Nonlinear Buckling Analysis of Polystyrene, Polyvinyl Chloride, and Polypropylene Cylindrical Nano-Composite Shells Reinforced by Carbon Nanotubes Based on Micro-Mechanics and Finite Element Method

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ABSTRACT

In this paper, we present nonlinear buckling instability analysis of polystyrene, polyvinyl chloride, and polypropylene nano-composite shell-structures reinforced by carbon nanotubes (CNTs) under the uni-axial compressive load to obtain a more conservative buckling response as compared with linear analysis. For this purpose, the Mori-Tanaka method was firstly utilized to estimate the effective elastic modulus of composites having aligned straight CNTs. Then, a novel model based on micro-mechanics and finite element method was developed for buckling analysis of a cylindrical nano-composite shell reinforced by CNTs and various effects of different types of polymer matrices (Polystyrene, Polyvinyl chloride, and Polypropylene), CNTs volume fraction, CNTs orientation angle, aspect ratio of cylinder, and different boundary conditions (simply supported and clamped ends) on critical buckling load of cylindrical nano-composite shells were discussed. The proposed model is based on Mori-Tanaka micro-mechanics which is developed in the ABAQUS finite element package. The numerical results showed different behavior from shell-type buckling to beam-type buckling in L/R =8 due to the change of the cylinder aspect ratios. Moreover, the developed finite element code and numerical results were compared and validated with Mori-Tanaka analytical model in the available literature and showed a good agreement.

1-Introduction

Polymer nano-composites are a novel and special group of materials that are gnerated when nano-scale fillers are introduced into a distinct polymer matrix. These new materials have attracted increasing attention due to their great enhancement of mechanical, thermal and barrier properties compared to traditional polymers [1-3]. Recently, nano-composites reinforced by carbon nanotubes (CNTs) dispersed in polymeric matrices have drawn great attention [4]. CNTs with their superior and exceptional mechanical properties have been regarded as an ideal reinforcement for advanced composites with high strength and low density. A number of experimental and theoretical studies have shown that CNTs have extraordinary mechanical properties.

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For example, their elastic modulus and tensile strength are estimated over 1 (TPa) and 150 (GPa), respectively, which makes them many times stiffer and stronger than steel while being about five times lighter [5-7]. In addition, the bonding at the CNT–polymer interface is strong which has been demonstrated in experimental works [8-10]. Therefore, the presence of the CNTs can improve the strength and stiffness of polymers as well as electrical and thermal conductivities of polymer-based composite structures [8].
Apart from that, a common concern in structures subjected to compressive loading is failure due to buckling. Buckling is a structural instability that can be addressed using both linear and nonlinear approaches. To obtain an indication of the potential of a structure to buckle under a particular loading, a linear buckling analysis can be undertaken. However, the nonlinear buckling analysis can yield a more conservative buckling response as compared with linear analysis. In addition, the buckling load of a cylindrical composite shell depends on different parameters, such as the geometry of the cylinder, properties of reinforcement, and the types of boundary conditions [11, 12]. In the present study, nonlinear buckling instability analysis of nano-composites reinforced by CNTs under uni-axial compressive load has been investigated based on micro-mechanics in ABAQUS finite element package. Hence, displacements vary non-linearly with the applied loads. Also, the stiffness varies as a function of the load and displacements can be very large and changes in geometry cannot be ignored. To this end, a finite element model is developed for nonlinear buckling analysis of polystyrene (PS), polyvinyl chloride (PVC), and polypropylene (PP) cylindrical nano-composite shell reinforced by CNTs and the effects of CNTs volume fraction, CNTs orientation angle, aspect ratio of the cylinder, and different boundary conditions are discussed and finally, numerical results are compared with Mori-Tanaka analytical model.

2- Micro-mechanical model

The micro-mechanical model involves the elastic behavior of polymeric nano-composite reinforced by aligned CNTs which are straight and infinitely long. In the micro-mechanical model, the CNTs are considered to be solid fibers with transversely isotropic material properties [13]. The bonding at the CNT–polymer interface is taken to be perfect. The composite is considered as transversely isotropic. The elastic tensor of an elementary cell of the composite material can be expressed as follows:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix}=\begin{bmatrix}k+m & l & k-m & 0 & 0 & 0\\ l & n & l & 0 & 0 & 0\\ k-m & l & k+m & 0 & 0 & 0\\ 0 & 0 & 0 & p & 0 & 0\\ 0 & 0 & 0 & 0 & m & 0\\ 0 & 0 & 0 & 0 & 0 & p\end{bmatrix}\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \varepsilon_{23}\\ \varepsilon_{13}\\ \varepsilon_{12}\end{Bmatrix} \quad (1)$$

where *k*, *l*, *m*, *n* and *p* are the Hill's elastic moduli: *k* is the plane strain bulk modulus normal to the fiber direction, *l* is the associated cross modulus, *m* and *p* are the shear moduli in planes normal and parallel to the fiber direction, *n* is the uni-axial tension modulus in the fiber direction (direction 1). Using the Mori-Tanaka approach, the Hill's elastic moduli are found to be as follows:

$$\begin{aligned}
k &= \frac{E_m\{E_m c_m + 2k_r(1+\nu_m)[1+c_r(1-2\nu_m)]\}}{2(1+\nu_m)[E_m(1+c_r-2\nu_m)+2c_m k_r(1-\nu_m-2\nu_m^2)]}\\
l &= \frac{E_m\{c_m\nu_m[E_m+2k_r(1+\nu_m)]+2c_r l_r(1-\nu_m^2)\}}{(1+\nu_m)[E_m(1+c_r-2\nu_m)+2c_m k_r(1-\nu_m-2\nu_m^2)]}\\
m &= \frac{E_m\{E_m c_m + 2m_r(1+\nu_m)[3+c_r-4\nu_m)]\}}{2(1+\nu_m)\{E_m[c_m+4c_r(1-\nu_m)]+2c_m m_r(3-\nu_m-4\nu_m^2)]}\\
n &= \frac{E_m^2 c_m(1+c_r-c_m\nu_m)+2c_r c_m(k_r n_r-l_r^2)(1+\nu_m)^2(1-2\nu_m)}{(1+\nu_m)\{2c_m k_r(1-\nu_m-2\nu_m^2)+E_m(1+c_r-4\nu_m)]}\\
&\quad+\frac{E_m[2c_m^2 k_r(1-\nu_m)+c_r n_r(1-2\nu_m+c_r)-4c_m l_r\nu_m\}}{E_m(1+c_r-2\nu_m)+2c_m k_r(1-\nu_m-2\nu_m^2)]}\\
p &= \frac{E_m\{E_m c_m + 2(1+c_r)p_r(1+\nu_m)\}}{2(1+\nu_m)[E_m(1+c_r)+2c_m p_r(1+\nu_m)]}
\end{aligned} \quad (2)$$

where c_m and c_r are the volume fractions of matrix and CNTs. Also, k_r , l_r , m_r , n_r and p_r are the Hill's elastic moduli for CNTs as the reinforcing phase, and E_m , v_m are the matrix Young's modulus and Poisson's ratio [8]. Therefore, for nano-composite reinforced by CNTs, the effective elastic moduli parallel (E_{II}) and normal ($E_{\perp}$) to CNTs are related to Hill's elastic moduli as follows:

$$E_{II} = n - \frac{l^2}{k}$$

$$E_{\perp} = \frac{4m(kn - l^2)}{kn - l^2 + mn} \qquad (3)$$

Finally, the proposed model is based on Mori-Tanaka micro-mechanics using effective elastic moduli in Eq. (3), and developed in ABAQUS finite element software based on the "Riks method" to capture nonlinearities which can arise from large-displacement effects. In fact, the "Riks method" is best suited to problems where there is unstable buckling or collapse and this procedure uses an arc-length method to determine the response of the loaded structure, where there are significant changes in the structure stiffness. In other words, the "Riks method" has a computational technique to handle the decreasing part of the deformation-load curve (zero or negative stiffness) while "General Statics" will diverge in this case.

3- Numerical results

Based on the novel model, nonlinear buckling of cylindrical nano-composite shells with different polymer matrices reinforced by CNTs is analyzed and the effects of CNTs volume fraction (C_r), CNTs orientation angle (ϕ), aspect ratio of cylinder (L/R), and various boundary conditions (simply supported and clamped) are discussed for different shell thicknesses (h). Also, the different polymeric matrices are specified as PS, PVC, and PP for nano-composite shells reinforced by carbon nanotubes which has demonstrated good dispersion and a strong interfacial bond with nanotubes in experimental works [8-10].)رابطه 3(

In addition, the mechanical constants for the uni-directional nano-composite shell are derived using micro-mechanical equations (1-3). The mechanical properties used in the present analysis are: the Young's modulus and Poisson's ratio of PS, PVC, and PP matrices are E_{PS} = 1.9 (GPa) and v_{PS} = 0.3 [8], E_{PVC} = 3 (GPa) and v_{PVC} = 0.3 [14], and E_{PP} = 1.38 (GPa) and v_{PP} = 0.36 [15], respectively.

Here, the CNTs are modeled as long, transversely isotropic fibers and the Hill's elastic moduli of CNTs are obtained as k_r = 30 (GPa), l_r= 10 (GPa), m_r =1 (GPa), n_r =450 (GPa), p_r =1 (GPa) [8].

Fig. 1 illustrates the representative volume element (RVE) of a cylindrical nano-composite shell including straight CNTs for FE simulations in the ABAQUS software.

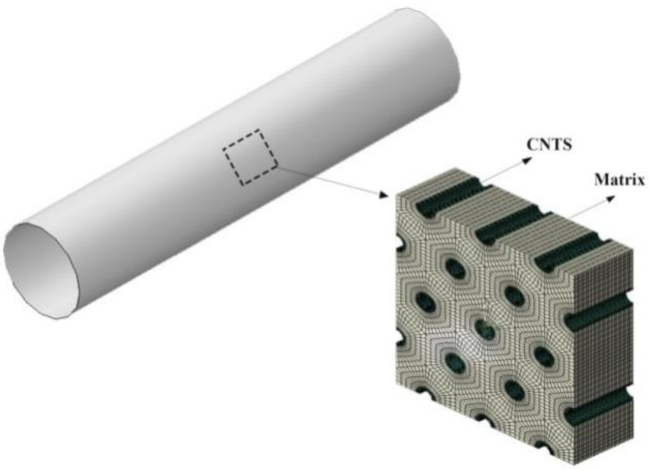

Fig. 1. Representative volume element (RVE) of the nano-composite cylindrical shell including straight CNTs

Fig. 2 illustrates the effects of CNTs volume fraction on critical buckling load for five CNTs orientation angles for PS, PVC, and PP polymer matrices.

Fig. 2 shows that critical buckling load increases with the increase of CNTs volume fraction. It is because of the high mechanical strength of CNTs in comparison with the polymer matrices which leads to increase the effective elastic moduli of nano-composites.

In addition, by increasing the CNTs orientation angle (ϕ) from 0° (perpendicular to the axial direction of cylinder) to 90° (parallel to the axial direction), the critical buckling load will increase and may lead to more stability of the structure. This result shows that reinforcements (CNTs) which are parallel to the axial direction of the cylinder can tolerate the axial stress more effectively as compared with perpendicular CNTs. Fig. 3 shows the effect of CNTs orientation angle on the buckling load of nano-composite shell with simply supported (S-S) and doubly clamped (C-C) boundary conditions.

As can be seen in Fig. 3, the critical buckling load for the clamped boundary condition is more than the simply supported boundary condition. Also, by increasing the orientation angle up to 90° (parallel to the axial structure), the buckling load will increase. Similar results have been reported by Eskandari Jam et al. [8], who analytically investigated the effects of CNT orientation angle and different boundary conditions on the critical buckling load of cylindrical nano-composite shell.

Additionally, the effect of different boundary conditions (S-S, C-C) on the buckling behavior of cylindrical nano-composite shell is shown in Fig. 4.

As it is illustrated in Fig. 4, structure with C-C boundary condition has more stability than S-S boundary condition. Also, the effect of length to radius ratio on the buckling of cylindrical nano-composite shell is illustrated in Fig. 5.

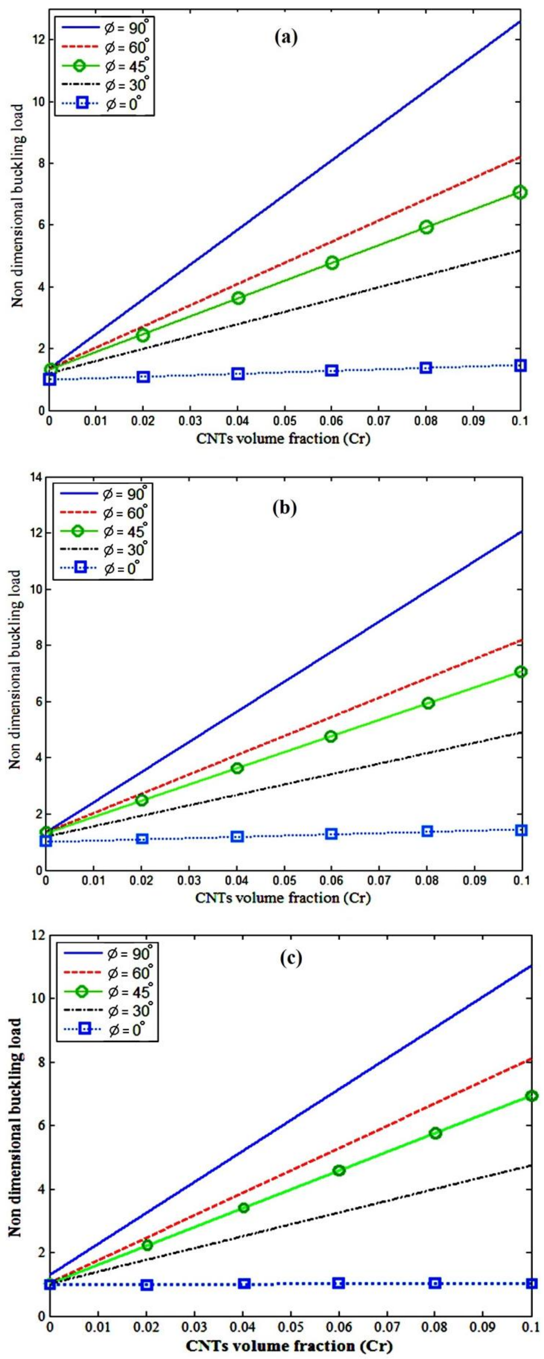

Fig. 2. Effects of CNTs volume fraction and orientation angles on critical buckling load of nano-composite shell with different matrices (a) PVC (b) PS (c) PP (h=2μm, R/h=10, L/R=4)

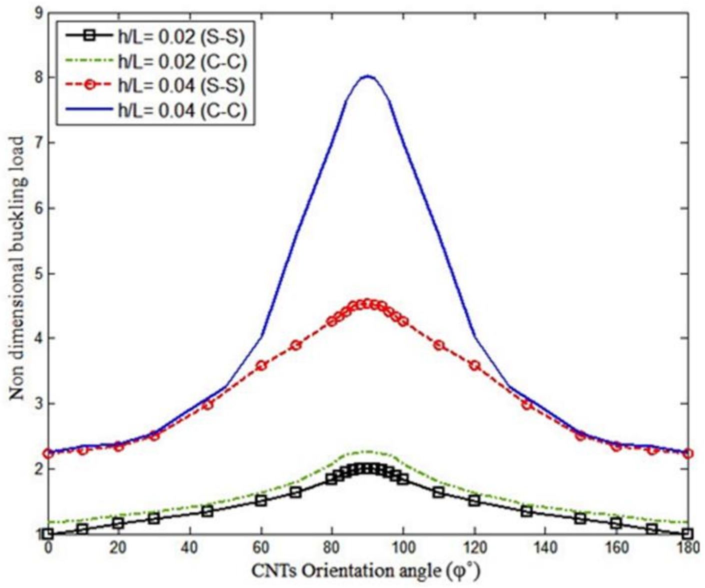

Fig. 3. Orientation angle and relation effects on the buckling load for S-S and C-C boundary condition (*L/R*= 5, *L*=100*μm*)

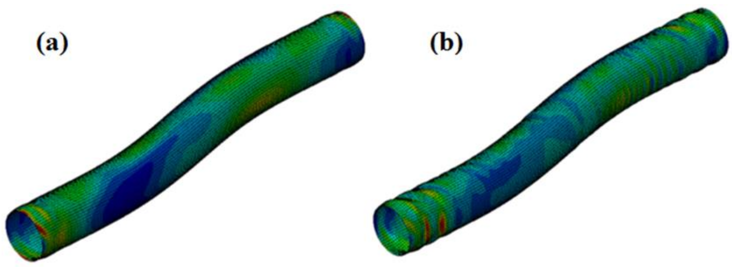

Fig. 4. Effect of different boundary conditions on critical buckling load (a) C-C, (b) S-S (*L/R*=20, *h*=2*μm*)

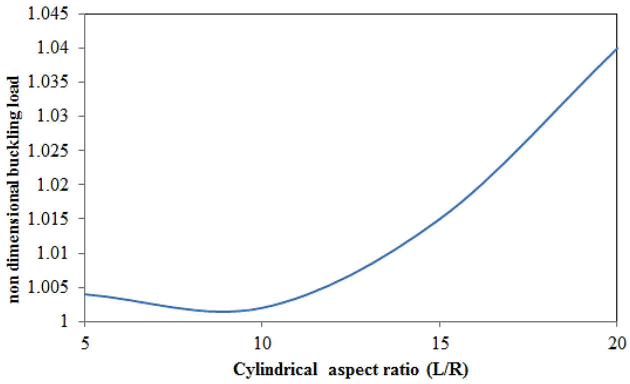

Fig. 5. The effect of length to radius ratio on buckling of cylindrical nano-composite shell (*R/h*=10, *h*=2*μm*)

Fig. 5 shows that with increasing the length to radius ratio, the critical buckling load decreases in the low cylinder aspect ratios (*L/R* <8); however, the critical buckling load increases for higher aspect ratios (*L/R* >8). This is because of the change in the buckling behavior from shell-type to beam-type in *L/R* =8. In fact, the mechanical behavior of a nano-composite cylindrical shell is a little different from that of a uniform cylinder, especially in the transition regime between shell buckling and Euler beam buckling modes. Therefore, for the shell buckling mode (*L/R* < 8), the highly local deformation occurs, where the local stiffness in the local buckled area is mainly dominated by a small number of chemical bonds between the matrix and the reinforcements located in this area. Thus, the local stiffness of the cylinder is comparatively lower. So, by decreasing the radius of the nano-composite cylinder or increasing the aspect ratio (*L/R*), the critical buckling load will decrease. However, in the case of Euler beam buckling (*L/R* >8), this kind of uniformly global deformation is dominated by the macroscopic or average stiffness of the cylinder which is clearly more than the local stiffness of nano-composite cylinder. This macroscopic or average stiffness of the cylinder is usually evaluated by considering the stiffness effect of a large number of chemical bonds on a long nano-composite cylinder. Thus, when the cylinder is comparatively long with a high aspect ratio, the non-axisymmetric buckling mode happens and the wave number along the axial direction becomes higher. Therefore, the critical buckling load will increase. Furthermore, when the wave number is much higher, the axisymmetric buckling mode happens and the results tend to be the same as the results of Timoshenko's shell buckling theory. Similar results have been reported by Eskandari Jam et al. [8], who analytically investigated the effects of aspect ratio (*L/R*) on the critical buckling load of nano-composite cylinder. The effect of length to radius ratio on the buckling behavior of cylindrical nano-composite shell is illustrated in Fig. 6.

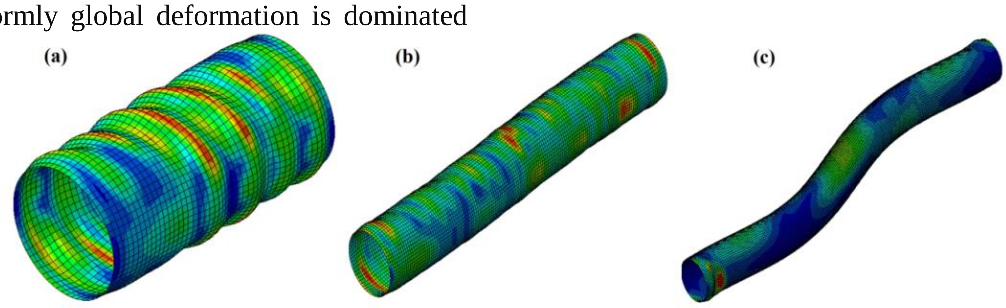

Fig. 6. Transition of buckling behavior from shell-type to beam-type for different aspect ratios (a) *L/R* = 5 (b) *L/R* = 10 (c) *L/R* = 20

Based on Fig. 6, with increasing the aspect ratio, the buckling type of shell structure changes from shell-type to beam-type, because by increasing the aspect ratio, the cylindrical structure behaves like a beam and non-axisymmetric buckling mode happens. Moreover, the effects of different polymeric matrices (PVC, PS, and PP) on the buckling loads are studied. These effects are shown in Fig. 7.

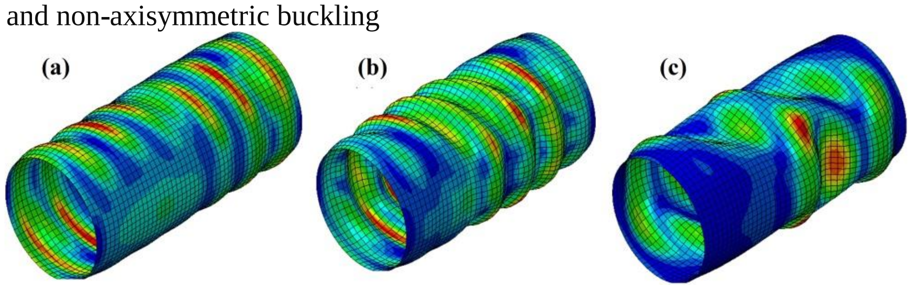

Fig. 7. Buckling behavior of nano-composite shell reinforced by CNTs with different matrices (a) PVC (b) PS (c) PP (h=2μm, *L/R*=5)

Fig. 7 shows that stability of the PVC matrix is more than PS and the stability of the PS matrix is more than that of the PP matrix. It is reasonable because the Young's modulus of PVC is more than PS and the Young's modulus of PS is more than PP. The comparison of critical buckling loads for these different matrices with different boundary conditions is shown in Fig. 8 for different CNTs volume fractions and thickness to length ratios.

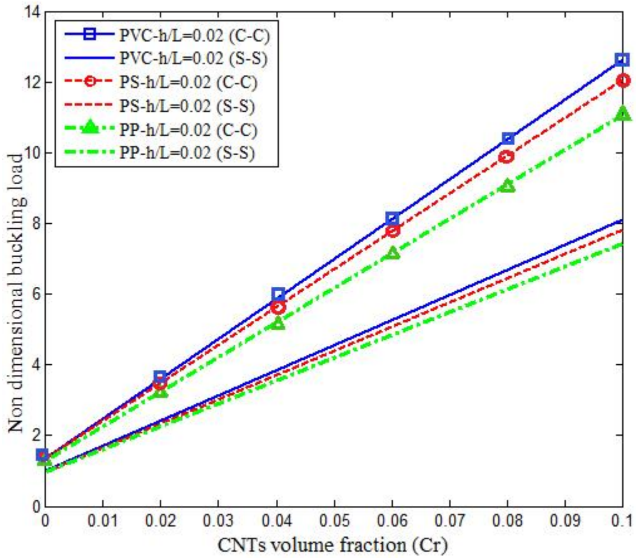

Fig. 8. Comparison of the buckling loads for the PVC, PS, and PP matrices

As can be seen in Fig. 8, the critical buckling loads of the PVC based nano-composites are more than those of the PS and PP matrices and the differences are more pronounced for the clamped boundary conditions in higher CNTs volume fractions. Again, it is concluded that the critical buckling load increases with the increase of CNTs volume fraction because of the high mechanical strength of CNTs in comparison with polymer matrices. Finally, in Fig. 9 the results are compared with the available literature [8] in order to validate the developed FE model.

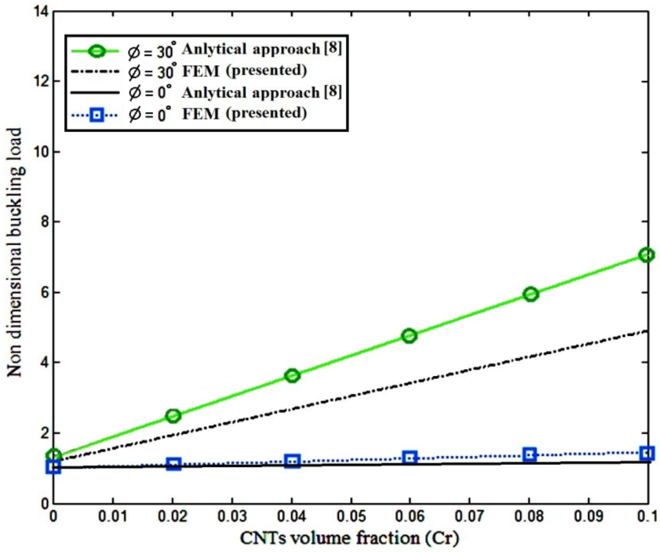

Fig. 9. Comparison of the presented FEM results with the analytical approach [8] for the buckling load of the PS matrix

As it is illustrated in Fig. 9, the presented FE simulation model is in good agreement with the reported results by Eskandari Jam et al. [8], who analytically investigated the effects of CNT orientation angle and CNTs volume fraction on the critical buckling load of cylindrical nano-composite shells.

4- Conclusions

In this paper, nonlinear buckling instability analysis of different polymeric nano-composite structures reinforced by CNTs under uni-axial compressive load was carried out based on a novel micro-mechanical and finite element model. In addition, the effects of carbon nanotubes volume fraction and orientation angle, and thickness to length ratio of cylinder were discussed for polystyrene (PS), polyvinyl chloride (PVC), and polypropylene (PP) nano-composite shells reinforced by carbon nanotubes with different boundary conditions. For this purpose, a finite element model was developed for the buckling analysis of a cylindrical nano-composite shell reinforced by CNTs. Generally, it is concluded that the critical buckling load increases with the increase of CNTs volume fraction. In addition, by increasing the CNTs orientation angles from 0° (perpendicular to the axial direction of cylinder) to 90° (parallel to the axial direction), the critical buckling load will increase and may lead to more stability for the structure. Furthermore, the stability of the PVC matrix is the most and that of the PP matrix is the least. In fact, critical buckling loads of PVC based nano-composites are more than PS and PP matrices and the differences are more pronounced for CNTs orientation angle of 90°. Also, it is concluded that the critical buckling load for clamped boundary condition is more than the simply supported boundary condition. Moreover, with increasing the length to radius ratio, critical buckling load decreases in the low cylinder aspect ratios (L/R <8); however, the critical buckling load increases for higher aspect ratios (L/R >8). This is because of changing the buckling behavior from shell-type to beam-type in L/R =8. In fact, by increasing the aspect ratio, the buckling type of shell structure changes from shell-type to beam-type, because by increasing the L/R ratio, cylindrical structure behaves like a beam. To validate the developed FE code, results were compared with available literature and showed a good agreement with the analytical results.

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