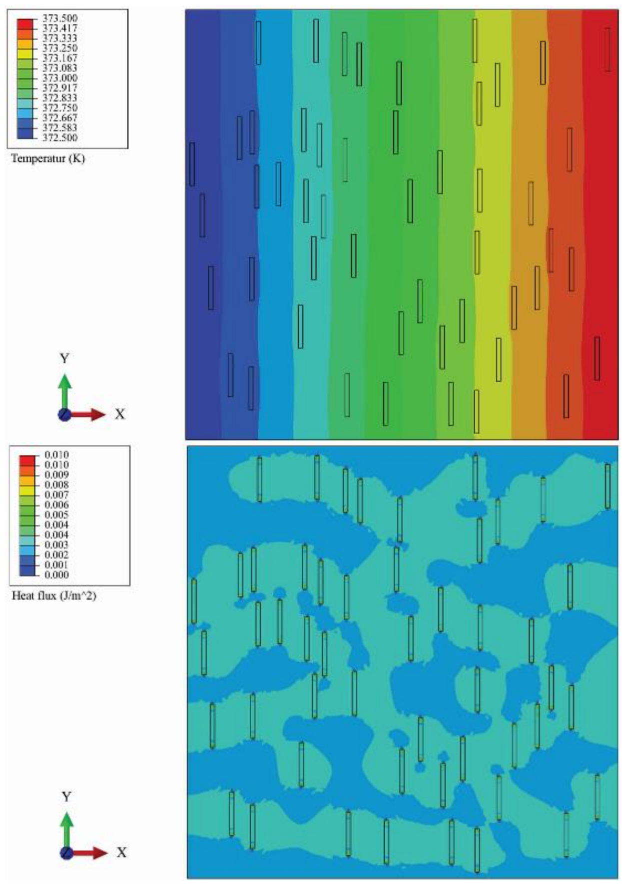


(c)

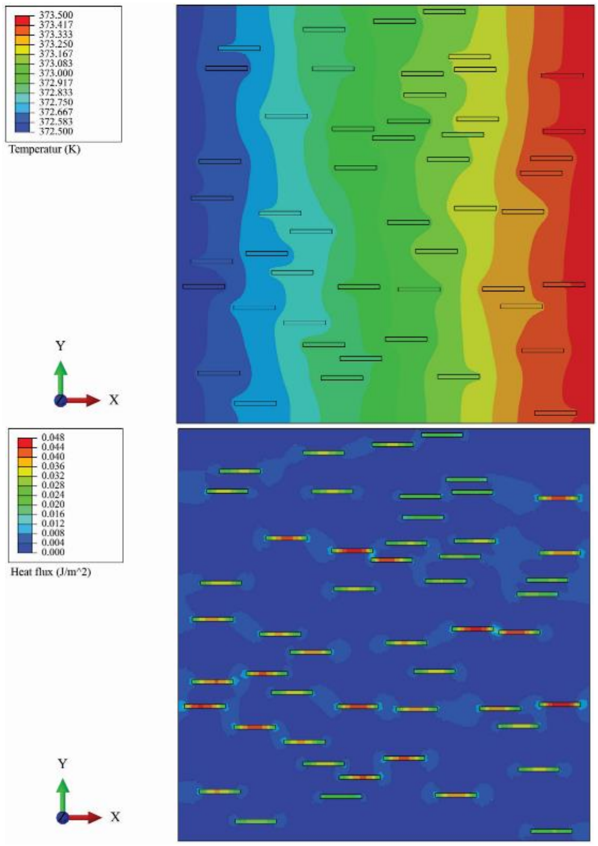
Figure 8. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 10, CNT volume percent = 3%, temperature = 100°C)



(a)



(b)

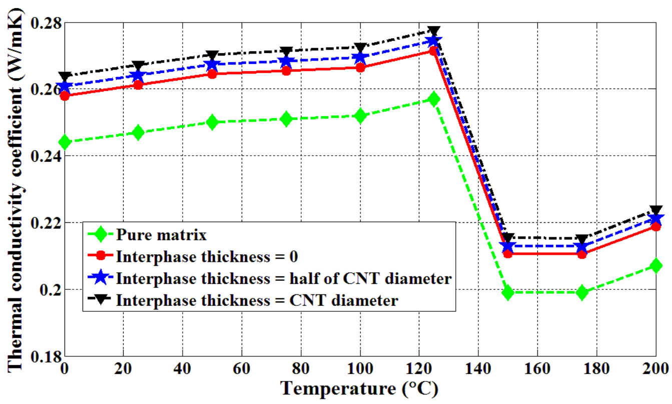


(c)

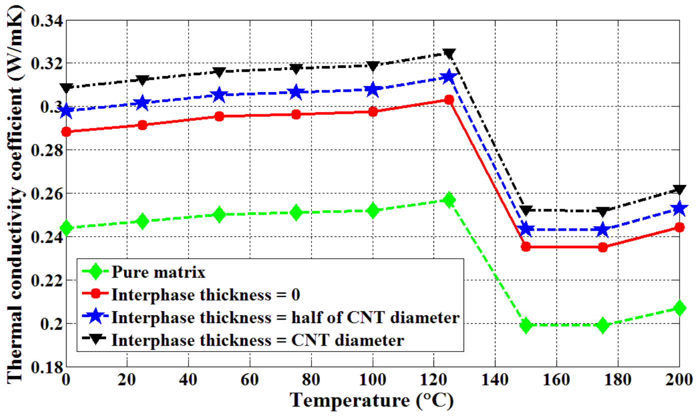
Figure 9. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 10, CNT volume percent = 5%, temperature =100°C)

3.3. Effect of interphase thickness

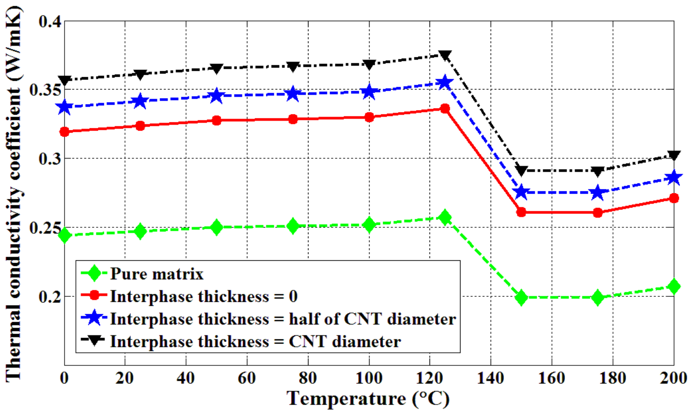
Fig. 10 shows the thermal conductivity coefficients of CNT/polypropylene nanocomposites with different interphase thicknesses. The aspect ratio is considered as 10. The CNTs are randomly dispersed in the polypropylene matrix. It is observed that for all of the selected CNT volume fractions, the largest thermal conductivity coefficients are those of RVEs in which the interphase thickness is considered as the diameter of CNT. Then, the RVEs with the interphase thickness as half of the CNT diameter. The lowest thermal conductivity coefficients are those of RVEs with perfect bonding between the CNTs and surrounded matrix. The effect of volume percentage is more observable for larger CNT volume fractions.



(a)



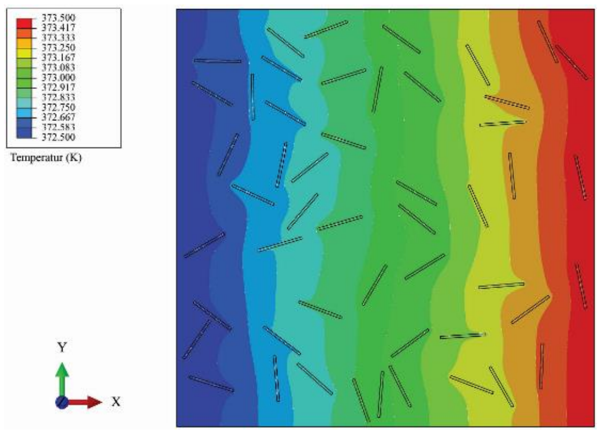
(b)

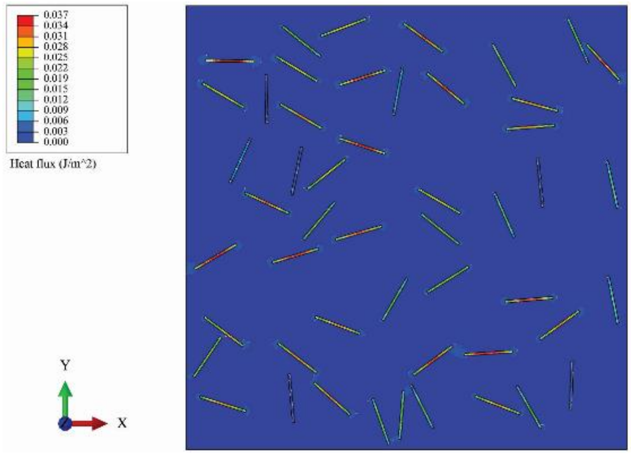


(c)

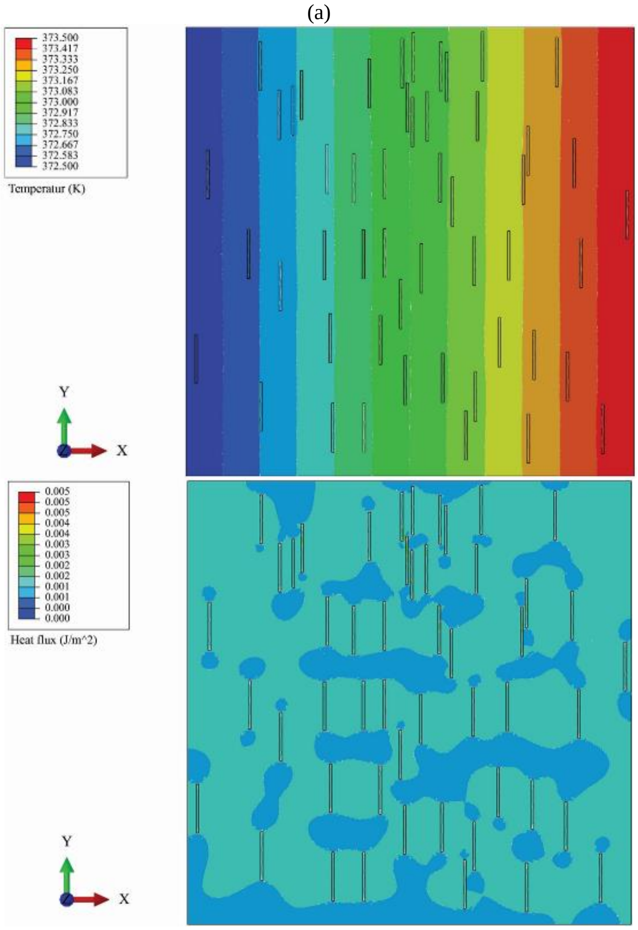
Figure 10. Thermal conductivity coefficient of polypropylene matrix reinforced by CNTs with different volume fractions versus temperature (random distribution, (a) 1%, (b) 3% and (c) 5% volume fraction)

Figs. 11-13 show the temperature and heat flux profiles of the CNT/polypropylene nanocomposites with different interphase thicknesses. CNT aspect ratio and volume fraction are selected as 20 and 5%, respectively. According to these figures, for none of the distribution patterns, considering the interphase thickness in the RVEs does not affect the constant temperature areas significantly. Besides, the heat fluxes are not affected by the CNT/polypropylene interphase thickness, either.

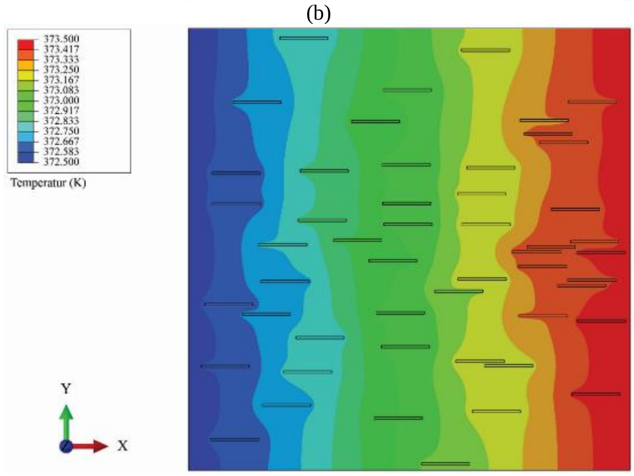


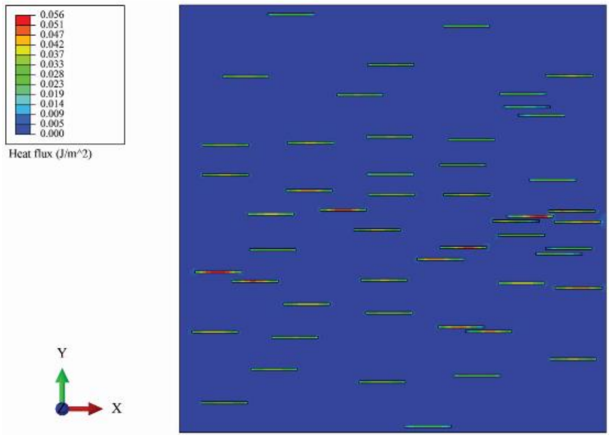


(a)



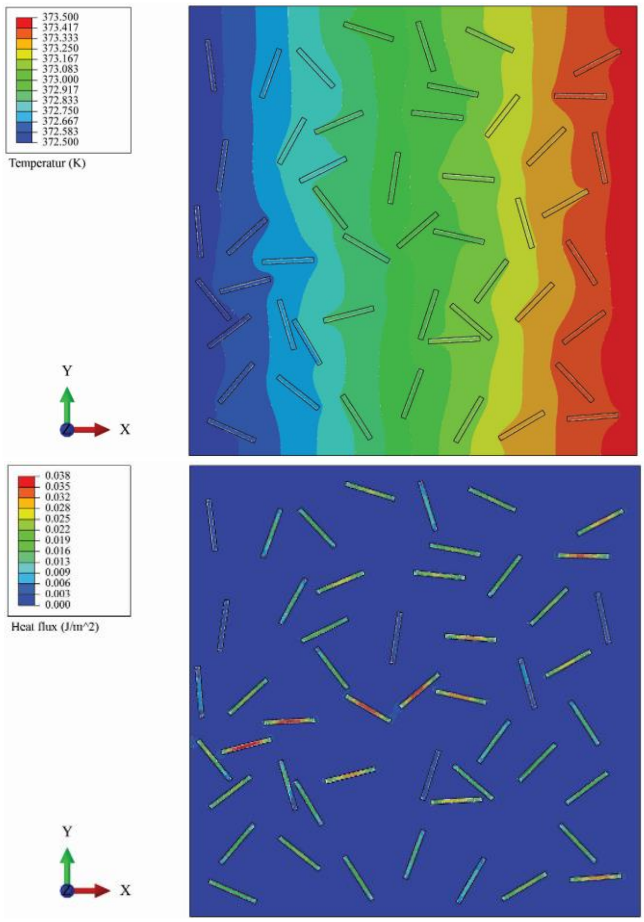
(b)



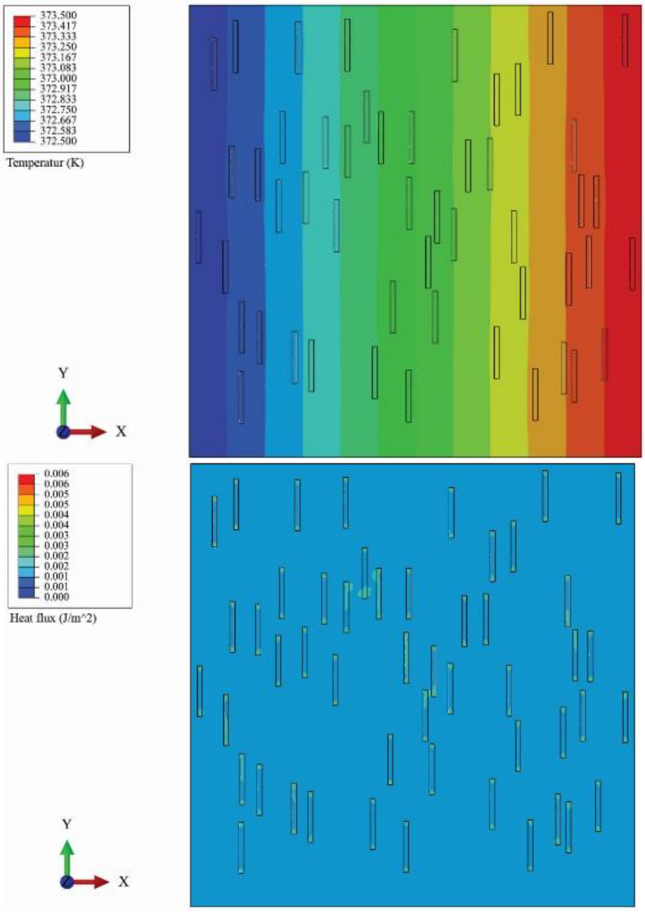


(c)

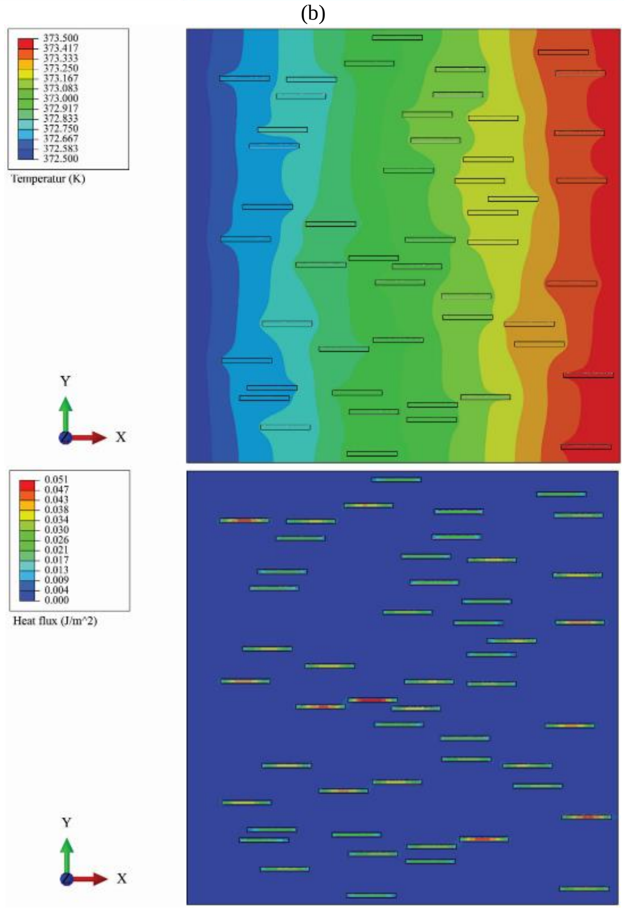
Figure 11. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 20, CNT volume percent = 5%, temperature = 100°C， interphase thickness= 0)



(a)

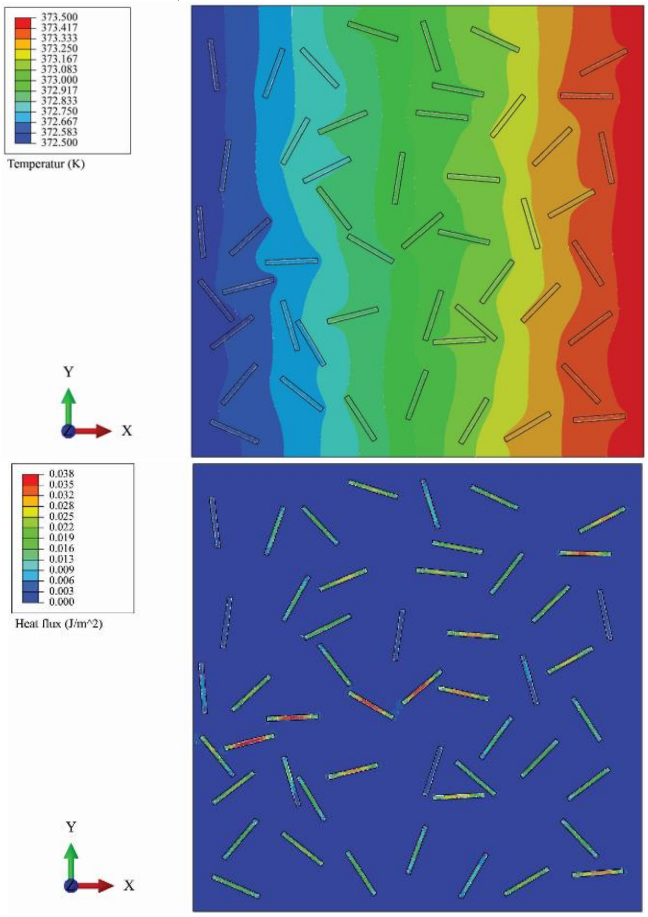


(b)

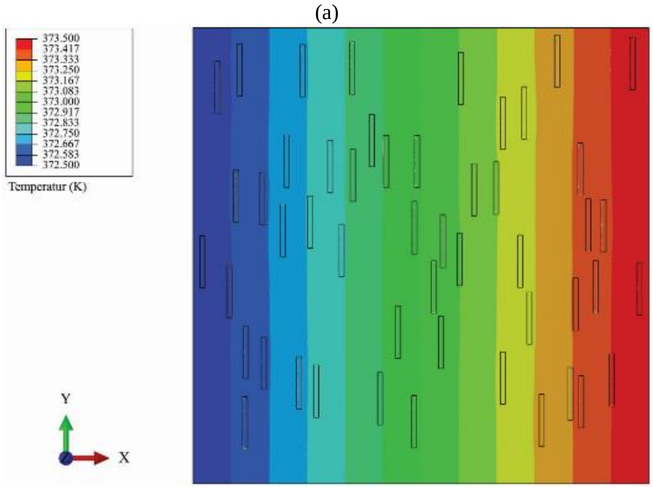


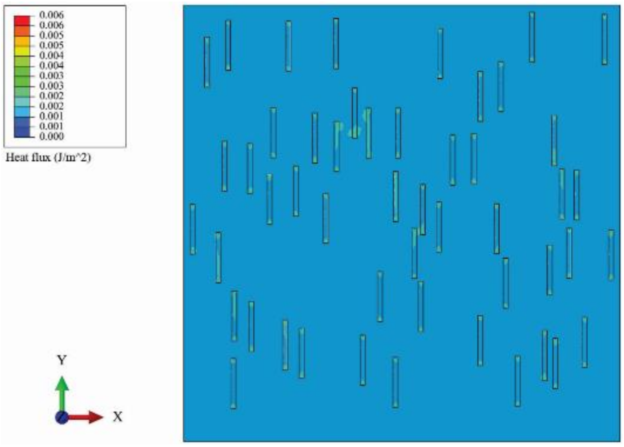
(c)

Figure 12. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 20, CNT volume percent = 5%, temperature = 100°C, interphase thickness= half of CNT diameter)

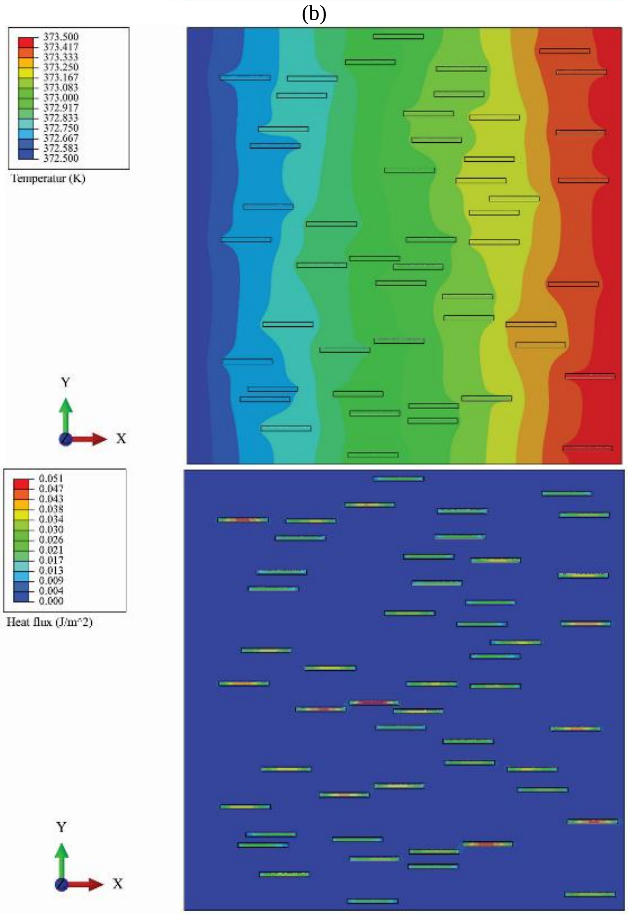


(a)





(b)



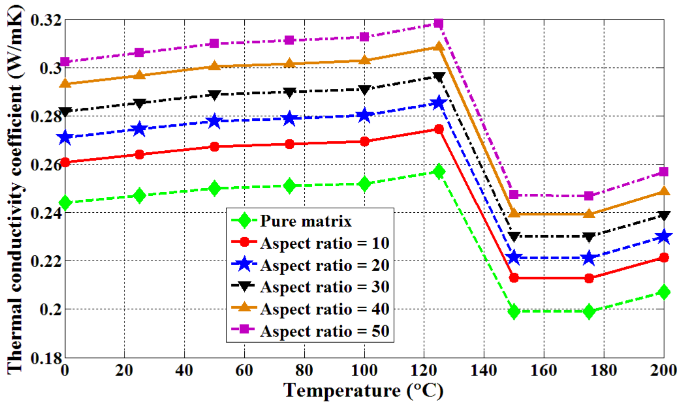
(c)

Figure 13. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 20, CNT volume percent = 5%, temperature = 100°C, interphase thickness= CNT diameter)

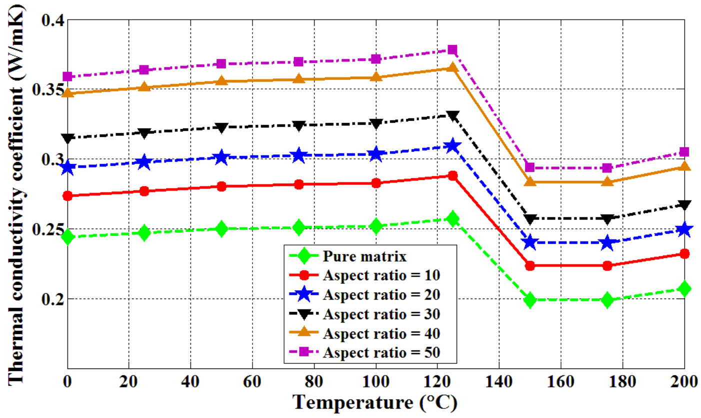
3.4. Effect of CNT aspect ratio

Figs. 14-16 show the effect of CNT aspect ratio on the thermal conductivity coefficient of CNT reinforced polypropylene matrix for the volume percent of 1%, 3% and 5%. The CNT aspect ratios are considered as 10, 20, 30, 40 and 50. The thickness of the interphase is considered as half of the CNT diameter. It is seen that increasing the nanotube aspect ratio leads to increasing the thermal conductivity coefficients of CNT/polypropylene nanocomposites for random distribution of CNT and regular distribution of CNT along the temperature difference. However, for polypropylene matrix reinforced by regular dispersed CNTs perpendicular to the temperature difference, an inverse phenomenon is seen. In other words, the polypropylene matrix reinforced by longer SWCNTs have smaller thermal conductivity coefficients than those reinforced by shorter nanotubes.

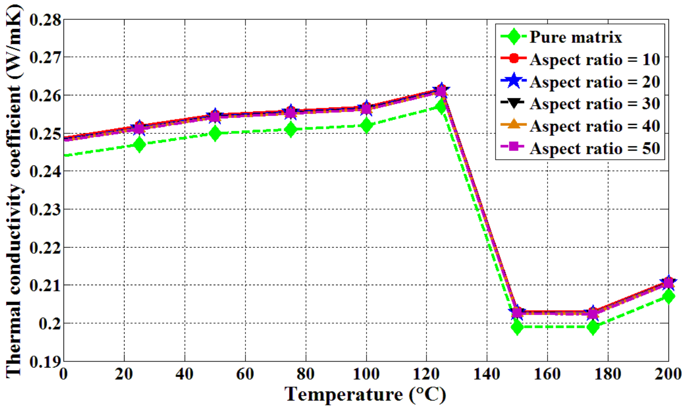
Moreover, the discrepancy of the curves is more for larger CNT volume fractions. Especially, for the CNT volume fraction of 1%, the curves associated with different CNT aspect ratios are almost coincident. Therefore, one can conclude that increasing aspect ratio leads to increasing the effect of aspect ratio on the thermal conductivity coefficient of polypropylene matrix reinforced by SWCNTs.



(a)

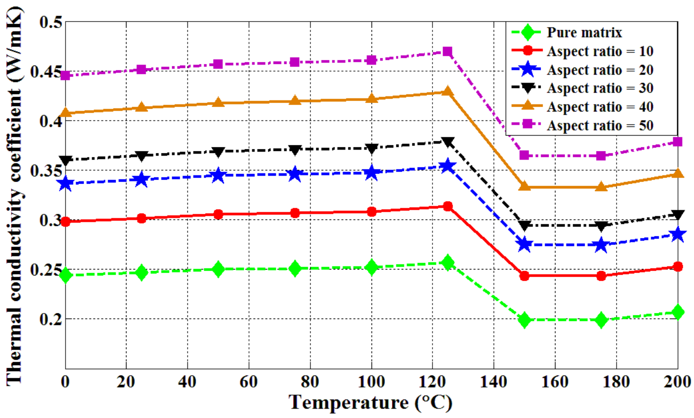


(b)

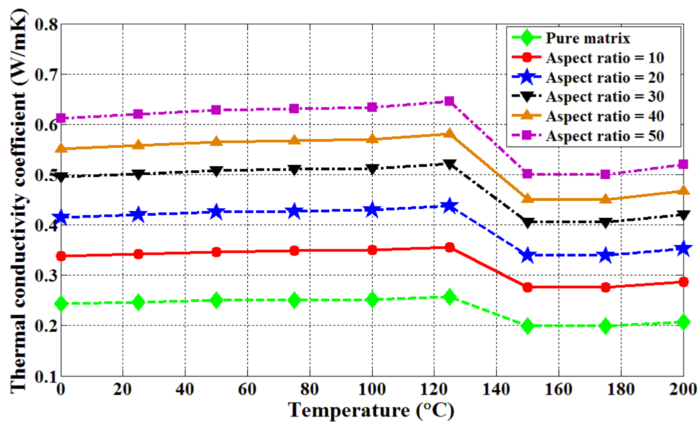


(c)

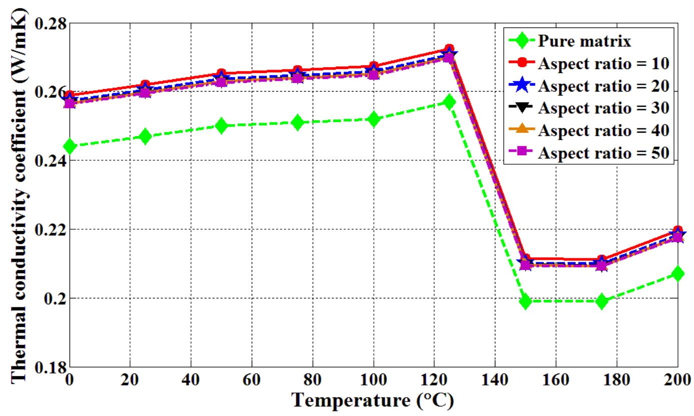
Figure 14. Thermal conductivity coefficient of polypropylene matrix reinforced by 1% volume percent CNTs with different aspect ratios versus temperature (interphase thickness = half of CNT diameter, (a) random distribution, (b) regular distribution along ΔT and (c) regular distribution perpendicular to ΔT)



(a)

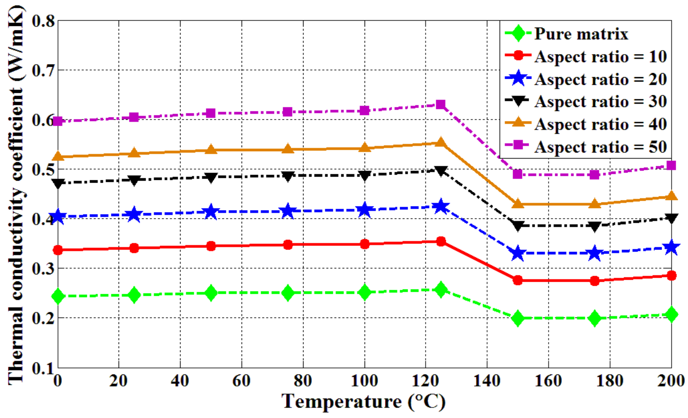


(b)

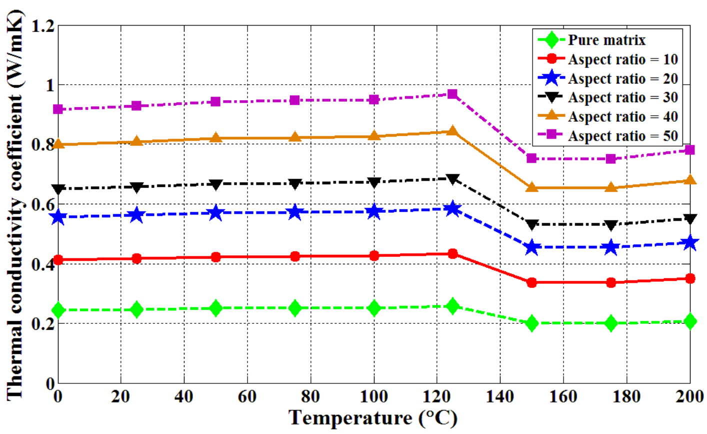


(c)

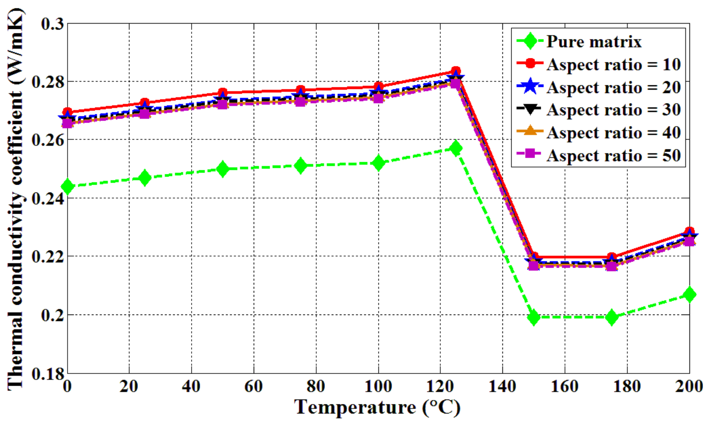
Figure 15. Thermal conductivity coefficient of polypropylene matrix reinforced by 3% volume percent CNTs with different aspect ratios versus temperature (interphase thickness = half of CNT diameter, (a) random distribution, (b) regular distribution along ΔT and (c) regular distribution perpendicular to ΔT)



(a)

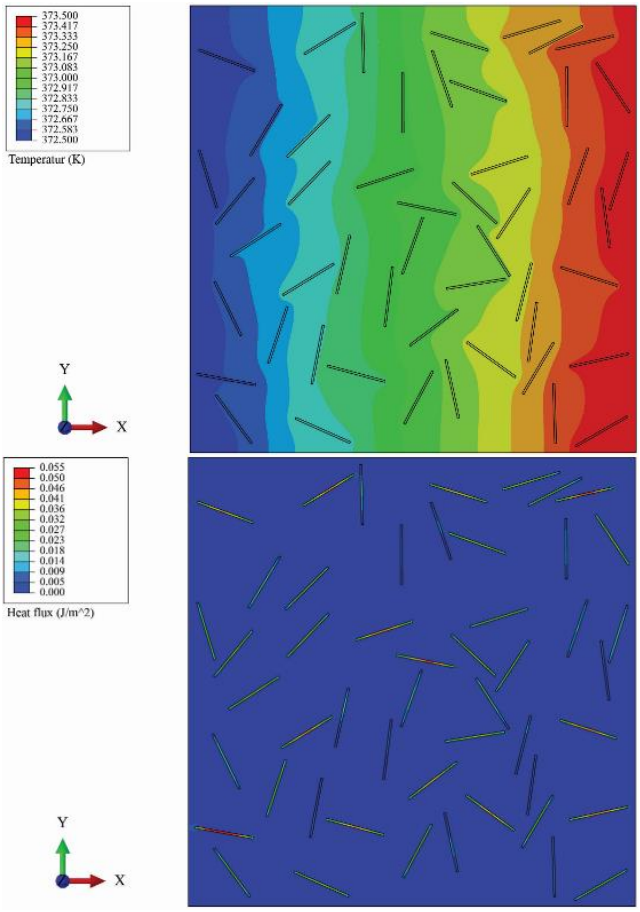


(b)

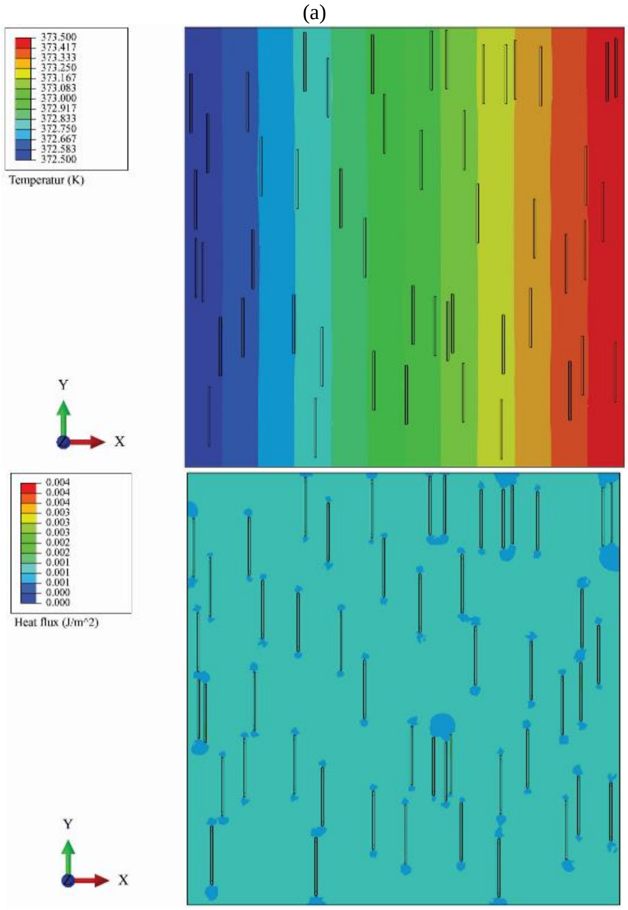


(c)

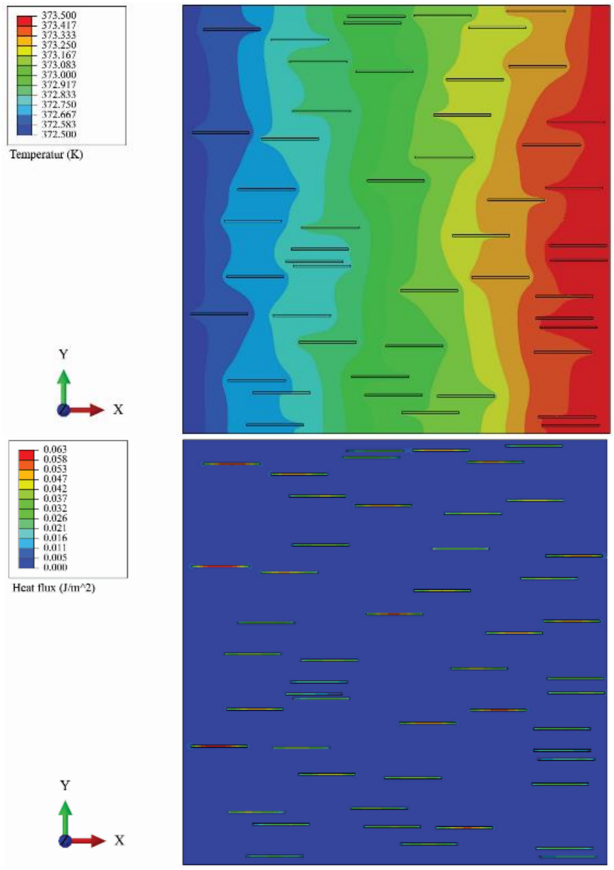
Figure 16. Thermal conductivity coefficient of polypropylene matrix reinforced by 5% volume percent CNTs with different aspect ratios versus temperature (interphase thickness = half of CNT diameter, (a) random distribution, (b) regular distribution along ΔT and (c) regular distribution perpendicular to ΔT)



(a)

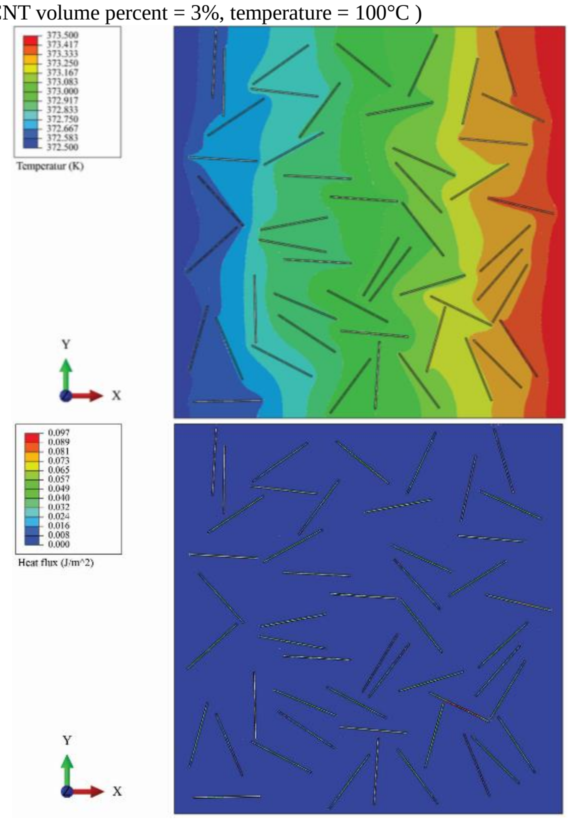


(b)

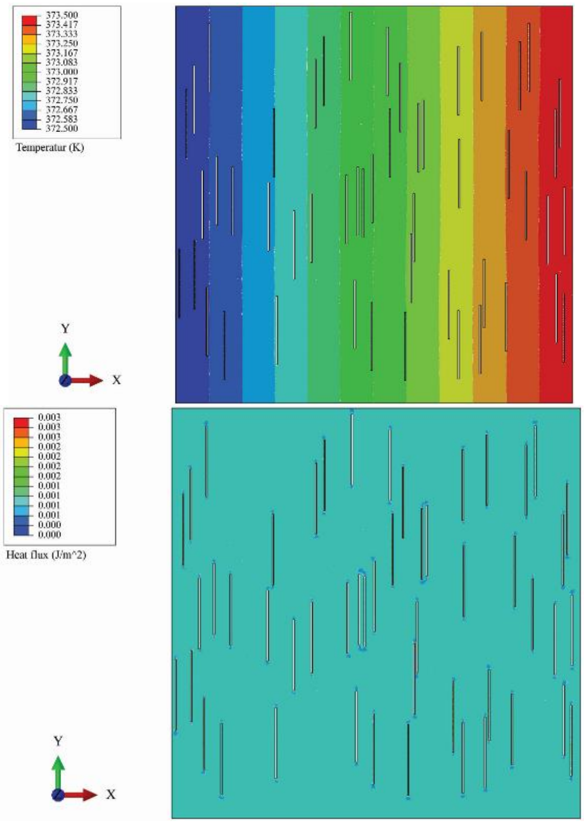


(c)

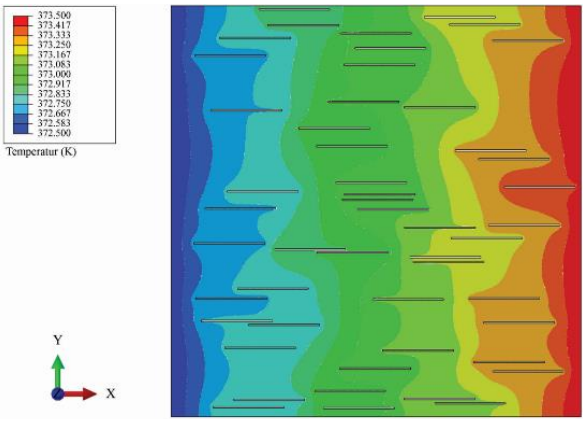
Figure 17. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 30, CNT volume percent = 3%, temperature = 100°C)

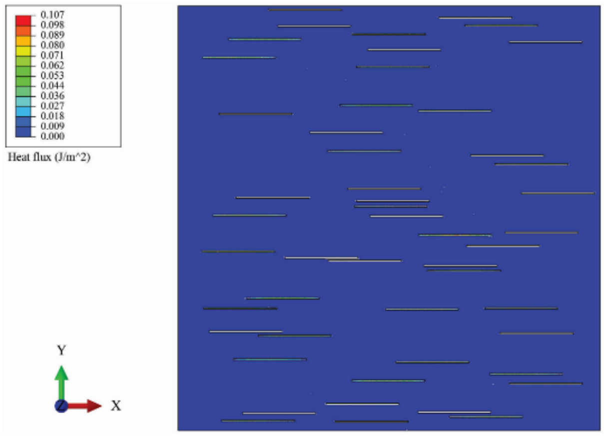


(a)



(b)





(c)

Figure 18. Thermal and heat flux distribution in polypropylene matrix reinforced by CNTs (a) random distribution, (b) regular distribution perpendicular to ΔT and (c) regular distribution along ΔT (CNT aspect ratio = 50, CNT volume percent = 3%, temperature = 100°C)

The effect of CNT aspect ratio on the temperature and heat flux profiles can be observed in Figs. 17 and 18. The CNT aspect ratios are considered as 3% and 5%. Moreover, the CNT volume percentage is 3%. As it is anticipated, the boundaries of constant temperature areas of RVEs reinforced by CNTs of larger aspect ratios, possess more nonlinearity. Besides, for random and regular dispersion along the temperature difference, the heat fluxes of the CNT/polypropylene nanocomposites with CNTs with larger aspect ratios are larger the heat fluxes of polypropylene reinforced by CNTs with smaller aspect ratios. However, for regular CNT dispersion perpendicular to the temperature difference, increasing aspect ratio adversely affect the heat flux.

4. Conclusions

In this paper, thermal conductivity coefficients of polypropylene matrix reinforced by SWCNTs were obtained by using FE method. It was shown that amongst the three considered CNT dispersion, including random dispersion, regular dispersion in the direction of temperature difference and regular dispersion perpendicular to the temperature difference, the second and third types possess the largest and smallest thermal conductivity coefficients, respectively. Furthermore, it was observed that the thermal conductivity coefficients of the RVEs with the first and the second dispersion types increase by the CNT aspect ratio. However, for the third dispersion pattern, increasing SWCNT aspect ratio inversely affects the thermal conductivity coefficient.

References

[1] S. Iijima, Helical microtubules of graphitic carbon, *nature*, Vol. 354, No. 6348, pp. 56, 1991.

[2] M. Mohammadi, M. Goodarzi, M. Ghayour, S. Alivand, Small scale effect on the vibration of orthotropic plates embedded in an elastic medium and under biaxial in-plane pre-load via nonlocal elasticity theory, 2012.

[3] M. Mohammadi, A. Farajpour, M. Goodarzi, R. Heydarshenas, Levy type solution for nonlocal thermo-mechanical vibration of orthotropic mono-layer graphene sheet embedded in an elastic medium, *Journal of Solid Mechanics*, Vol. 5, No. 2, pp. 116-132, 2013.

[4] S. R. Asemi, M. Mohammadi, A. Farajpour, A study on the nonlinear stability of orthotropic single-layered graphene sheet based on nonlocal elasticity theory, *Latin American Journal of Solids and Structures*, Vol. 11, No. 9, pp. 1515-1540, 2014.

[5] M. Mohammadi, A. Moradi, M. Ghayour, A. Farajpour, Exact solution for thermo-mechanical vibration of orthotropic mono-layer graphene sheet embedded in an elastic medium, *Latin American Journal of Solids and Structures*, Vol. 11, No. 3, pp. 437-458, 2014.

[6] M. Goodarzi, M. Mohammadi, A. Farajpour, M. Khooran, Investigation of the effect of pre-stressed on vibration frequency of rectangular nanoplate based on a visco-Pasternak foundation, 2014.

[7] M. Mohammadi, A. Farajpour, M. Goodarzi, H. Mohammadi, Temperature effect on vibration analysis of annular graphene sheet embedded on visco-Pasternak foundation, 2013.

[8] P. Malekzadeh, A. Farajpour, Axisymmetric free and forced vibrations of initially stressed circular nanoplates embedded in an elastic medium, *Acta Mechanica*, Vol. 223, No. 11, pp. 2311-2330, 2012.

[9] M. Mohammadi, M. Safarabadi, A. Rastgoo, A. Farajpour, Hygro-mechanical vibration analysis of a rotating viscoelastic nanobeam embedded in a visco-Pasternak elastic medium and in a nonlinear thermal environment, *Acta Mechanica*, Vol. 227, No. 8, pp. 2207-2232, 2016.

[10] M. Safarabadi, M. Mohammadi, A. Farajpour, M. Goodarzi, Effect of surface energy on the vibration analysis of rotating nanobeam, *Journal of Solid Mechanics*, Vol. 7, No. 3, pp. 299-311, 2015.

[11] M. Baghani, M. Mohammadi, A. Farajpour, Dynamic and stability analysis of the rotating nanobeam in a nonuniform magnetic field considering the surface energy, *International Journal of Applied Mechanics*, Vol. 8, No. 04, pp. 1650048, 2016.

[12] M. R. Farajpour, A. Rastgoo, A. Farajpour, M. Mohammadi, Vibration of piezoelectric nanofilm-based electromechanical sensors via higher-order non-local strain gradient theory, *Micro & Nano Letters*, Vol. 11, No. 6, pp. 302-307, 2016.

[13] M. Danesh, A. Farajpour, M. Mohammadi, Axial vibration analysis of a tapered nanorod based on nonlocal elasticity theory and differential quadrature method, *Mechanics Research Communications*, Vol. 39, No. 1, pp. 23-27, 2012.

[14] H. Moosavi, M. Mohammadi, A. Farajpour, S. Shahidi, Vibration analysis of nanorings using nonlocal continuum mechanics and shear deformable ring theory, *Physica E: Low-dimensional Systems and Nanostructures*, Vol. 44, No. 1, pp. 135-140, 2011.

[15] A. Farajpour, A. Rastgoo, M. Farajpour, Nonlinear buckling analysis of magneto-electro-elastic CNT-MT hybrid nanoshells based on the nonlocal continuum mechanics, *Composite Structures*, Vol. 180, pp. 179-191, 2017.

[16] S. Rouhi, Y. Alizadeh, R. Ansari, On the interfacial characteristics of polyethylene/single-walled carbon nanotubes using molecular dynamics simulations, *Applied Surface Science*, Vol. 292, pp. 958-970, 2014.

[17] S. Rouhi, Y. Alizadeh, R. Ansari, Molecular dynamics simulations of the single-walled carbon nanotubes/poly (phenylacetylene) nanocomposites, *Superlattices and Microstructures*, Vol. 72, pp. 204-218, 2014.

[18] S. Rouhi, Y. Alizadeh, R. Ansari, On the elastic properties of single-walled carbon nanotubes/poly (ethylene oxide) nanocomposites using molecular dynamics simulations, *Journal of molecular modeling*, Vol. 22, No. 1, pp. 41, 2016.

[19] S. Rouhi, Y. Alizadeh, R. Ansari, M. Aryayi, Using molecular dynamics simulations and finite element method to study the mechanical properties of nanotube reinforced polyethylene and polyketone, *Modern Physics Letters B*, Vol. 29, No. 26, pp. 1550155, 2015.

[20] S. Rouhi, R. Ansari, M. Ahmadi, Finite element investigation into the thermal conductivity of carbon nanotube/aluminum nanocomposites, *Modern Physics Letters B*, Vol. 31, No. 06, pp. 1750053, 2017.

[21] R. Ansari, S. Rouhi, M. Eghbalian, On the elastic properties of curved carbon nanotubes/polymer nanocomposites: A modified rule of mixture, *Journal of Reinforced Plastics and Composites*, Vol. 36, No. 14, pp. 991-1008, 2017.

[22] S. Rouhi, S. H. Alavi, On the mechanical properties of functionally graded materials reinforced by carbon nanotubes, *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, pp. 0954406217706096, 2017.

[23] M. Ahmadi, R. Ansari, S. Rouhi, Finite element investigation of temperature dependence of elastic properties of carbon nanotube reinforced polypropylene, *The European Physical Journal Applied Physics*, Vol. 80, No. 3, pp. 30401, 2017.

[24] R. S. Ruoff, D. C. Lorents, Mechanical and thermal properties of carbon nanotubes, *carbon*, Vol. 33, No. 7, pp. 925-930, 1995.

[25] J. Che, T. Cagin, W. A. Goddard III, Thermal conductivity of carbon nanotubes, *Nanotechnology*, Vol. 11, No. 2, pp. 65, 2000.

[26] K. I. Winey, T. Kashiwagi, M. Mu, Improving electrical conductivity and thermal properties of polymers by the addition of carbon nanotubes as fillers, *Mrs Bulletin*, Vol. 32, No. 4, pp. 348-353, 2007.

[27] S.-Y. Yang, C.-C. M. Ma, C.-C. Teng, Y.-W. Huang, S.-H. Liao, Y.-L. Huang, H.-W. Tien, T.-M. Lee, K.-C. Chiou, Effect of functionalized carbon nanotubes on the thermal conductivity of epoxy composites, *Carbon*, Vol. 48, No. 3, pp. 592-603, 2010.

[28] A. M. Marconnet, N. Yamamoto, M. A. Panzer, B. L. Wardle, K. E. Goodson, Thermal conduction in aligned carbon nanotube–polymer nanocomposites with high

packing density, *ACS nano*, Vol. 5, No. 6, pp. 4818-4825, 2011.

[29] W. Park, K. Choi, K. Lafdi, C. Yu, Influence of nanomaterials in polymer composites on thermal conductivity, *Journal of Heat Transfer*, Vol. 134, No. 4, pp. 041302, 2012.

[30] R. Gulotty, M. Castellino, P. Jagdale, A. Tagliaferro, A. A. Balandin, Effects of functionalization on thermal properties of single-wall and multi-wall carbon nanotube–polymer nanocomposites, *ACS nano*, Vol. 7, No. 6, pp. 5114-5121, 2013.

[31] H. Liem, H. Choy, Superior thermal conductivity of polymer nanocomposites by using graphene and boron nitride as fillers, *Solid State Communications*, Vol. 163, pp. 41-45, 2013.

[32] S. Araby, Q. Meng, L. Zhang, H. Kang, P. Majewski, Y. Tang, J. Ma, Electrically and thermally conductive elastomer/graphene nanocomposites by solution mixing, *Polymer*, Vol. 55, No. 1, pp. 201-210, 2014.

[33] R. S. Kapadia, B. M. Louie, P. R. Bandaru, The influence of carbon nanotube aspect ratio on thermal conductivity enhancement in nanotube–polymer composites, *Journal of Heat Transfer*, Vol. 136, No. 1, pp. 011303, 2014.

[34] P. Ding, S. Su, N. Song, S. Tang, Y. Liu, L. Shi, Influence on thermal conductivity of polyamide-6 covalently-grafted graphene nanocomposites: varied grafting-structures by controllable macromolecular length, *RSC Advances*, Vol. 4, No. 36, pp. 18782-18791, 2014.

[35] Y. Çelik, A. Çelik, E. Flahaut, E. Suvaci, Anisotropic mechanical and functional properties of graphene-based alumina matrix nanocomposites, *Journal of the European Ceramic Society*, Vol. 36, No. 8, pp. 2075-2086, 2016.

[36] T. C. Clancy, T. S. Gates, Modeling of interfacial modification effects on thermal conductivity of carbon nanotube composites, *Polymer*, Vol. 47, No. 16, pp. 5990-5996, 2006.

[37] A. Bagchi, S. Nomura, On the effective thermal conductivity of carbon nanotube reinforced polymer composites, *Composites science and technology*, Vol. 66, No. 11-12, pp. 1703-1712, 2006.

[38] C. Guthy, F. Du, S. Brand, K. I. Winey, J. E. Fischer, Thermal conductivity of single-walled carbon nanotube/PMMA nanocomposites, *Journal of heat transfer*, Vol. 129, No. 8, pp. 1096-1099, 2007.

[39] J. Yu, T. E. Lacy Jr, H. Toghiani, C. U. Pittman Jr, Micromechanically-based effective thermal conductivity estimates for polymer nanocomposites, *Composites Part B: Engineering*, Vol. 53, pp. 267-273, 2013.

[40] B. Mortazavi, M. Baniassadi, J. Bardon, S. Ahzi, Modeling of two-phase random composite materials by finite element, Mori–Tanaka and strong contrast methods, *Composites Part B: Engineering*, Vol. 45, No. 1, pp. 1117-1125, 2013.

[41] B. Mortazavi, J. Bardon, S. Ahzi, Interphase effect on the elastic and thermal conductivity response of polymer nanocomposite materials: 3D finite element study, *Computational Materials Science*, Vol. 69, pp. 100-106, 2013.

[42] B. Mortazavi, O. Benzerara, H. Meyer, J. Bardon, S. Ahzi, Combined molecular dynamics-finite element multiscale modeling of thermal conduction in graphene epoxy nanocomposites, *Carbon*, Vol. 60, pp. 356-365, 2013.

[43] B. Mortazavi, F. Hassouna, A. Laachachi, A. Rajabpour, S. Ahzi, D. Chapron, V. Toniazzo, D. Ruch, Experimental and multiscale modeling of thermal conductivity and elastic properties of PLA/expanded graphite polymer nanocomposites, *Thermochimica Acta*, Vol. 552, pp. 106-113, 2013.

[44] E. Fiamegkou, N. Athanasopoulos, V. Kostopoulos, Prediction of the effective thermal conductivity of carbon nanotube-reinforced polymer systems, *Polymer Composites*, Vol. 35, No. 10, pp. 1997-2009, 2014.

[45] I. E. Afrooz, A. Öchsner, Effect of the Carbon Nanotube Distribution on the Thermal Conductivity of Composite Materials, *Journal of Heat Transfer*, Vol. 137, No. 3, pp. 034501, 2015.

[46] Y. Wang, C. Yang, Q.-X. Pei, Y. Zhang, Some aspects of thermal transport across the interface between graphene and epoxy in nanocomposites, *ACS applied materials & interfaces*, Vol. 8, No. 12, pp. 8272-8279, 2016.

[47] M. A. Osman, D. Srivastava, Temperature dependence of the thermal conductivity of single-wall carbon nanotubes, *Nanotechnology*, Vol. 12, No. 1, pp. 21, 2001.

[48] A. Dawson, M. Rides, J. Urquhart, C. Brown, Thermal conductivity of polymer melts and implications of uncertainties in data for process simulation, *Cerca con Google*, 2000.

[49] Y. S. Song, J. R. Youn, Evaluation of effective thermal conductivity for carbon nanotube/polymer composites using control volume finite element method, *Carbon*, Vol. 44, No. 4, pp. 710-717, 2006.