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VIBRATION ANALYSIS OF DRUG DELIVERY CNTS USING TRANSFER MATRIX METHOD

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ABSTRACT

The free vibration and instability of fluid-conveying multi-wall carbon nanotubes (MWCNTs) are studied based on an Euler-Bernoulli beam model. A theory based on the transfer matrix method (TMM) is presented. The validity of the theory was confirmed for MWCNTs with different boundary conditions. The effects of the fluid flow velocity were studied on MWCNTs with simply-supported and clamped boundary conditions. Furthermore, the effects of the CNTs' thickness, radius and length were investigated on resonance frequencies. The CNT was found to posses certain frequency behaviors at different geometries. The effect of the damping corriolis term was studied in the equation of motion. Finally, a useful simplification is introduced in the equation of motion.

KEYWORDS: Vibration, fluid conveying CNT, instability, transfer matrix method.

INTRODUCTION

In recent years, carbon nanotubes (CNTs) have attracted a great deal of attention. Their excellent mechanical properties, chemical and thermal stability and hollow cylindrical geometry have led to several potential applications such as; fluid transport (nanopipes), nanocontainers, biosensors and drug-delivery systems (DDS). As a result of such interesting characteristics, dynamic and vibration analysis of CNTs has been of great interest to many researchers. However, due to experimental difficulties at the nano-scale, theoretical analysis is found to be the best solution for the investigation of CNT properties. Theoretical analyses at the nano-scale are divided into: (1) molecular dynamic simulations and (2) continuum elastic models. Since molecular dynamic simulations are expensive, complex and time consuming, especially for large-scale systems, continuum elastic models remain the best way for the study of CNTs.

Because of their superior elastic properties, in most of the above applications, CNTs are widely used for holding or transporting fluids (e.g. DDS and nanopipes). The vibration behavior of fluid-conveying CNTs is expected to be different from their macro/micro counterparts, especially because of their very small nano-scale dimensions. Therefore, studying the dynamic behavior of fluid-conveying nanotubes has become a complicated and challenging research topic over the past few years.

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Yoon *et al*. [1, 2] investigated the influence of internal moving fluid on free vibration and fluid flow instability of carbon nanotubes by utilizing different methods *i.e.* Galerkin procedure. Reddy *et al.* [3] studied the free vibration and instability of single-walled carbon nanotubes (SWCNTs) conveying fluid. They attempted to find a method for measuring the mass flow rate of the fluid by using the atomistic simulations and continuum beam models. Wang *et al.* [4] used multi elastic beam models to analyze the buckling instability of double-wall carbon nanotubes conveying fluid. They also regarded the inter-tube radial displacements and the related internal degrees of freedom in their analyses. In more comprehensive study, Wang and Ni [5] employed the differential quadrature method (DQM) for flutter instability in conveying fluid CNTs which occurs at higher flow velocities. Subsequently, vibration characteristics of single-walled [6], double-walled [7, 8] and multi-walled [9, 10] CNTs were investigated. The effects of viscous [11] and non-viscous [5, 6-10] fluids on the free vibration of CNTs were also studied. In most references the classical Euler–Bernoulli beam model was utilized [5, 9]. However, some other researchers have employed the Timoshenko beam model for the vibration and instability analysis of multi-walled CNTs conveying fluid [11, 12].

The main objective of the present study is to investigate an optimum model, for a CNT drug delivery system. In order to understand the effects of fluid-structure interactions on the dynamic behavior of multi-wall carbon nanotubes (MWCNT), a theory based on the Euler-Bernoulli beam model is presented. By exerting the transfer matrix method (TMM), the vibration analysis of a fluid-conveying MWCNT is developed. By comparing present results with those obtained by former researchers, the validity of the theory was first investigated. The theory was found to be accurate and simple to apply. The first few resonance frequencies and critical flow velocities were calculated for MWCNTs with simply supported and clamped boundary conditions. The effects of fluid flow velocity and linear elastic Winkler foundation on the resonance frequencies were studied. It was observed that the instability of MWCNTs occurs at a critical flow velocity. MWCNTs with different thickness/radius and length/radius ratios were compared. Resonance frequencies were found to possess certain variations with geometrical changes, especially thickness changes. Finally, the effect of damping coriolis term was investigated. Based on such an investigation, a useful simplification is introduced in the equation of motion. Interesting designing considerations are obtained, which are crucial in the designing process of a MWCNT.

MECHANICAL MODELING FOR FLUID CONVEYING CNTS

As show in Fig. 1, a fluid conveying CNT can be illustrated as an elastic hollow tube conveying fluid with various boundary conditions. As described in Ref. [13], continuum elastic-beam models have been effectively used to study static and dynamic structural behavior of CNTs. Here, as usual, we shall neglect gravity effect and assume that the constraint for axial displacement of the CNT is absent or negligible. Thus, vibration and structural instability of a fluid conveying CNT can be declared by the following model [14]:

$$\begin{aligned}&EI\frac{\partial^4 u_y}{\partial x^4}+(m_f V^2+P_0 A_f-F_{xt})\frac{\partial^2 u_y}{\partial x^2}+\\&2m_f V\frac{\partial^2 u_y}{\partial x\partial t}+(m_f+m_p)\frac{\partial^2 u_y}{\partial t^2}+k u_y=0\end{aligned}\quad (1)$$

In Eq. (1), x is the axial coordinate, t is time, $u_y(x, t)$ is the transverse deflection of the CNT, E and I are the Young's modulus and the moment of inertia of the cross-section of the CNT, m_p and m_f are the mass of the CNT and the fluid, per unit axial length respectively. k is the Winkler constant of the surrounding elastic medium described as a Winkler-like elastic foundation [14], F_{xt} and P_0 are the externally applied tension on the CNT and the global pressure exerted on fluid equally at both ends of CNT, respectively. In Eq. (1), the term $2m_f V\partial^2 u_y/(\partial x\partial t)$ is called the damping term. Due to the relative motion of the fluid inside the CNT, the coriolis damping term is associated with the coriolis acceleration, which has an angular velocity. It should be noticed that the wall–fluid interaction and the viscosity of fluid is not considered on the mean flow velocity V.

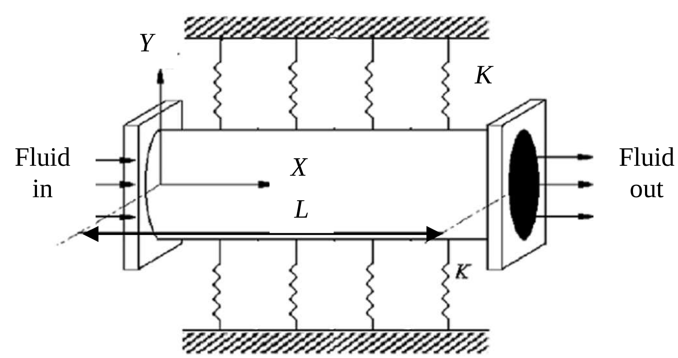

Fig. 1 Schematic of fluid conveying CNT on a Winkler foundation.

In this paper, we shall consider a simply-supported or clamped CNT. The boundary conditions of a simply supported-simply supported (*SS-SS*) CNT are as follows:

$$u_y(0,t)=\frac{\partial^2 u_y(0,t)}{\partial x^2}=u_y(l,t)=\frac{\partial^2 u_y(l,t)}{\partial x^2}=0 \quad (2)$$

The boundary conditions of a clamped-clamped (*C-C*) CNT are as follows:

$$u_y(0,t)=\frac{\partial u_y(0,t)}{\partial x}=u_y(l,t)=\frac{\partial u_y(l,t)}{\partial x}=0 \quad (3)$$

SOLUTIONS BY THE TRANSFER MATRIX METHOD (TMM)

In order to solve the equation of motion, consider solutions of the form:

$$u_y(x,t)=\mathrm{Re}\left[\sum_{n=1}^{4} B e^{i\lambda x} e^{i\omega t}\right] \quad (4)$$

where B is a constant and ω is the complex circular frequency. Substitution of Eq. (4) into Eq. (1) gives:

$$\lambda^4-\sigma_f\,\lambda^2-\gamma\lambda+\tau_f=0 \quad (5)$$

in which:

$$\sigma_f=(m_f V^2+P_0 A_f-F_{xt})/(E I_p)\,, \quad (6)$$
$$\gamma=(2 m_f V\omega)/(E I_p) \text{ and}$$
$$\tau_f=(k-(m_f+m_p)\omega^2)/(E I_p)\,.$$

In Eq. (5), four complex roots λ_n (n=1, 2, 3 and 4) are functions of ω. The transverse shear force $\hat{f}_y$, rotation angle $\hat{\varphi}_z$ and bending moment $\hat{M}_z$ can be represented as:

$$\hat{f}_y=-\frac{\partial \hat{M}_z}{\partial x} \quad (7)$$

$$\hat{\varphi}_z(x,t)=\frac{\partial \hat{u}_y}{\partial x} \quad (8)$$

$$\hat{M}_z(x,t)=E I_p\frac{\partial \hat{\varphi}_z}{\partial x} \quad (9)$$

Now, Eq. (4) must be expanded in terms of λ_n and B_n (n=1, 2, 3 and 4) as follows:

$$u_y(x,t)=\mathrm{Re}\{(B_1 e^{i\lambda_1 x}+B_2 e^{i\lambda_2 x} + B_3 e^{i\lambda_3 x}+B_4 e^{i\lambda_4 x})e^{i\omega t}\} \quad (10)$$

The coefficients B_n (n=1, 2, 3 and 4) are constant values. Substitution of Eq. (10) into Eqs. (7 and 8) and substitution of Eq. (8) into Eq. (9), yields four equations in terms of the constant values B_n (n=1, 2, 3 and 4). These four equations can be written in a matrix form:

$$\begin{Bmatrix}\hat{u}_y\\ \hat{\varphi}_z\\ \hat{M}_z\\ \hat{f}_y\end{Bmatrix}=\begin{bmatrix} q_1 & q_2 & q_3 & q_4\\ S_1 q_1 & S_2 q_2 & S_3 q_3 & S_4 q_4\\ D_1 q_1 & D_2\, q_2 & D_3 q_3 & D_4\, q_4\\ T_1 q_1 & T_2 q_2 & T_3 q_3 & T_4 q_4\end{bmatrix}\begin{Bmatrix}B_1\\ B_2\\ B_3\\ B_4\end{Bmatrix} \quad (11)$$

where:

$$q_n=e^{i\lambda_n x}\,,\ S_n=i\lambda_n\,,\ D_n=-E I_p\lambda^2{}_n\,, \quad T_n=iE I_p\lambda^3{}_n\,, \ (n\text{=1, 2, 3 and 4}). \quad (12)$$

Eq. (11) can be written in short form as:

$$\{Z\}=[Q(x)]\{B\} \quad (13)$$

Assume for the ith CNT's element that, at x=0, $Z=Z_{i-1}$ and at x=l, $Z=Z_i$ in which Z is the state vector corresponding to both ends of the CNT and l is the length of the CNT's element. $\{B\}$ can be expressed by $\{Z\}_{i-1}$ by letting x=0 in Eq. (13):

$$\{B\}=[Q(0)]^{-1}\{Z\}_{i-1} \quad (14)$$

Substituting Eq. (15) into Eq. (13), the vector $\{Z\}$ can be written as:

$$\{Z\}=[Q(x)][Q(0)]^{-1}\{Z\}_{i-1}\,. \quad (15)$$

Applying $Z=Z_i$ at x=l, gives:

$$\{Z\}_i=[Q(l)][Q(0)]^{-1}\{Z\}_{i-1} \quad (16)$$

where $[TM]=[Q(l)][Q(0)]^{-1}$ is the transfer matrix of the CNT's element. Suppose [RL] and [RR] to be the boundary conditions of the left and right side of the CNT, respectively. By consideration of just one element for the CNT, applying the boundary conditions of the CNT in Eq. (16) would cause:

$$[R_R]\,[TM][R_L]\{Z\}_0=\{0\} \quad (17)$$

where the vector $\{Z\}_0$ represents non-zero vector. Eq. (17) is usually written in the form:

$$[RTM]\{Z\}_0=\{0\} \quad (18)$$

where $[RTM]$ is the reduced size of matrix [*TM*] due to exerting the boundary conditions. For achieving a non-trivial solution for Eq. (18), one should have:

$$\left|RTM\right| = \{0\}. \tag{19}$$

Eq. (19) is called the frequency equation and the components of the $\left|RTM\right|$ are the functions of the natural frequencies of the CNT.

RESULTS AND DISCUSSION

Based on the above formulations for a fluid conveying CNT, the vibration behavior of MWCNTs are discussed in detail. The effects of steady flow velocity, surrounding elastic medium, geometrical properties and the damping coriolis term are studied on the resonant frequencies and the instability of MWCNTs. In order to calculate the natural frequencies, a computer program based on the transfer matrix method (TMM) was written. In the following examples, water is considered as the internal fluid of the CNT with a density of 1 g/cm^3. The density of the CNT is assumed to be 2.3 g/cm^3 and its Young's modulus (E) is equal to 1 TPa. According to available data in the literature [15, 16], flow velocities inside the CNT range from 400 m/s to 2000 m/s. However in Ref. [17], velocities of up to 50,000 m/s are also reported.

In Figs. 2 and 3, resonance frequencies of simply-supported MWCNTs with two different outermost radiuses (R_{out}=10 nm and R_{out}=20 nm) are plotted as a function of fluid flow velocity. In these figures the first four vibration modes of the MWCNTs are presented. The following results are obtained from Figs. 2 and 3:

1. Resonance frequencies are highly dependent upon the fluid flow velocity. For each resonance mode in Figs. 2 and 3, in the first part of the ω-*V* diagram, as the flow velocity increases, resonance frequencies decrease. Such decrease continues until the frequency equals to zero at a certain velocity. The velocity in which the frequency tends to zero is called the critical flow velocity. For each resonance mode a critical flow velocity occurs. At such a velocity, a static structural instability characterized by adjacent neutral equilibrium states takes place (divergence instability). Therefore, at the critical velocity of each mode, the MWCNT becomes unstable and tends to buckle.

2. By comparing Figs. 2 and 3 with R_{out}=10 nm and R_{out}=20 nm respectively, it can be concluded that; as the radius decreases, the critical flow velocities and resonance frequencies of the MWCNT increase. In order to understand such a behavior, consider the following formula for the moment of inertia of the CNT's cross-section:

$$I = \frac{\pi}{4}(R_{out}^4 - R_{in}^4)\,. \tag{20}$$

   in which R_{out} and R_{in} are the outermost and innermost radius of the CNT respectively. Hence, according to Eq. (20) as the outermost radius of the CNT decreases, the moment of inertia decreases likewise. According to the fundamentals of vibration, as the moment of inertia of a system decreases, the natural frequencies of the system increase. Therefore, the larger the CNT's radius, the higher its resonance frequencies.

   As a result, the first mode (fundamental mode) of Figs. 2 and 3 becomes unstable at *V*=8645 m/s and *V*=5202 m/s respectively. However, the second, third and fourth modes are still stable at these velocities. For higher modes the critical velocities occur at higher velocities.

3. At a certain flow velocity after the critical velocity, each mode appears again in the ω-*V* diagram and starts to rise with the increase of velocity. Such can be observed for mode one in Fig. 2 and modes one and two in Fig 3. In Fig. 2 the second part of the first mode starts to increase right after the critical velocity at *V*=8659 m/s, whereas, in Fig. 3 a bigger gap exists between the decreasing and increasing parts of the first and second mode. As an example, in Fig. 3 the critical velocity of the first mode is *V*=5202 m/s, while the first mode starts to rise again at *V*=5516 m/s. Hence, in Fig. 3 for R_{out}=20 nm, the first mode becomes unstable at 5202<*V* <5516 m/s, whereas in Fig. 2 for R_{out}=10 nm, the instability of the first mode occurs only at 8645<*V*<8659 m/s. Therefore, the divergence instability of each mode occurs at a certain velocity range. The length of such a velocity range is dependent upon the outermost radius of the MWCNT. As a result, the greater the radius of the MWCNT, the larger the velocity range of the divergence instability.

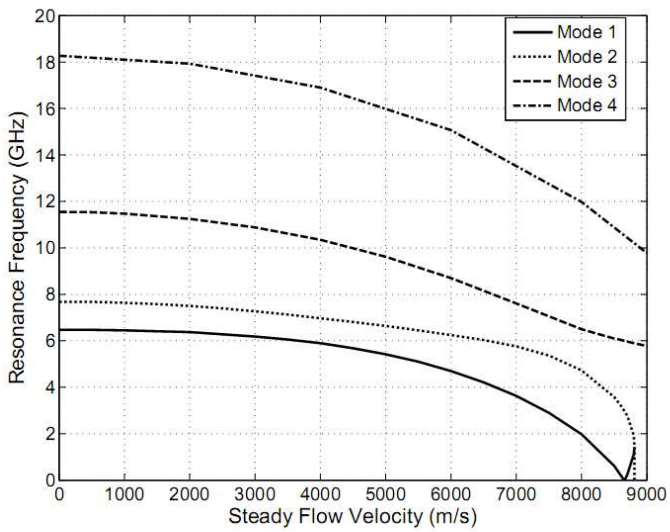

Fig. 2 Flow velocity dependence of the lowest four modes of a simply supported MWCNT with R_{out} =10nm, L/R_{out} =40, h=5nm and k=0.

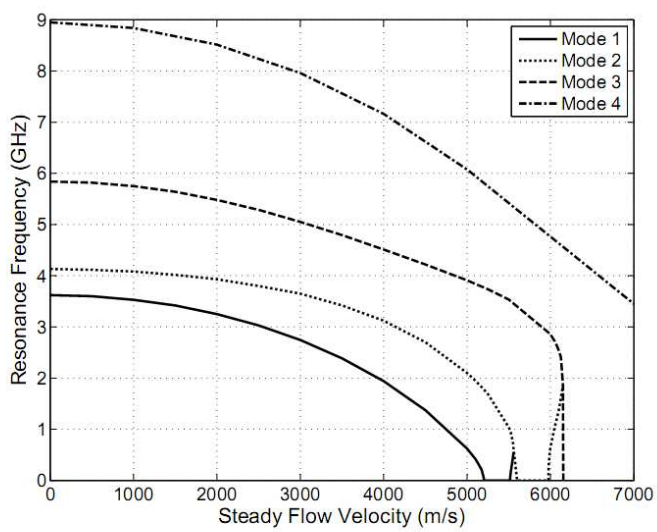

Fig. 3 Flow velocity dependence of the lowest four modes of a simply supported MWCNT with R_{out} =20nm, L/R_{out} =40, h=5nm and k=0.

In order to evaluate the validity of the present method, results were compared with those given in the literature. A MWCNT with outermost radius R_{out}=50 nm, thickness h=10 nm and length L=2000 nm was considered. In Table 1 critical flow velocities obtained by the TMM are compared to those given by Yoon et al. [1] and Wang et al. [5]. According to Table 1, compared to other methods the TMM yields results with a maximum error of less than 0.009 %. Therefore the TMM is found to be highly accurate for both simply supported (SS-SS) and clamped (C-C) boundary conditions. The effects of the Winkler foundation k, on the critical flow velocity could also be observed in Table 1. According to Table 1, the presence of a surrounding elastic medium (k=1 GPa), increases the critical flow velocity of the MWCNT. An elastic foundation k, represents the distributed support provided to the MWCNT. Thus the Winkler elastic foundation can be modeled as distributed springs over the CNT's length (Fig. 1). The additional stiffness supplied by the Winkler elastic foundation makes the system stiffer. Therefore, the presence of the elastic medium increases the natural frequencies and critical flow velocities of the whole system, by increasing its stiffness. Such a statement is correct for both simply supported and clamped boundary conditions.

Table 1 Critical flow velocities obtained by the TMM compared with previous stdies.

Boundary Condition	***Present Study***	***[1]***	***[5]***
SS-SS (k=1 GPa)	4666	4660	-
SS-SS (k=0)	1193	1190	1190
C-C (k=1 GPa)	5175	5200	-
C-C (k=0)	2385	2380	2390

Now, let us consider the effects of the CNT's wall thickness h, on its resonance frequencies. Consider a MWCNT surrounded by an elastic medium (k=1 GPa), with variable thickness and constant dimensions; R_{out} =50 nm and L/R_{out} =40. In Fig. 4 the ω-V diagrams of the fundamental frequency (first mode) have been plotted, for MWCNTs with six various thicknesses. It is clear from Fig. 4 that the CNT with the largest thickness yields the highest critical velocity. Generally, as the thickness of the CNT decreases, the critical velocity decreases likewise. However, the resonance frequency behavior of the CNTs with variable thickness is different. Results in Fig. 4 show that, a transient region exists in the ω-V diagrams of CNTs with different thicknesses. This region has been marked in Fig. 4. Interesting phenomena happen in this region. For the flow velocities before the transient region (V<1000 m/s), the CNTs with less thickness possess higher resonance frequencies, compared to those with larger thicknesses. Though, for velocities after the transient region (V>2300 m/s) vice versa occurs; the thinner the CNTs, the lower the resonance frequencies. However, for flow velocities inside the transient region (1000<V<2300 m/s), no consistent relationship exists between the resonance frequencies and the tube's thickness. In the transient region some abnormal and unpredicted behaviors occur for the nanotubes.

According to the fundamentals of vibration, the resonance frequency of a one-degree freedom system is as follows:

$$\omega = \sqrt{\frac{k_s}{m}} \tag{21}$$

in which k_s and m are the stiffness and the mass of the system, respectively.

The additional stiffness supplied by the Winkler elastic foundation makes the system stiffer. Thus, when a CNT is supported by a Winkler elastic foundation ($k \neq 0$), according to Eq. (21) its resonance frequency increases. However, when a CNT's thickness is decreased, the system becomes less stiff and therefore the resonance frequency decreases.

According to Fig. 4, at low flow velocities (before the transient region), the increasing effect of the Winkler foundation on resonance frequencies, is more effective on the thinner CNTs. Hence, at low flow velocities, due to the Winkler foundation stiffness, the thinner CNTs possess higher resonance frequencies. However, at high flow velocities (after the transient region), the decreasing effect of the CNT's thickness on resonance frequencies, is more effective on the thinner CNTs. Therefore, at high flow velocities, due to the thickness decrease (which causes stiffness decrease), the thinner CNTs possess lower resonance frequencies. Such a phenomenon causes the thinner CNTs to posses lower critical flow velocities. The effectiveness of the Winkler foundation or the thickness of the CNT, at low and high flow velocities respectively, is due to the characteristics of the equation of motion.

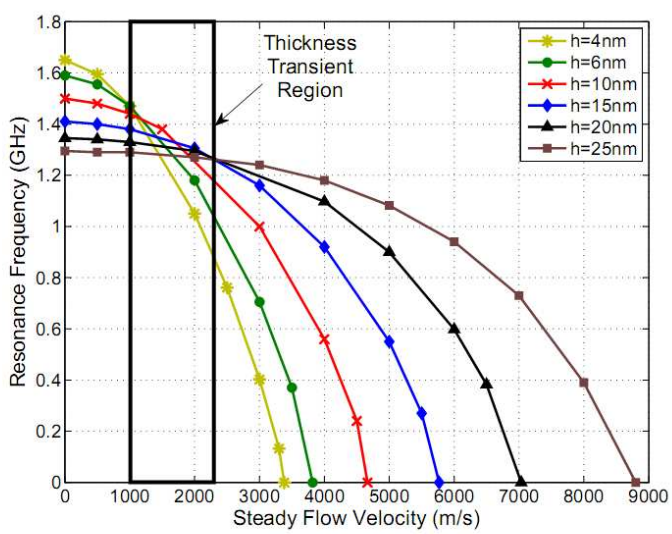

Fig. 4 Frequency variations of the fundamental mode of simply supported MWCNTs with the nanotubes thickness and the flow velocity (R_{out} =50nm, L/R_{out} =40 and k=1GPa).

Hence, the frequency behavior of variable thickness CNTs, surrounded by an elastic medium (k=1 GPa), is totally dependent upon a transient region. Therefore, in order to calculate a CNT's thickness, recognizing and defining the thickness transient region is of crucial importance.

Next, let us consider a MWCNT having similar dimensions to the above MWCNT (R_{out} = 50 nm and L/R_{out} =40), however this time with no surrounding elastic medium (k=0 GPa). In Fig. 5 the ω-V diagrams of these MWCNTs have been plotted for five different thicknesses. In Fig. 5 similar to Fig. 4, the critical velocity decreases with the thickness decrease of the CNT. However, in Fig. 5 no transient region exists for the CNT. The frequency behavior of various thickness CNTs without a surrounding elastic medium (k=0), is consistent, throughout all flow velocities. Therefore, according to Fig. 5, the CNTs with less thickness possess lower resonance frequencies, in all flow velocities.

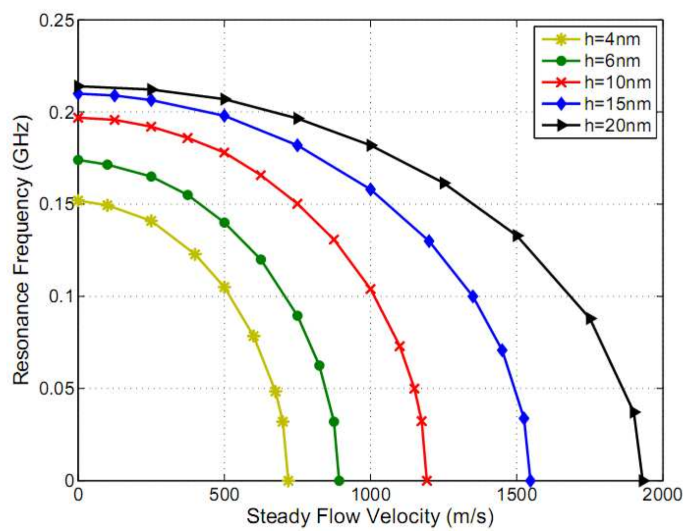

Fig. 5 Frequency variations of the fundamental mode of simply supported MWCNTs with the nanotubes thickness and the flow velocity (R_{out} =50nm, L/R_{out} =40 and k=0GPa).

By comparing Figs. 4 and 5, the effects of the surrounding elastic medium k, on the frequency behavior of a CNT are observed. It was observed for a CNT surrounded by an elastic medium k=1GPa (Fig. 4), that different thicknesses possess different frequency behaviors before and after a certain thickness transient region. Whereas, for the same CNTs without an elastic medium, no such transient region exists and different thicknesses possess similar frequency behaviors throughout all flow velocities. Furthermore, comparing resonance frequencies of Figs. 4 and 5, it is noticed that CNTs surrounded by an elastic medium have higher resonance frequencies and critical flow velocities.

Effect of coriolis damping term

One of the aims of the present study is to investigate the effects of the Coriolis damping term on the equation of motion Eq. (1). In order to study such an effect, critical flow velocities of several MWCNTs are presented in Table 2, with and without the coriolis damping term in the equation of motion. As it can be observed in Table 2, neglecting the coriolis damping term for both simply supported and clamped CNTs, results in 0% error for all aspect ratios ($\frac{L}{R_{out}}$). It is to note that, in the present study of MWCNTs, $\frac{m_f}{m_f + m_p} < 0.5$. According to Table 2, the coriolis damping term does not have a substantial effect on the calculation of the critical flow velocities of CNTs having $\frac{m_f}{m_f + m_p} < 0.5$. This is because, when $\frac{m_f}{m_f + m_p} < 0.5$, the Coriolis damping term becomes an skew-symmetric matrix, therefore, it does not have a large effect on the resonance frequencies of the system [18, 19]. Therefore, for CNTs having $\frac{m_f}{m_f + m_p} < 0.5$, if interested in only finding the critical flow velocities, one could neglect the coriolis damping term in Eq. (1). This claim is in complete agreement with Refs. [18, 19]. The equation of motion is therefore simplified and the solving procedure is made easy by considering such an assumption.

Table 2 Critical flow velocities with and without the coriolis damping term.

	SS-SS		***C-C***	
Aspect Ratio (L/R_{out})	With Coriolis Damping Term	Without Coriolis Damping Term	With Coriolis Damping Term	Without Coriolis Damping Term
20	5085	5085	6110	6110
40	4666	4666	5175	5175

Conclusions

The free vibration and instability of fluid conveying CNTs were studied, considering the effects of internal moving fluid. The analysis was carried out using the transfer matrix method (TMM). The TMM was found to be efficient and simple to apply. It was observed that the divergence instability of the CNT occurs at a certain critical velocity domain. The length of such a domain is dependent upon the geometry of the CNT, especially the outermost radius. The variations of critical flow velocities and resonance frequencies with the thickness of the CNT were also examined. It was noticed that CNTs with different thicknesses posses different frequency behaviors. A thickness transient region, which has an important role in the designing process of a CNT was also obtained. Moreover, the Winkler elastic foundation was also found to have a notable effect on the frequency behavior of CNTs with different thicknesses. Finally, the effect of the coriolis damping term was investigated in the equation of motion and on the critical flow velocities. It was observed that, for CNTs having $\frac{m_f}{m_f + m_p} < 0.5$, the neglect of the coriolis damping term did not have any effects on the final critical velocity results. Interesting results were obtained in which a simplified equation of motion was resulted.

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