Prediction of the elastic behaviour of HDPE/SWCNTs nanocomposites with FEM approach

R.T. Tebeta 1, A.M. Fattahi 1, and N.A. Ahmed 2

1Mechanical Engineering Science Department, Faculty of Engineering and Built Environment, University of Johannesburg, 2006, South Africa.
2Mechanical Engineering Science Department, Faculty of Engineering and Built Environment, University of Johannesburg, 2006, South Africa.
Corresponding Author; thapelotrt@gmail.com, 201217480@student.uj.ac.za

Abstract.
Prediction of elastic behaviour of polymer-based nanocomposite using finite element method (FEM) has attracted the attention of many researchers in the past few years. In this study, ANSYS 19.2 software was used to predict the elastic modulus of high-density polyethylene (HDPE) reinforced with single-walled carbon nanotubes (SWCNTs) at different weight fractions. Three-dimensional (3-D) representative volume element (RVE) was created by FEM using ANSYS software to estimate the elastic modulus of HDPE based nanocomposite reinforced with SWCNTs nanoparticles at 0.2 wt%, 0.4 wt%, 0.6 wt%, 0.8 wt%, and 1 wt% weight fractions. To present the FEM model for predicting the elastic modulus of HDPE/SWCNT nanocomposite, the results from atomic modelling were extracted and used for properties of matrix and fibre interface. The interfacial region was used in the model to separate the conditions of load transfer between the HDPE matrix and SWCNT fibre. Two density fractions of HDPE/SWCNTs nanocomposite were also used in terms of two different densities for both HDPE and SWCNT to investigate their effect on the elastic modulus. The modelling results showed that the increase of weight fraction of single-walled carbon nanotubes (SWCNTs) results with the increase of relative elastic modulus of the nanocomposite. The results also showed that the elastic modulus of low-density fraction HDPE/SWCNTs nanocomposite improves more compared to one of the high-density fractions at the same SWCNTs weight fraction. Rule of the mixture was also used to predict the elastic behaviour of HDPE/SWCNT nanocomposite and the results were compared to those of the FEM model for validation.

Keywords: FEM, HDPE, SWCNTs, RVE, Elastic modulus, Model, Nanocomposite, weight fraction, density fraction.

1. Introduction
Improving polymer-based nanocomposites elastic properties by increasing the weight fraction of the reinforcement into the matrix have attracted many researchers and manufacturing industries. This is due to the increase in the demand of improved polymer-based nanocomposites materials in the new technological applications such as in automotive and aeronautical industries for strong but lightweight components, thermal insulators in electrical and electronics, coating and many others [1]. However, past researchers used different approaches to improve the elastic properties of the polymer-based nanocomposite, some used an experimental approach, some numerical approach and others used an analytical approach. Thakur et al. [2] showed by an experimental approach that if volume fraction of carbon nanotubes (CNTs) is increased in a matrix, it caused the increase or improvement on young's
modulus, toughness and stiffness of polymer. It has also been shown by Fattahi et al. [3] by using a numerical approach that increases in the weight fraction of single-walled carbon nanotubes (SWCNTs) improved the elastic properties of polyethylene. In this study numerical approach was used to help predict the elastic behaviour of high-density polyethylene (HDPE) reinforced with single-walled carbon nanotubes (SWCNTs) at various weight fractions. The main goal of using the numerical approach in this study was to save time and costs for experimentation. Because if the boundary conditions, material properties, intermediate phase, fibre weight fraction and the loads imposed are known, then it will be easy to predict the elastic behaviour of any composite material using numerical simulation. The biggest challenge of using a numerical approach for the prediction of the mechanical, electrical, and thermal behaviour of composite materials is to generate the model that resembles the real-life situation. Composites are known as heterogeneous materials either natural or man-made, and to model such material is difficult because two or more material with different properties must be considered as one material [4]. In the composite material reinforcement phase properties, shape and size affect the mechanical property of the entire composite and this macroscopic behaviour can only be explained by the overall behaviour of the composite [4]. There are few numerical studies available in the literature based on carbon nanotube (CNT) polymer composite assumed to be isotropic but in nature knowing that CNT polymer composite exists as anisotropic [4], [3]. This assumption is made to ensure that the numerical model is easy to generate and avoiding the complexity in generating the model. The estimation of effective elastic properties of CNT polymer-based composites have been studied and reported for the past decade and some limitations on how to apply the numerical simulation were found [5], [6]. According to Kumar et al. [7] the overall effective elastic properties of CNT-reinforced composites can be predicted using micromechanics laws if the arrangements, properties, and weight fraction of constituent phases are known. However, CNTs or SWCNTs are not a continuum media but they are a mesh structure like and for this type of structures micromechanics rules does not apply [7]. In this affection, to calculate the mechanical properties of CNT-reinforced composites several nanomechanical models are developed [8], [9], [10]. Methods such as continuum mechanics and molecular dynamics play an important role in the development of CNT-reinforced composites. According to Joshi et al and Safaei et al. [11], [12] the continuum mechanics method is regarded as perfect because it has been successfully used in the mechanical modelling of CNTs which could be in the solid cylinder, shell, or beam modes. To model CNT-reinforced composites at a different weight fraction of CNT, continuum mechanics-based methods can be applied to parametrically evaluate the effective elastic properties [7]. This method has the potential to model transition from nano-scales to macro scales such as properties of the interphase between the different materials and chemical bonds. Most of the researches and existing literature reported continuum mechanics methods using finite element method (FEM) which are based on three-dimensional (3-D) Representative Volume Element (RVE) concept [13], [14]. In this work, the mechanical properties of HDPE/SWCNTs nanocomposite were investigated using 3-D RVE. Its elastic behaviour was simulated by creating RVE using finite element method. The properties of fibre, intermediate phase, and matrix used were extracted based on atomic modelling results and a model for the prediction of elastic modulus of HDPE/SWCNTs nanocomposite was developed. Also, the Rule of mixture was used to calculate the elastic modulus of HDPE/SWCNTs nanocomposite and the results were compared to that of simulated results for validation.
The effect of reinforcing polymer with nanoparticles such as CNTs at different weight fraction to improve its elastic and thermal properties have been widely investigated using various approaches including experimental, analytical, and numerical methods. Among all the approaches used Finite element method (FEM) which is part of the numerical approach has attracted great attention because of its ability to save time and costs. The main goal of this work was to use ANSYS 19.2 software to develop a modelling system for the prediction of the elastic behaviour of HDPE/SWCNT nanocomposite and find the vital equations to extract the results from the software. In this work, the effect of adding SWCNTs into HDPE matrix at different weight fraction was examined using RVE method and rule of mixture equation to vary the volume fractions of the matrix at the constant fibre volume fraction. To achieve this SWCNTs fibre and HDPE matrix within RVE were assumed to be an elastic continuum, homogeneous, linear, elastic, isotropic, and their Poisson’s ration and Young’s moduli were known. Also, for the intermediate phase between SWCNT fibre and HDPE matrix, the section was created, and its properties were determined with atomic simulations [3], [15]. The obtained results were compared and validated with the aid of experimental results [16], [2], and the numerical results [3].

2. Methodology

2.1 Finite element modelling approaches

The method used for the modelling of the HDPE/SWCNTs nanocomposite was FEM by means of the RVE technique. To generate a model the RVE was created using the test section of the reinforced tensile test sample with randomly dispersed SWCNTs nanoparticles as illustrated in Figure 1. At the test section, the SWCNTs are assumed to be dispersed homogeneously in the HDPE matrix and there is no existence of SWCNTs aggregation in the nanocomposite [17]. The RVE consists of three phases, including SWCNT fibre, intermediate phase located between fibre and matrix, and HDPE matrix. It is noted that the SWCNTs are modelled as nanofibers and they are surrounded by the intermediate phase region of distinct thickness [18], [19], [20], [21]. To obtain the elastic properties of the HDPE/SWCNTs nanocomposite, a uniform pressure of -100 MPa was applied on the edge of the RVE, while the opposite edge fixed along the z-direction. Figure 2 presents the two views of the cylindrical geometry of the RVE obtained from the test section of the reinforced tensile sample in Figure 1.
Figure 1: RVE from the test section of the reinforced tensile test sample with random microstructure

Figure 2 illustrate the load and boundary conditions on the RVE of HDPE/SWCNTs nanocomposite with random microstructure. The microstructure RVE was assumed to have been obtained from the centre test sample where x and z are fixed so that it can respond to the applied load the same way as the reinforced tensile test sample due to the symmetry along z-x region [22].

Figure 2: two views and boundary conditions of RVE obtained from the test section of the reinforced tensile sample

To generate a 3-dimensional (3-D) model for the matrix, intermediate phase and fiber presented in Figure 2, a quarter of cylindrical RVE was created to represent HDPE/SWCNTs nanocomposite. Figure 3 Illustrates the 3-D RVE of the short SWCNT fiber and intermediate phase in the HDPE matrix. This RVE of the nanocomposite was made from three layers of different colors to show how actually SWCNT is bonded to HDPE by intermediate phase. Figure 4 shows the assembling order of the three layers that make up the RVE of HDPE/SWCNTs nanocomposite. It shows that SWCNT was modeled as a tube-like structure covered with the layer of the intermediate phase.
2.2 HDPE/SWCNTs nanocomposite RVE modelling

The effect of reinforcing HDPE matrix with SWCNTs at different weight fractions have been investigated using the material properties listed in Table 1. Last two rows of Table 1 contain different densities for both HDPE and SWCNTs. This is due to the products manufactures, for example, HDPE has a density ranging from 0.940 g/cm³ to 0.959 g/cm³ [23] available in the markets. SWCNTs also exist with the density range from 1.65 g/cm³ to 1.90 g/cm³. Since HDPE and SWCNTs exist in different densities, then tow ranges of their densities were used for the investigation.

Figure 3: 3-D view Quarter-sectional of a cylindrical RVE

Figure 4: Assembly order for fiber, intermediate phase, and matrix in the RVE
Table 1: Properties and the dimensions of the RVE with HDPE matrix parameters represented by x [3].

| Properties         | Intermediate phase | (HDPE) Matrix | (SWCNTs) Fibre |
|--------------------|--------------------|---------------|----------------|
| Length (nm)        | 150                | 150           |                |
| Internal radius (nm)| 5                  | Change with x| 4.6           |
| Outer radius (nm)  | 5.4                |               | 5              |
| Elastic modulus (GPa)| 4.06              | 1000          |                |
| Poisson's ration   | 0.3                | 0.3           |                |
| Density (g/cm³)    | --                 | 0.940         | 1.68           |
| Density (g/cm³)    | --                 | 0.950         | 1.90           |

To achieve different weight and volume fractions symmetric model of the RVE in Figure 5 was developed such that change in x parameter affect the weight fractions. It was used to studying the effect of the addition of SWCNTs into the HDPE matrix. In this study, it was assumed that the material properties of RVE in Table 1 are like the real properties of the HDPE/SWCNT nanocomposite [24], [25], [26].

![Figure 5: Schematic of HDPE/SWCNT nanocomposite RVE](image)

To determine the value of x parameter for a given weight fraction of SWCNTs, the volume of SWCNT and the volume of RVE were calculated as follows:

\[
V_{SWCNT} = \pi ((5)^2 - (4.6)^2)(150) = 576\pi \\
V_{RVE} = \pi \left(\frac{(2x+10)^2}{2}\right)(2x + 150) \tag{1}
\]

The volume fraction was also calculated using equation 2 that relates the volume of SWCNT and the of RVE as:

\[
V_f = \frac{V_{SWCNT}}{V_{RVE}} = \frac{wt\%}{wt\% + \left(\frac{\rho_f}{\rho_m}\right)(1-wt\%)} \tag{2}
\]

Where wt\% is the specific weight fraction of fiber (WSCNT) into the matrix (HDPE), \(\rho_f\) is the density of the fiber (WSCNT), and \(\rho_m\) is the density of the matrix (HDPE).
From equation 2 the density fraction of fiber and matrix is represented as $\left( \frac{\rho_f}{\rho_m} \right)$. Since in this study two densities for SWCNT and HDPE were used, then two density fractions was calculated for each x parameter as:

$\left( \frac{\rho_f}{\rho_m} \right) = \left( \frac{1.68}{0.940} \right) = 1.79$ for first HDPE/SWCNTs nanocomposite properties and the second HDPE/SWCNTs nanocomposite was found to be $\left( \frac{\rho_f}{\rho_m} \right) = \left( \frac{1.90}{0.950} \right) = 2$. These density fractions were used in equation 2 to calculate the volume fractions of each HDPE/SWCNTs nanocomposite at different weight fractions of SWCNTs.

Equation 1 and 2 were then equated to come up with equation 3 that was used to calculate parameter x as follows:

$$V_{RVE} = \frac{V_{SWCNT}}{V_f} \times 100 = \pi \left( \frac{(2x+10)^2}{2} \right) \left( 2x + 150 \right) = \frac{576\pi}{V_f} \times 100$$

Equation 3 was then simplified to the third order equation as:

$$2x^3 + 170x^2 + 1550x + 3750 = \frac{576}{V_f} \times 100$$

The value of x for any given weight fraction of SWCNTs was obtained by solving equation 4. The RVE diameter and the length were calculated according to Fig 5, using the following equations:

$$D_{RVE} = 2x + 10, \quad L_{RVE} = 2x + 150$$

To comply with the experimental results of [2, 16] and the numerical results of [3], the weight fractions were considered to be 0.2 wt%, 0.4 wt%, 0.6 wt%, 0.8 wt%, and 1 wt%. At this given weight fractions, x parameter was obtained by solving equation 4 using volume fraction. The calculated value of the x parameter for each weight fraction was used to obtain the dimensions of RVE presented in Table 2 and Table 3 based on density fractions.

**Table 2**: Volume fraction, parameter x and the dimensions of RVE at different weight fractions for the density fraction of 1.79.

| SWCNTs Weight fraction (wt%) | Volume Fraction | Parameter x (nm) | The diameter of RVE (nm) | The length of RVE (nm) |
|-----------------------------|-----------------|-----------------|-------------------------|------------------------|
| 0.2                         | 0.112           | 41.90           | 93.80                   | 233.80                 |
| 0.4                         | 0.224           | 29.99           | 69.98                   | 209.98                 |
| 0.6                         | 0.337           | 24.33           | 58.66                   | 198.98                 |
| 0.8                         | 0.449           | 20.87           | 51.74                   | 191.74                 |
| 1                           | 0.562           | 18.42           | 46.84                   | 186.84                 |

**Table 3**: Volume fraction, parameter x and the dimensions of RVE at different weight fractions for the density fraction of 2.

| SWCNTs Weight fraction (wt%) | Volume Fraction | Parameter x (nm) | The diameter of RVE (nm) | The length of RVE (nm) |
|-----------------------------|-----------------|-----------------|-------------------------|------------------------|
|                            |                 |                 |                         |                        |
2.3 ANSYS Simulation
The parameters in Table 2 and Table 3 were used to generate a model for FEM simulation using ANSYS Mechanical APDL 19.2 file. The preferences on ANSYS mechanical was set to structural and the Element type was set as solid 10 nodes 187. The material properties for materials were used as listed in Table 1 and they were assumed to be linear, elastic, and isotropic. The model was created a quarter of a cylinder as illustrated in Figure 3 and Figure 4. Figure 6 demonstrate the lead application on the HDPE/SWCNTs nanocomposite geometry used for simulation.

|   |   |   |   |
|---|---|---|---|
| 0.2 | 0.1 | 44.16 | 98.32 | 238.32 |
| 0.4 | 0.201 | 31.65 | 73.30 | 213.30 |
| 0.6 | 0.301 | 25.81 | 61.62 | 201.62 |
| 0.8 | 0.402 | 22.16 | 54.32 | 194.32 |
| 1   | 0.503 | 19.60 | 49.20 | 189.20 |

Figure 6: Load application on the HDPE/SWCNT nanocomposite RVE
Figure 7 illustrates the meshed HDPE/SWCNT nanocomposite RVE with the two longitudinal sides along z-direction assumed to be symmetric. The load of -100 MPa was applied to the red striped area and the opposite area was fixed as shown by the purple arrows. The mesh size of the model was improved to a global mesh fine of 4 as shown in Figure 8.
The nodal solutions for both displacement and stress transfer in the z-direction of the parament $x = 18.42$ nm from Table 2 are presented in Figure 9 and Figure 10 respectively.
Figure 9: Nodal displacement in the z-direction of HDPE/SWCNTs nanocomposite

Figure 10: Nodal Stress transfer in HDPE/SWCNTs nanocomposite
The nodal displacement and stress transfer were simulated for every x-parameter as presented in both Table 2 and Table 3. The results and the discussion for the model are presented in section 3.

### 3. Result and discussions

The results obtained from FEM and rule of the mixture are summarised in Table 4 and Table 5 for both density fractions. The elastic modulus of FEM results and the rule of mixture results presented in Tables 4 and 5 were calculated as follows:

For FEM as illustrated in Fig. 10 that the maximum displacement of HDPE/SWCNTs nanocomposite reinforced at 1 wt% weight fraction of SWCNT with the x parameter of 18.42 nm is 4.96128 nm. Then the elastic modulus was calculated as:

$$E_c = \frac{P_L}{\text{DMX}} = \frac{(100 \times 10^6)(186.84)}{4.96128} = 3.77 \text{ GPa} \quad (6)$$

Where $E_c$ is the elastic modulus of the composite/nanocomposite, $P$ is the applied load, $L$ is the length of the RVE of HDPE/SWCNT nanocomposite, and DMX is the FEM maximum displacement. Since the dimensions of RVE of the nanocomposite were changing with respect to x parameter, equation 6 was used to calculate the elastic modulus of other HDPE/SWCNTs nanocomposite at different weight fractions and density fraction as illustrated in Table 4 and Table 5. The FEM for each RVE dimensions were performed at a constant load of -100 GPa at various DMX based on the simulation.

For the Rule of mixture elastic modulus of HDPE/SWCNTs nanocomposite was calculated as:

$$E_c = V_f E_f + V_m E_m + V_I E_I \quad (7)$$

Where, $V_f$ is the volume fraction of the fibre (SWCNT), $E_f$ is the elastic modulus of the fibre (SWCNT), $V_m$ is the volume fraction of the matric (HDPE), $E_m$ is the elastic modulus of the matrix (HDPE), $V_I$ is the volume fraction of the intermediate phase, and $E_I$ is the elastic modulus of the intermediate phase.

In equation 7, the elastic modulus of fibre, matrix and intermediate phase was kept constant for according to Table 1 and the changes were made for volume fraction based on the change in x parameter affected by weight fractions. The volume fractions of fibre, matrix and intermediate phase for each weight fraction were calculated as follows:

$$V_f = \frac{\pi ((r_{of})^2 - (r_{if})^2)(150)}{\pi ((r_{im}+x)^2 - (r_{im})^2)(150) + \pi ((r_{im}+x)^2)(2x)} \quad (8)$$

$$V_I = \frac{\pi ((r_{im}+x)^2 - (r_{im})^2)(150) + \pi ((r_{im}+x)^2)(2x)}{\pi ((r_{ol})^2 - (r_{il})^2)(150)} \quad (9)$$

$$V_m = 1 - V_f - V_I \quad (10)$$

Where, $r_{of}$ is the outer radius of the fiber, $r_{if}$ is the inner radius of the fibre, $r_{im}$ is the inner radius of the matrix, $r_{ol}$ is the outer radius of the intermediate phase, $r_{il}$ is the inner radius of the intermediate phase, 150 is the length of fiber and intermediate phase in (nm), and $x$ is the parameter that changes with the weight fraction as shown in Table 4 and Table 5.
Table 4: The FEM and rule of mixture elastic modulus of HDPE/SWCNTs nanocomposite and different weight fractions for the density fraction 1.79.

| SWCNTs Weight fraction (wt%) | Parameter x (nm) | Elastic modulus from ANSYS FEM (GPa) | Elastic modulus from the Rule of mixture (GPa) |
|-----------------------------|------------------|-------------------------------------|---------------------------------------------|
| 0.2                         | 41.90            | 2.16                                | 3.13                                        |
| 0.4                         | 29.99            | 2.28                                | 4.25                                        |
| 0.6                         | 24.33            | 3.10                                | 5.38                                        |
| 0.8                         | 20.87            | 3.43                                | 6.52                                        |
| 1                           | 18.42            | 3.77                                | 7.69                                        |

Table 5: The FEM and rule of mixture elastic modulus of HDPE/SWCNTs nanocomposite and different weight fractions for the density fraction of 2

| SWCNTs Weight fraction (wt%) | Parameter x (nm) | Elastic modulus from ANSYS FEM (GPa) | Elastic modulus from the Rule of mixture (GPa) |
|-----------------------------|------------------|-------------------------------------|---------------------------------------------|
| 0.2                         | 44.16            | 2.37                                | 3.01                                        |
| 0.4                         | 31.65            | 2.69                                | 4.02                                        |
| 0.6                         | 25.81            | 3.00                                | 5.02                                        |
| 0.8                         | 22.16            | 3.30                                | 6.04                                        |
| 1                           | 19.60            | 3.60                                | 7.08                                        |

Figure 11: The effect of SWCNT weight fraction on HDPE/SWCNTs nanocomposite Elastic modulus
Figure 12: The effect of SWCNT weight fraction on HDPE/SWCNTs nanocomposite Elastic modulus

Figure 13: Comparison of the effect of the density fraction on HDPE/SWCNTs nanocomposite at a different weight fraction of SWCNTs
Figure 14: Comparison of the effect of the density fraction on HDPE/SWCNTs nanocomposite at a different weight fraction of SWCNTs

The results obtained from ANSYS FEM model and rule of mixture were presented in the form of Tables and graphs. According to Figure 11 generated from Table 4, the results obtained by FEM modelling and the rule of mixture showed that the increase of SWCNTs weight fraction significantly increases the elastic modulus of the HDPE/SWCNTs nanocomposite. However, the difference between FEM results and the Ruler of mixture results was higher of which it might have been caused by the assumptions made for FEM modelling. Figure 13 demonstrate the effect of the density fractions on the elastic modulus of HDPE/SWCNTs nanocomposite for Rule of mixture results, which showed that even if the weight fraction of SWCNTs is the same, elastic modulus differs. This displayed that the elastic modulus of HDPE/SWCNTs nanocomposite with low-density fraction improver better at the same weight fraction compared to one with high-density fraction.

The effect of adding SWCNTs weight fraction into HDPE is directly proportional to the improvement of the elastic modulus of HDPE/SWCNTs regardless of density fraction, this is also shown in Figure 12 created form Table 5. The results obtained were found to be in line with the existing literature results. Though, Figure 14 illustrated the effect of density fractions for FEM results on the elastic modulus of HDPE/SWCNTs nanocomposite at specific weight fraction. At the weight fractions 0.2 wt% and 0.4 wt% it seemed like high-density fraction shows more improvement compared to the low-density fraction, then at the weight fractions 0.6 wt%, 0.8 wt%, and 1 wt% high elastic modulus improvement was shown by nanocomposite with low-density fraction. The density fraction of fibre (SWCNTs) and matrix (HDPE) affects the elastic modulus of HDPE/SWCNTs nanocomposite.

4. Conclusion
The study showed that the addition of SWCNTs weight fractions into HDPE matrix advances the elastic modulus of HDPE/SWCNTs nanocomposite. These results were obtained by modeling the 3-D RVE of HDPE/SWCNTs nanocomposite at different weight fractions of SWCNTs by means of FEM approach using ANSYS 19.2. It was also found that the elastic
modulus of HDPE/SWCNTs nanocomposite improved by 74.54% at the weight fraction of 1 wt% for the density fraction of 1.79 and at the same weight fraction for the density fraction of 2 the improvement was found to be 51.90%. This shows that the low-density fraction of SWCNTs fibre and HDPE matrix results with higher improvement on elastic modulus HDPE/SWCNTs nanocomposite compare to the high-density ratio at the same weight fraction.

The modelling results showed that the elastic modulus of polymers or polymer-based nanocomposites (HDPE) can be enhanced by addition the weight fraction of nanoparticles (SWCNTs). This was also proved by the rule of mixture results.

5. Recommendation
For further recommendation, experimental tests should be conducted at the same weight fractions and same material properties to investigate the elastic behaviour of HDPE/SWCNTs nanocomposite using tensile testing. Further numerical methods should be conducted for validation and the improvement of the modelling approach.

Acknowledgements
The authors wish to acknowledge the National Research Foundation (NRF) for the financial support and the University of Johannesburg department of mechanical engineering science for the facility and academic support with supervision.

References
[1] Giannopoulos, G.I., 2019. Linking MD and FEM to predict the mechanical behaviour of fullerene reinforced nylon-12. Composites Part B: Engineering, 161, pp.455-463.
[2] Thakur, S.K., Sharma, A. and Batra, N.K., 2012. Tribological characterization of CNT/HDPE polymer nano-composites. Int. J. Theor. Appl. Res. Mech. Eng., 1, pp.32-36.
[3] A. Fattahi, S. Roozpeikar and N. Ahmed, "FEM modeling based on molecular results for PE/SWCNT nanocomposites," International Journal of Engineering & Technology, www.sciencepubco.com/index.php/IJET, vol. 7, pp. 1-12, 2018.
[4] Arora, G. and Pathak, H., 2019. Modeling of transversely isotropic properties of CNT-polymer composites using meso-scale FEM approach. Composites Part B: Engineering, 166, pp.588-597.
[5] Shokrieh, M.M. and Rafee, R., 2010. Prediction of mechanical properties of an embedded carbon nanotube in polymer matrix based on developing an equivalent long fiber. Mechanics Research Communications, 37(2), pp.235-240.
[6] Bhuiyan, M.A., Pucha, R.V., Worthy, J., Karevan, M. and Kalaitzidou, K., 2013. Defining the lower and upper limit of the effective modulus of CNT/polypropylene composites through integration of modeling and experiments. Composite Structures, 95, pp.80-87.
[7] Kumar, P. and Srinivas, J., 2014. Numerical evaluation of effective elastic properties of CNT-reinforced polymers for interphase effects. Computational Materials Science, 88, pp.139-144.
[8] Chowdhury, S.C., Haque, B.G., Okabe, T. and Gillespie Jr, J.W., 2012. Modeling the effect of statistical variations in length and diameter of randomly oriented CNTs on the
properties of CNT reinforced nanocomposites. Composites Part B: Engineering, 43(4), pp.1756-1762.

[9] Joshi, U.A., Sharma, S.C. and Harsha, S.P., 2012. A multiscale approach for estimating the chirality effects in carbon nanotube reinforced composites. Physica E: Low-dimensional Systems and Nanostructures, 45, pp.28-35.

[10] Jarali, C.S., Patil, S.F., Pilli, S.C. and Lu, Y.C., 2013. Modeling the effective elastic properties of nanocomposites with circular straight CNT fibers reinforced in the epoxy matrix. Journal of Materials Science, 48(8), pp.3160-3172.

[11] Joshi, U.A., Sharma, S.C. and Harsha, S.P., 2011. Analysis of elastic properties of carbon nanotube reinforced nanocomposites with pinhole defects. Computational Materials Science, 50(11), pp.3245-3256.

[12] Safaei, B., Naseradinmousavi, P. and Rahmani, A., 2016. Development of an accurate molecular mechanics model for buckling behavior of multi-walled carbon nanotubes under axial compression. Journal of Molecular Graphics and Modelling, 65, pp.43-60.

[13] Bhuiyan, M.A., Pucha, R.V., Karevan, M. and Kalaitzidou, K., 2011. Tensile modulus of carbon nanotube/polypropylene composites—A computational study based on experimental characterization. Computational Materials Science, 50(8), pp.2347-2353.

[14] Rahmat, M. and Hubert, P., 2011. Carbon nanotube–polymer interactions in nanocomposites: a review. Composites Science and Technology, 72(1), pp.72-84.

[15] Namilae, S. and Chandra, N., 2005. Multiscale model to study the effect of interfaces in carbon nanotube-based composites. Journal of Engineering materials and technology, 127(2), pp.222-232.

[16] Najipour, A. and Fattahi, A.M., 2017. Experimental study on mechanical properties of PE/CNT composites. Journal of Theoretical and Applied Mechanics, 55(2), pp.719-726.

[17] Hassanzadeh-Aghdam, M.K. and Ansari, R., 2017. A micromechanical model for effective thermo-elastic properties of nanocomposites with graded properties of interphase. Iranian Journal of Science and Technology, Transactions of Mechanical Engineering, 41(2), pp.141-147.

[18] Ngabonziza, Y., Li, J. and Barry, C.F., 2011. Electrical conductivity and mechanical properties of multiwalled carbon nanotube-reinforced polypropylene nanocomposites. Acta mechanica, 220(1-4), pp.289-298.

[19] Wang, T.Y., Liu, S.C. and Tsai, J.L., 2016. Micromechanical stick-slip model for characterizing damping responses of single-walled carbon nanotube nanocomposites. Journal of Composite Materials, 50(1), pp.57-73.

[20] Thomas, B. and Roy, T., 2016. Vibration analysis of functionally graded carbon nanotube-reinforced composite shell structures. Acta Mechanica, 227(2), pp.581-599.

[21] Hassanzadeh-Aghdam, M.K., Ansari, R. and Darvizeh, A., 2018. Micromechanical analysis of carbon nanotube-coated fiber-reinforced hybrid composites. International Journal of Engineering Science, 130, pp.215-229.

[22] Azizi, S., Fattahi, A.M. and Kahnamouei, J.T., 2015. Evaluating mechanical properties of nanoplatelet reinforced composites under mechanical and thermal loads. Journal of Computational and Theoretical Nanoscience, 12(11), pp.4179-4185.
[23] Cheng, J.J., 2008. Mechanical and chemical properties of high density polyethylene: effects of microstructure on creep characteristics.

[24] Kulkarni, M., Carnahan, D., Kulkarni, K., Qian, D. and Abot, J.L., 2010. Elastic response of a carbon nanotube fiber reinforced polymeric composite: a numerical and experimental study. Composites Part B: Engineering, 41(5), pp.414-421.

[25] Zuberi, M.J.S. and Esat, V., 2015. Investigating the mechanical properties of single walled carbon nanotube reinforced epoxy composite through finite element modelling. Composites Part B: Engineering, 71, pp.1-9.

[26] Snipes, J.S., Robinson, C.T. and Baxter, S.C., 2011. Effects of scale and interface on the three-dimensional micromechanics of polymer nanocomposites. Journal of Composite Materials, 45(24), pp.2537-2546.