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Evaluating the Ability of Modified Adomian Decomposition Method to Simulate the Instability of Freestanding Carbon Nanotube: Comparison with Conventional Decomposition Method

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Abstract: In recent years, the buckling of freestanding Carbon Nanotube (CNT) in the vicinity of graphite has become of great interest for scientists. In this work, the ability of modified Adomian decomposition methods for modeling the nonlinear instability of cantilever and doubly-supported CNT was investigated. The obtained results were compared with those of conventional decomposition method as well as numerical solutions. The critical value of CNT-graphite attraction at the onset of the instability was computed as the basic parameter for engineering applications. It was found that modified Adomian method is highly reliable for simulating the CNT-graphite interaction. On the other hands, using conventional decomposition method in solving CNT problems might lead to physically incorrect results in some cases. These shortcomings were not observed for modified Adomian series.

Key words: Freestanding CNT, instability, nonlinear differential equation, modified adomian decomposition, conventional adomian decomposition

INTRODUCTION

Carbon Nanotubes (CNT) are increasingly used in developing nano-actuators, nano-switches, nano-probes, nano-sensors and other nano-devices (Paradise and Goswami, 2007; Yazdi and Mashadi, 2007; Mohammadpour *et al*., 2011). Consider a typical CNT which is suspended over a graphite surface. There is a small gap between the CNT and the graphite surface. As the gap decreases from micro to nano-scale, the van der Waals interaction deflects the CNT to the graphite. When the separation is small enough, the nanotube buckles onto the graphite surface. Prediction of the instability of CNT near the graphite surface is a critical subject in designing CNT-based nano-devices (Koochi *et al*., 2011a). A reliable trend to simulate the CNT-graphite interaction is to apply nano-scale continuum models. However, this approach often leads to nonlinear equations in the form of Eq. 1 that might not be accurately worked out by analytical methods (Koochi *et al*., 2011b):

$$w^{(IV)}-f_n z^{-n} = 0 \ (n = 4,5) \tag{1}$$

In recent decades, various mathematical methods, such as adomian decomposition (Adomian, 1983; Wazwaz, 2000), variational iteration (He, 1997, 1999; Noorzad *et al*., 2008; Shakeri *et al*., 2009; Barari *et al*., 2008), homotopy perturbation (He, 2000, 2006; Sharma and Methi, 2011; Fazeli *et al*., 2008) etc., have been proposed for solving nonlinear problems. Among these methods, the decomposition method proposed by Adomian has been widely used to solve stochastic systems (Adomian and Rach, 1983; Adomian, 1983; Rach, 1984; Jaradat, 2008) due to the convenience of the computations. Furthermore, this method has been applied to investigate engineering problems such as oscillation (Momani *et al*., 2008), heat transfer (Chiu and Chen, 2002; Luo *et al*., 2006) etc. Several investigators made attempt to improve Adomian decomposition (Adomian, 1986; Gabet, 1994). Rach (1984) proposed a systematic formula for computing the Adomian's polynomials. Further modification of the polynomials was also provided by Gabet (1994). A powerful modification of the Adomian decomposition method was proposed by Wazwaz and El-Sayed (2001). This modification highly accelerates the convergence of the decomposition polynomials and it is applied for solving higher order boundary value problems (Wazwaz, 2000, 2001). A modified Adomian decomposition method was applied to simulate the static deflection of electrostatic beam-type micro-actuators (Kuang and Chen, 2005).

The aim of this study was to investigate the potentials of Modified Adomian Decomposition (MAD) in solving constitutive equation of CNT (Eq. 1). In order to evaluate the abilities of this method, the precision and convergence speed of MAD is compared with those of

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Conventional Adomian Decomposition (CAD). In addition, numerical solution is obtained using MAPLE commercial software and analytical solutions are compared with the numerical results.

GOVERNING EQUATION OF FREESTANDING CNT

Figure 1 depicts schematic cantilever and doubly-supported CNTs suspended over graphite with small gap between them. With the decrease in dimensions from micro to nano-scale, CNT deflects to the substrate due to the van der Waals interaction between CNT and graphite. Especially, when the separation is sufficiently small, the nanotube becomes unstable and buckles onto the graphite layers.

Based on continuum mechanics, the governing equation of a freestanding single-walled CNT over graphite surface can be derived as Koochi *et al.* (2011a):

$$E_{eff}I\frac{d^4W}{dZ^4} = \begin{cases} \dfrac{C_6\sigma^2\pi^2R}{d(D-W)^4} & \text{For large number of graphene layers} \\ \dfrac{4C_6\sigma^2\pi^2NR}{(D-W+Nd/2)^5} & \text{For small number of graphene layers} \end{cases} \tag{2a}$$

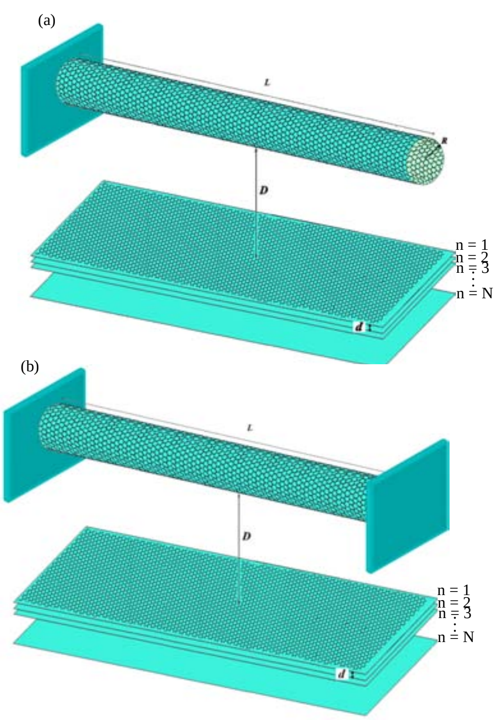

Fig. 1 (a-b): A CNT over a graphite ground plane (a) Cantilever CNT and (b) doubly-supported CNT

$$W(0) = \frac{dW}{dZ}(0) = 0 \tag{2b}$$

$$\frac{d^2W}{dZ^2}(L) = \frac{d^3W}{dZ^3}(L) = 0 \qquad \text{(For Cantilever CNT)} \tag{2c}$$

$$W(L) = \frac{dW}{dZ}(L) = 0 \qquad \text{(For Doubly-supported CNT)} \tag{2d}$$

where, Z is the position along the CNT measured from the clamped end (s) and W is the deflection of CNT. The length of CNT is L and the initial gap between CNT and the ground is D. In above relation, E_{eff}, I, σ and C_6 are the CNT Young's modulus, cross-sectional moment of inertia, graphene surface density and attractive constant, respectively. The constants d and N are the graphite interlayer distance and number of layers, respectively. Equation 1 and 2a-d can be made dimensionless using the following substitutions:

$$z = Z/L \tag{3a}$$

$$w = \begin{cases} \dfrac{W}{D} & \text{For large number of layers } (n = 4) \\ \dfrac{W}{D+Nd/2} & \text{For small number of layers } (n = 5) \end{cases} \tag{3b}$$

$$f_n = \begin{cases} \dfrac{C_6\sigma^2\pi^2RL^4}{dE_{eff}ID^5} & \text{For large number of layers} \\ \dfrac{4C_6\sigma^2\pi^2NRL^4}{E_{eff}I(D+Nd/2)^6} & \text{For small number of layers} \end{cases} \tag{3c}$$

These transformations yield:

$$\frac{d^4w}{dz^4} = \frac{f_n}{(1-w(z))^n} \tag{4a}$$

$$w(0) = w\ (0) = 0 \ \text{(BC. For Cantilever and Doubly-supported CNT)} \tag{4b}$$

$$w(1) = w\ (1) = 0 \ \text{(BC. For Cantilever CNT)} \tag{4c}$$

$$w(1) = w\ (1) = 0 \ \text{(BC. For Doubly-supported CNT)} \tag{4d}$$

Note that parameter f_n in above equations, physically corresponds to the van der Waals attraction. At the onset of the buckling instability, the maximum deflection of the CNT increases abruptly. In mathematical view, the slope of w-f_n curve reaches infinity when instability occurs, i.e., $dw/df_n\,(z = 1)\rightarrow\infty$ and $dw/df_n\,(z = 0.5)\rightarrow\infty$ for cantilever and doubly-supported CNT, respectively. As a convenient approach, the values of critical van der Waals force, f_n^*

and the corresponding CNT critical deflection can be acquired via plotting w (z = 1) vs. f_n for cantilever and w (z = 0.5) vs. f_n for doubly-supported CNT. In order to apply decomposition methods for simulating the deflection and the instability of CNT, the substitution y = 1-w is used to rewrite Eq. 3 into the following form:

$$\frac{d^4y}{dz} = -\frac{f_n}{y(z)^n} \tag{5a}$$

$$y(0) = 1\ ,\ y'(0) = 0 \tag{5b}$$

$$y''(1) = 0\ ,\ y'''(1) = 0 \text{ (For Cantilever CNT)} \tag{5c}$$

$$y(1) = 1\ ,\ y'(1) = 0 \text{ (For Doubly-supported CNT)} \tag{5d}$$

FUNDAMENTALS OF DECOMPOSITION METHODS

Consider a differential equation of a fourth-order boundary-value problem:

$$y^{(IV)}(x) = N(x,y),\ 0 \le x \le L_b \tag{6a}$$

$$y(0) = \alpha_0,\ y'(0) = \alpha_1 \tag{6b}$$

Equation 6 can be represented as:

$$L^{(IV)}[y(x)] = N(x,y) \tag{7}$$

where, $L^{(IV)}$ is a differential operator which is defined as:

$$L^{(IV)} = \frac{d^{(4)}}{dx^{(4)}} \tag{8a}$$

The corresponding inverse operator $L^{-(IV)}$ is defined as a 4-fold integral operator, that is:

$$L^{-(IV)} = \underbrace{\int_0^x \dots \int_0^x (.)dx\dots dx}_{4} \tag{8b}$$

By employing the decomposition method (Kuang and Chen, 2005), the dependent variable in Eq. 6 can be written as:

$$y(x) = \sum_{n=0}^{\infty} y_n(x) = \alpha_0 + \alpha_1 x + \frac{1}{2}C_1 x^2 + \frac{1}{3!}C_2 x^3 + L^{-(IV)}\left[\sum_{n=0}^{\infty} A_n\right] \tag{9}$$

where, constants C_1 and C_2 can be determined from the boundary condition at x = L_b. In above relations f_n function approximates the nonlinear f (x,y) function and it is determined as a polynomial series (Adomian, 1983):

$$N(x,y) = \sum_{n=0}^{\infty} A_n \tag{10}$$

In order to compute A_n terms let us define f_v as the following:

$$f_v(y_0) = \frac{d^v}{dy^v}\left[f(y(\lambda))\right]_{\lambda=0} \tag{11}$$

Then, according to Conventional Adomian Decomposition (CAD), A_n is obtained using the following formula:

$$A_n = \frac{1}{n!} f_v(y_0) \tag{12}$$

On the other hand, according to Modified Adomian Decomposition (MAD), the above can be further presented as the following convenient equations (Rach, 1984; Adomian, 1986):

$$A_n = \sum_{v=1}^{n} C(v,n) f_v(y_0) \tag{13}$$

Where:

$$C(n,v) = \sum_{p_i} \prod_{i=1}^{v} (1/k_i!) f_{p_i}^{k_i}$$

$$\sum_{i=1}^{v} k_i p_i = n$$

n>0, 0≤i≤n, 1 ≤p_i≤n-v+1 and k_i is the number of repetition of the f_{pi}, the values of p_i are selected from the above range by combination without repetition.

According to decomposition methods, the recursive relations of Eq. 6 can be provided as follows:

$$\begin{aligned} &y_0(x) = \alpha_0, \\ &y_1(x) = \alpha_1 x + \frac{1}{2}C_1 x^2 + \frac{1}{3!}C_2 x_3 + L^{-(IV)}[f_0], \\ &y_{k+1}(x) = L^{-(IV)}[f_k], \qquad k \ge 1 \end{aligned} \tag{14}$$

Now, the solution of Eq. 5 can be represented as:

$$y(z) = \sum_{n=0}^{\infty} y_n = 1 + \frac{C_1 z^2}{2!} + \frac{C_2 z^3}{3!} - f_n L^{-(IV)}\left[\sum_{m=0}^{\infty} A_m\right] \tag{15}$$

where, the constants C_1 and C_2 can be determined by solving the resulted algebraic equations from B.C. at z = 1, i.e. using Eq. 5c or 5d for cantilever and doubly-supported cases, respectively.

Modified Adomian (MAD) series solution: In the case of modified domain method:

$$\begin{aligned}
&A_0 = f_0(y_0),\\
&A_1 = C(1,1)f_1(y_0) = y_1 f_1(y_0),\\
&A_2 = C(1,2)f_1(y_0) + C(2,2)f_2(y_0) = y_2 f_1(g_0) + \frac{1}{2!}y_1^2 f_2(y_0),\\
&A_3 = C(1,3)f_1(y_0) + C(2,3)f_2(y_0) + C(3,3)\\
&f_3(y_0) = y_3 f_1(y_0) + y_1 y_2 f_2(y_0) + \frac{1}{3!}y_1^3 f_3(y_0),\\
&\ldots\ldots
\end{aligned} \tag{16}$$

and:

$$\begin{aligned}
&y_0 = 1\\
&y_1 = \frac{1}{2!}C_1 z^2 + \frac{1}{3!}C_2 z^3 - \frac{f_n}{4!}z^4\\
&y_2 = nf_n(\frac{1}{6!}C_1 z^6 + \frac{1}{7!}C_2 z^7 - \frac{1}{8!}f_n z^8)\\
&y_3 = -3n(n+1)f_n\frac{C_1^2}{8!}z^8 - 10n(n+1)\frac{C_1C_2}{9!}f_n z^9\\
&+\frac{n^2C_1 + n(n+1)(15C_1 - 10C_2^2)}{10!}f_n^2 z^{10}\\
&+\frac{(n^2+35n(n+1))C_2}{11!}f_n^2 z^{11} - \frac{n^2f_n^2 + 35n(n+1)f_n^3}{12!}z^{12}
\end{aligned} \tag{17}$$

Therefore, the solution of Eq. 4 can be summarized to:

$$\begin{aligned}
w(z) &= -C_1\frac{z^2}{2!} - C_2\frac{z^3}{3!} + f_n\frac{z^4}{4!} - C_1 nf_n\frac{z^6}{6!}\\
&-C_2 nf_n\frac{z^7}{7!} + (3n(n+1)C_1^2 + nf_n)f_n\frac{z^8}{8!} + 10n(n+1)C_1C_2f_n\frac{z^9}{9!}\\
&-\left(n^2C_1 + n(n+1)(15C_1 - 10C_2^2)\right)f_n^2\frac{z^{10}}{10!}\\
&-(n^2+35n(n+1))f_n^2C_2\frac{z^{11}}{11!} + \left(n^2f_n^2 + 35n(n+1)f_n^3\right)\frac{z^{12}}{12!} + \ldots
\end{aligned} \tag{18}$$

Conventional Adomian (CAD) series solution: In order to solve Eq. 5 using CAD, the formula (12) is expanded to obtain:

$$\begin{aligned}
&A_0 = y_0^{-n},\\
&A_1 = -ny_0^{-n-1}y_1,\\
&A_2 = \frac{1}{2}n(n+1)y_0^{-n-2}y_1^2 - ny_0^{-n-1}y_2\\
&A_3 = -\frac{1}{6}n(n+1)(n+2)y_0^{-n-3}y_1^3 + n(n+1)y_0^{-n-2}y_1y_2 - ny_0^{-n-1}y_3\\
&\vdots = \quad \vdots
\end{aligned} \tag{19}$$

Substituting relation (19) in Eq. 14, we obtain:

$$\begin{aligned}
&y_0 = 1,\\
&y_1 = 0,\\
&y_2 = \frac{C_1 z^2}{2},\\
&y_3 = \frac{C_2 z^3}{6},\\
&y_4 = -f_n\frac{z^4}{24},\\
&y_5 = 0,\\
&y_6 = C_1 nf_n\frac{z^6}{720},\\
&y_7 = C_2 nf_n\frac{z^7}{5040},\\
&y_8 = -\left[\frac{n(n+1)}{2}f_nC_1^2 + \frac{nf_n^2}{6}\right]\frac{z^8}{6720},\\
&\ldots
\end{aligned} \tag{20}$$

where, n = 5 holds for small number of layers and n = 4 for very large number of layers, respectively. Therefore, the polynomial solution of Eq. 4 is obtained which can be summarized to:

$$\begin{aligned}
w(x) &= -\frac{C_1z^2}{2!} - \frac{C_2z^3}{3!} + f_n\frac{z^4}{4!} - nf_n\frac{C_2z^6}{6!}\\
&- nf_n\frac{C_2z^7}{7!} + \left[C_1^2\frac{n(n+1)}{2}f_n + \frac{nf_n^2}{6}\right]\frac{z^8}{8!} + \ldots
\end{aligned} \tag{21}$$

SIMULATING INSTABILITY OF CNT

To evaluate MAD methods, typical cantilever and doubly-supported CNTs are modeled and the results are compared with numerical solution.

Cantilever CNT: Figure 2 and 3, respectively show the variation of tip deflection (w (z = 1)) of typical cantilever CNT with large and small number of layers obtained by MAD method using various series terms (f_n = 0.5). As seen, the MAD series converges faster to the numerical solution in comparison with the conventional series.

The centerline shape of the cantilever CNT has been depicted in Fig. 4 and 5 while van der Waals force increases from zero to the critical instability point. When f_n exceeds the critical value, f_n^*, no solution exists for w and the buckling occurs. While Fig. 4 corresponds to large number of graphene layer, small number of layer is considered in Fig. 5.

Similar behavior is observed for nano-actuators (Ramezani *et al*., 2006), nano-tweezers (Wang *et al*., 2004) and nano-switches (Zhao *et al*., 2003) where van der Waals force makes the freestanding cantilever structures unstable.

Table 1 shows the convergence of instability characteristics (f_n^*) for cantilever CNT obtained by

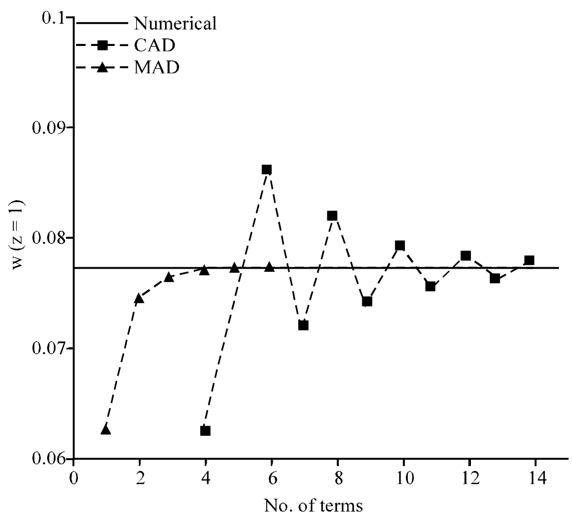

Fig. 2: Variation of tip deflection as a function of selected Adomian series terms for typical cantilever CNT with large number of layer (f_4 = 0.5)

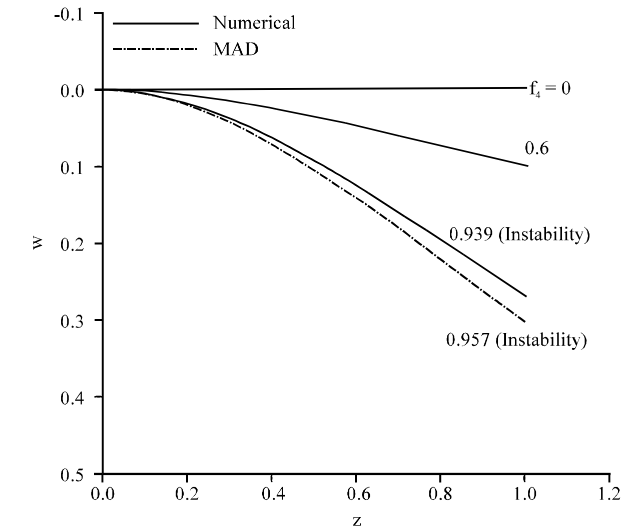

Fig. 4: Deflections of typical cantilever CNT for different values of f_n. MAD method is used and large number of layers is considered

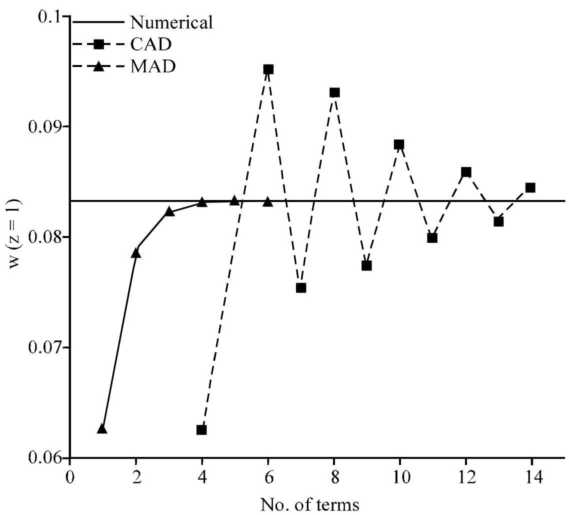

Fig. 3: Variation of tip deflection as a function of selected Adomian series terms for typical cantilever CNT with small number of layer (f_5 = 0.5)

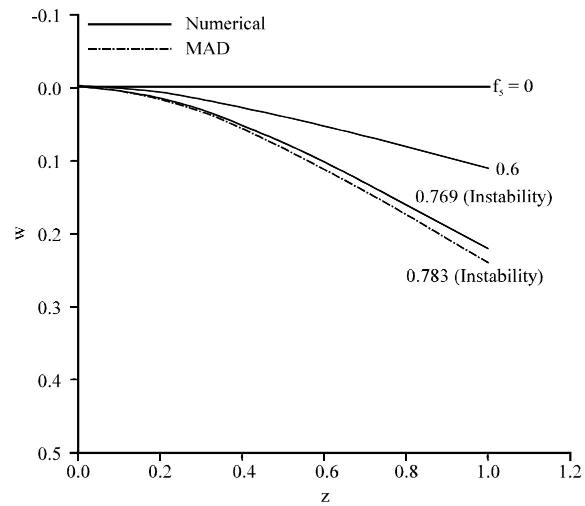

Fig. 5: Deflections of typical cantilever CNT for different values of f_n. MAD method is used and small number of layers is considered

Table 1: Convergence check of critical van der Waals force (f_n^*) for cantilever CNT. Despite conventional Adomian, the f_n^* values obtained by modified decomposition series converge to those of numerical values

f_n^*	Method	3 terms	5 terms	6 terms	8 terms	10 terms	Numerical
For n = 4	CAD	Can't determine	Can't determine	2	0.8146	0.7853	0.9391
	Difference with numerical solution (%)	-	-	112.9699	13.2574	16.3774	
	MAD	1.1551	0.9577	Can't determine			
	Difference with numerical solution (%)	23.00075	1.98062	-			
For n = 5	CAD	Can't determine	Can't determine	1.6	0.6616	0.6434	0.7695
	Difference with numerical solution (%)	-	-	107.9272	14.0221	16.3873	
	MAD	0.9360	0.7827	Can't determine			
	Difference with numerical solution (%)	21.63743	1.7154	-			

various series terms. This table reveals that CAD converges to an instability value which is different from the numerical one. However, this shortcoming is not observed in the case of the modified series and the instability value obtained by MAD method converges to that of numerical solution.

The values of f_n^* obtained using CAD series (using 8 terms) are the same as those predicted using Homotopy perturbation method (Koochi *et al*., 2011b) and are very close to those predicted using Green's function method (Koochi *et al*., 2011a). Interestingly, the critical values of CNT-graphite attraction obtained in the case of large number of layers are the same as the critical values of Casimir force obtained in reference (Abadyan *et al*., 2010; Soroush *et al*., 2010) for freestanding nano-electromechanical actuators. Note that the dimensionless constitutive equations are mathematically the same in these two cases. However, the physical implication of f_n^* is completely different in these problems.

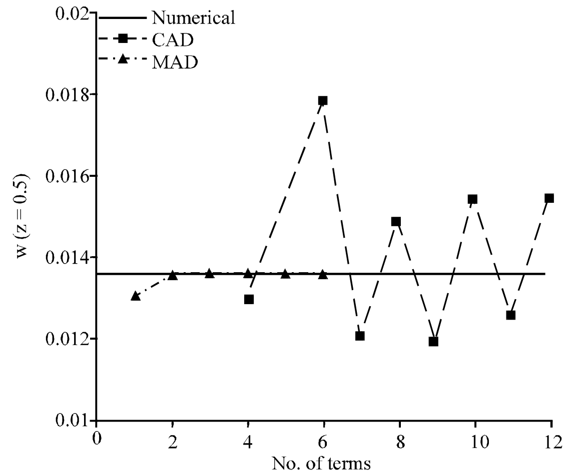

Fig. 6: Variation of tip deflection as a function of selected Adomian series terms for typical doubly-supported CNT with large number of layer ($f_4 = 5$)

Doubly-supported CNT: Figure 6 and 7, respectively show the variation of mid-point deflection for typical doubly-supported CNT with large and small number of layers as a function of series terms. The value of van der Waals attraction is chosen as $f_n = 5$ for both number of layers. These figures reveal that conventional decomposition can not be applied for modeling the CNT/graphite interaction. As seen, while the MAD method rapidly converges to the numerical solution, CAD series diverges from it.

The centerline shape of the doubly-supported freestanding CNT has been depicted in Fig. 8 and 9 while van der Waals force increases from zero to the critical instability point. While Fig. 8 corresponds to large number of layer, small number of layer is considered in Fig. 9.

Furthermore, Table 2 shows the convergence of f_n^* for doubly-supported CNT obtained by MAD using various series terms. As seen, f_n^* values obtained by MAD series converge to that of numerical value. In Table 2, only the f_n^* values obtained by MAD are presented since the CAD method is not able to model the double-supported CNT/graphite interaction. In the case of doubly-supported CNT, the instability value computed by conventional decomposition series is very different from that of numerical method.

Interestingly the f_n^* values of doubly-supported CNT is considerably larger than those of cantilever one due to higher elastic stiffness of doubly-supported structure. Similar difference has been observed between cantilever and doubly-supported nano-beams (Koochi *et al*., 2010), where higher elastic stiffness of the doubly-supported nano-structure leads to higher instability characteristics.

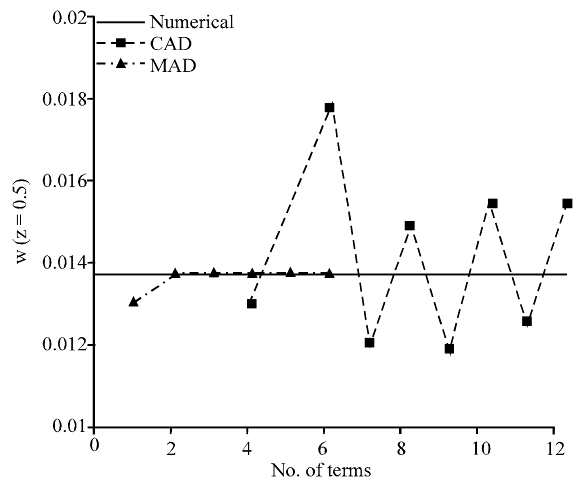

Fig. 7: Variation of tip deflection as a function of selected Adomian series terms for typical doubly-supported CNT with small number of layer ($f_5 = 5$)

Note that while Fig. 6 and 7 reveal some series (Even term series) are able to approximate the CNT deflection (for f_n values which are far from the instability point of the system), they can not determine the instability of the CNT. This limitation should be considered in simulations to avoid physically worthless results.

Table 2: The critical van der Waals force (f_n^*) for doubly-supported CNT

Force	1 terms	2 terms	3 terms	4 terms	5 terms	6 terms	Numerical
f_n^* (for n = 4)	Can't determine	Can't determine	49.1626	Can't determine	39.3133	Can't determine	38.9976
Difference with numerical solution (%)	-	-	22.91387	-	1.71085	-	-
f_n^* (for n = 5)	Can't determine 31.9301	Can't determine	39.8103	Can't determine	32.1010	Can't determine	
Difference with numerical solution (%)	-	-	19.73499	-	0.427998	-	-

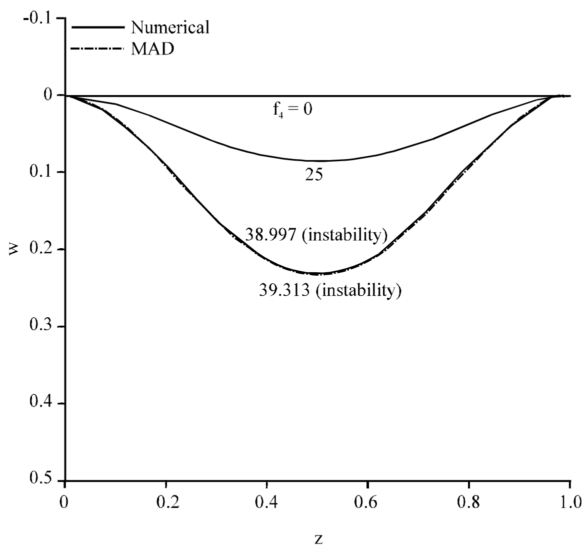

Fig. 8: Deflections of typical doubly-supported CNT for different values of f_n. MAD method is used and large number of layers is considered

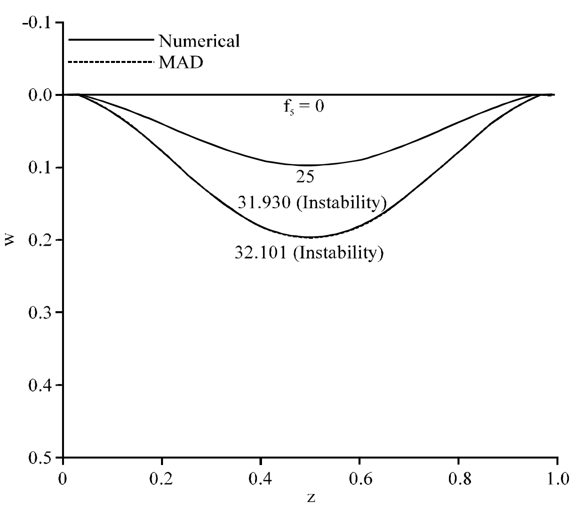

Fig. 9: Deflections of typical doubly-supported CNT for different values of f_n. MAD method is used and small number of layers is considered

CONCLUSION

In this study, the modified Adomian decomposition methods were applied to simulate the mechanical behavior of cantilever and doubly-supported CNT suspending over graphite surface. The critical van der Waals force at the onset of the instability was computed and the results were compared with numerical solution and conventional Adomian decomposition.

Results revealed that the modified Adomian series provides accurate results, converges rapidly to numerical solution. Therefore this method could easily be utilized to simulate the van der Waals force-induced deflection and instability of CNT. Compared to modified Adomian method, conventional decomposition might provides computational errors in simulating CNT deflection. Moreover the values of instability characteristics computed by conventional Adomian series converged to the values which differ from those obtained by numerical methods. Interestingly, none of the mentioned shortcomings were observed for modified Adomian series. Note that although some MAD series could approximate the CNT deflection but they could not determine the instability of the nanotube. This limitation should be considered in CNT modeling to avoid physically meaningless results.

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