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Molecular Dynamics Simulation of Stationary and Rotating Nanotube in Uniform Liquid Argon Flow

S.M. HOSSEIN KARIMIAN[1, 2], S.M. HASHEMINASAB[1, 2, *], MASOUD ARABGHAHESTANY[1, 2]

*** Corresponding author: Tel.: +989123622379; Email: smhasheminasab@aut.ac.ir**
1 Department of Aerospace Engineering, Amirkabir University of Technology (Tehran Polytechnic), Iran
2 Center of Excellence in Computational Aerospace Engineering, Tehran, Iran

Abstract In this paper molecular dynamics (MD) simulation is used to investigate the liquid argon flow past a stationary and rotating carbon nanotube. The main purpose of this work is to estimate flow forces on the nanotube and compare them with classical continuum results. The simulation is 3D and consists of 33,700 liquid argon atoms as fluid and 240 atoms of carbon as the nanotube. The single walled nanotube is simulated as a rigid cylinder of fixed carbon atoms. For simulation of rotating carbon nanotube, carbon atoms are rotated around center axes of the nanotube in each times step according to the desired angular velocity. Both argon-argon and carbon-argon interactions are modeled by Lennard-Jones potential function. Periodic boundary condition is used for the whole system. Flow is driven by rescaling velocities at the inlet each 50 time steps. The results show that the rotation of nanotube causes a reduction in drag force, up to rotation rate of 3.0 where the drag force is about 78% of the stationary one. Above the rotation rate of 3.0 drag coefficient is almost constant. Lift coefficient of stationary nanotube is negligible in comparison with drag coefficient and the rotation of nanotube has a little influence on the lift coefficient.

Keywords: Molecular Dynamics, Carbon Nanotube, Rotating, Drag Coefficient

1. Introduction

For many years the physical interactions between Macro-scale fluid flow passing stationary and rotating cylinders have been subject of a large number of investigations. In recent years, many researches have been done on adsorption of many gas flows by carbon nanotubes [1, 2, and 3]. One of thorough study of flow around rotating and stationary circular cylinders has been done by Mittal and Kumar [4]. They presented an incompressible finite-element simulation of fluid flow of Reynolds 200 around a spinning circular cylinder in wide range of non-dimensional rotation rates varying between 0 and 5. They concluded that very large lift coefficients can be produced for large rotation rates because of Magnus effect, however, the power required to rotate cylinder increases rapidly with rotation rate. From this one can conclude that there is a fast increase of drag force at large rotation rates.

In recent years, study of nano-scale fluid flow has been one of the subjects of interest. Due to lack of experimental information in nano-scales, the roles of numerical methods are very significant in this regard [5]. Due to the failure of continuum theories in atomistic level of fluid flow, the common macro-scale numerical methods are not applicable here and therefore other types of simulation must be used [6]. A very powerful method for such simulation is molecular dynamics (MD), which is specifically suitable for problems with length scales below 10 nm [7].

Walther et al. [8] performed a non-equilibrium molecular dynamics (NEMD)

simulation of uniform liquid argon flow passing over a stationary carbon nanotube. They presented a detailed study on drag forces and coefficients of nanotubes using direct summation of molecular forces exerted from fluid molecules on CNT molecules, for different sizes of carbon nanotubes in flows with velocities between 15-320 m/s. Comparing their results with results of FE analysis, they realized that in low speed flows MD simulation results did not match those obtain from macro scale analysis, so they concluded that continuum mechanics cannot be used for nano-flows simulations.

Kang and Hwang [9] investigated fluidic Gas-driven carbon-nanotube motors that works based on multi-wall CNT and fluidic gas flow. They demonstrated the performance of fluidic gas-driven CNTs for flow velocities in range of 20-40A/ps. They concluded that rotational motion of CNT motors accelerates as time increases and also the angular velocity of the nano-motor increases with the stream velocity increases.

Despite wide range of application for rotating nanotube cylinders, little research has been devoted to determine the exerted forces on CNTs, especially drag force, which are the base of most nano-engineering machines. Therefore we decided to investigate the detail of interaction between nano-flows and spinning CNTs.

In this paper, behavior of nano-scale flow passing a spinning nanotube cylinder has been investigated. Effects of non-dimensional rotation rate of nanotubes on drag coefficient have been studied. We have verified our MD results, specifically the drag coefficient with the results obtained from LAMMPS open-source code. Our results are also compared with results obtained from macro-scale simulation of the same problem. It seems that drag force on a spinning nanotube decreases as its rotation increases in low Reynolds.

2. SIMULATION

In this paper amount of parameters and results will be presented in reduced molecular dynamics units. The molecular mass (*m*) and diameter (σ) of liquid argon are used as units of mass and length, respectively. The ε which is the strength of interaction for Lennord-Jones Potential, is considered as unit of energy. Amounts of these parameters are given in Table 1. Also the units of time, force and velocity are derived using reference molecular units.

Table 1
Molecular units

Quantity	Symbol	Equivalent in SI
Length	σ	**3.40×10-10 *(m)***
Mass	m	**6.625×10-26 *(kg)***
Energy	ε	**1.657×10-21 *(J)***
Other parameters based on molecular units		
Time	$\tau \equiv (\sigma^2 m/\varepsilon^{-1})^{1/2}$	**2.15×10-12 *(s)***
Force	$F \equiv \varepsilon\sigma^{-1}$	**4.873×10-12 *(N)***
Velocity	$U \equiv \sigma\tau^{-1}$	**1.58×102 *($m.s^{-1}$)***

2.1. Solution domain

Schematic of simulation domain illustrated in Fig.1,the system consists of two types of atoms; the argon atoms as fluids, and the carbon atoms forming the carbon nanotube (CNT). The CNT is assuming to be a rigid body which means carbon atoms do not move relative to each other and only can only rotating around its center of mass with each other. Domain of simulation is a box with the dimensions of 50×60 molecular diameter in *z* and *y* direction. Domain width in *x*

direction equals the length of nanotube. Periodic boundary condition is applied to the solution domain in all directions.

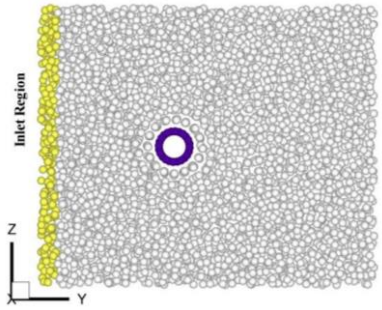

Fig. 1. Schematic of the system

First, nanotube assumed to be fixed and flow over a fixed nanotube is fully analyzed. In the second step of this simulation, in the MD code CNT atoms rotate to its center of mass with non-dimensional rotation rate of α and drag force's dependency to carbon nanotube rotation rate is investigated. In this paper for analysis of convergence of drag force, huge number of simulations were conducted with various number of non-dimensional rotation rate in range of 0.1-5.

2.2. Initial setup and rotation technique

Argon atoms are initially distributed in the channel in a lattice form of FCC with the liquid argon density of 0.8 consists of 14964 argon atoms. Initial thermal velocities of atoms are assigned according to their initial temperature of 95K. Velocity components of atoms are assigned based on Maxwell–Boltzmann distribution that results in a zero resultant velocity and no flow in the channel. Initial flow is generated by adding a velocity of U_0=1.0 in *y* direction to all argon atoms. To maintain the flow, velocities of atoms located in the $0.03L_y$ of the inlet region are reset every 50 time steps. Resetting or rescaling of velocity is applied by setting the initial random thermal velocity of the atoms in the inlet region and then adding U_0 to their velocities in y direction. In addition to maintaining the flow, this technique removes excess heat from the system as well [10] and there is no need to use thermostat or other techniques.

For rotating the nanotube, the non-dimensional rotation rate is defined as:

$$\alpha = \frac{r\omega}{U_0} \qquad (1)$$

Where r is the nanotube radius and ω is the desired angular velocity. In each time step the carbon atoms are rotated around the center mass of nanotube with an angle of $\Delta\theta$ and the new position of each atom is obtained.

$$\Delta\theta = \omega.\Delta t = \frac{\alpha.U_0}{r}.\Delta t \qquad (2)$$

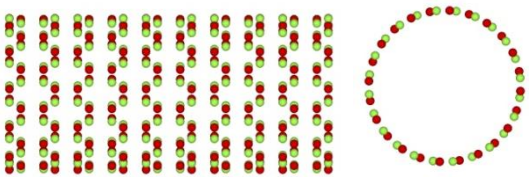

Fig. 2. Rotation of carbon atoms

2.3. MD simulation

All the atoms in the system interact by Lennard-Jones (LJ) 12-6 potential function but with different parameters for argon-argon and carbon-argon interactions.

$$V_{ij} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \qquad (3)$$

Where V_{ij} is the LJ potential, ε is the strength of interaction, σ is the molecular diameter of argon and r_{ij} is the distance between a pair of atoms. Based on LJ potential, the interaction force between a pair of atoms is calculated by

$$\boldsymbol{F}_{ij} = \frac{48\varepsilon}{\sigma^2}\left[\left(\frac{\sigma}{r_{ij}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma}{r_{ij}}\right)^{8}\right]\boldsymbol{r}_{ij} \qquad (4)$$

Where r_{ij} is the position vector from atom i to atom j and r_c is the cut-off distance beyond which the forces are neglected. The interaction forces between argon-argon and carbon-argon atoms are computed using the parameters as in Table 2.

Table 2
LJ potential parameters

	Argon-Argon	Carbon-Argon
ε	1.6567×10^{-21} J	1.9646×10^{-21} J
σ	3.4×10^{-10} m	3.573×10^{-10} m

A cut-off distance of 2.5σ is used for both interactions and neighbor list method is used to calculate interactions between atoms. Equation of motion is integrated using a Verlet scheme with a time step of $\Delta t = 0.001\tau$ equals 2.15×10^{-15}s. With these assumptions a parallel MD code is developed using atom decomposition approach to reduce computational time. The simulation is performed for 8×10^5 time steps corresponding to 1.7 ns.

3. RESULTS

To evaluate the drag and lift forces of nanotube, simulations are performed to reach an equilibrium time t_{eq} and then continued to a desired time t to get enough data for extracting forces and other macroscopic properties. Some of the methods reported in the literature to detect system equilibration are to record instantaneous values of the energies and pressure during this period [11], or to monitor the positional disorder and velocity distribution of atoms [12]. In this work trend of kinetic energy is used to detect the equilibrium time. Change of kinetic energy during the simulation is shown in Fig. 2.

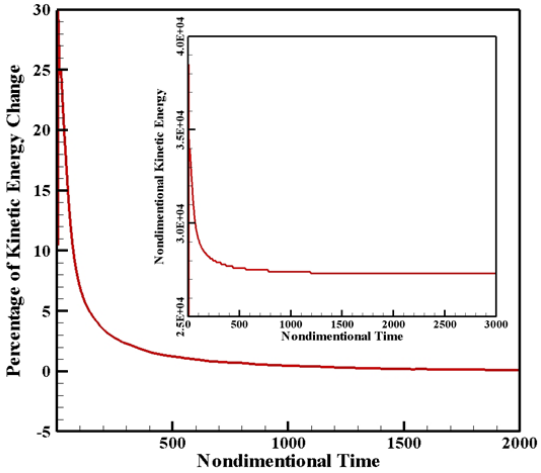

Fig. 3. Kinetic energy during the simulation

As shown in Fig. 3, after the time of 1000 the percentage of kinetic energy change is less than 1%. So we can assume that the system has been reached to equilibrium after this time corresponding to the iteration of 10^6 and the t_{eq}=1000 is considered for all the simulations in this work.

3.1. Force Evaluation

In MD simulations, lift and drag forces are calculated directly from the forces exerted on the solid atoms by fluid atoms [5]. The drag and lift are obtained using the summation of forces applied on the carbon atoms by the argon atoms in y and z direction, respectively. In this way the instantaneous forces are calculated in each iteration. Using this method the instantaneous forces on the nanotube in x direction (along the nanotube) and y direction (flow direction) are obtained. As shown In Fig. 4, the forces in both directions fluctuate around a value. In x direction fluctuations are around zero as expected but in flow direction (y) the instantaneous forces fluctuate around a higher value.

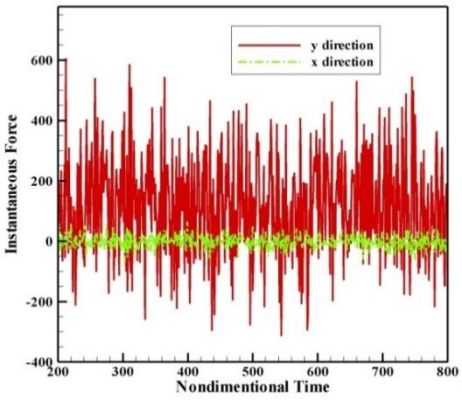

Fig. 4. Instantaneous forces in *x* and *y* direction

To determine the mean forces on the nanotube the instantaneous forces should be average over a period of time after equilibrium. There are two more common averaging methods that can be used for the measurement of mean drag force, one denoted by sample-averaged measurement (SAM), and the other denoted by cumulative average measurement (CAM) [13].

$$D_{ave}(t) = \frac{1}{N_{t_{eq}-t}} \sum_{t_{eq}}^{t} D_{inst} \qquad (5)$$

Where $N_{t_{eq}-t}$ is the number of time steps from equilibrium time (t_{eq}) to time (t)used for data averaging. As mentioned before, in these cases according to convergence trend of kinetic energy the value of 1000 and 3000 are considered for t_{eq} and t respectively. Results of averaging the instantaneous forces can be seen in Fig. 5, in flow direction (y) an average force of about 115 is obtained and in two other directions average force is about zero as expected.

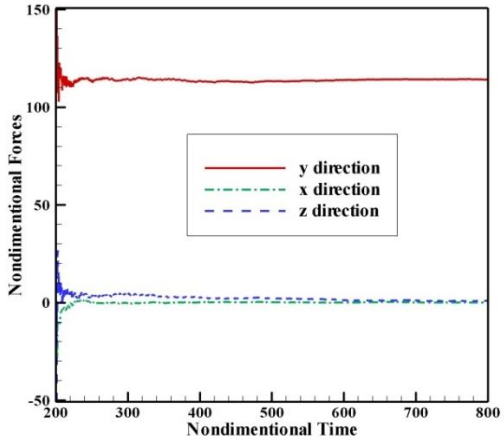

Fig. 5. Averaged forces in *x, y* and *z* direction

3.2. Verification

The results obtained for mean drag force in different domain sizes are compared with the existing results of reference [5] as shown in Fig. 6.

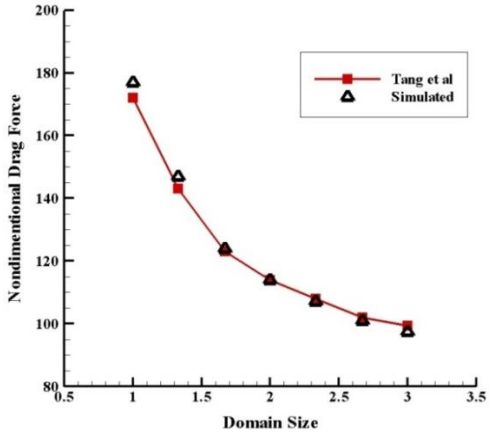

Fig. 6.Comparison of drag forces obtained from present simulation and reference [5]

As it can be seen in Fig. 6,there is a good agreement between the results of two simulations, the differences of two simulations are less than 4% in all the cases as calculated in Table 4.

Table 4
Comparison of mean drag force of present work and reference [5]

Domain Size	Tang and Advani	Present Work	Percentage Difference
1	172.37	176.57	2.44%
1.33	142.76	147.05	3.21%
1.67	123.03	124.26	1.00%
2	113.65	114.15	0.43%
2.33	107.73	107.19	0.50%
2.67	102.3	100.91	1.36%
3	99.34	97.36	2.10%

Also the same simulation was done with LAMMPS software. Drag and lift coefficient obtained from the LAMMPS simulation for domain 2 with rotation rate of 1 is compared with those obtained from the present simulation and is showed in Table 5.

Table 5
Comparison of drag and lift coefficient of present work and LAMMPS simulation, α=1.0

	C_L	C_D
Present Work	-0.313	24.65
LAMMPS	-0.318	25.47
Difference	1.47%	3.22%

The difference is less than 5% and shows that the lift and drag forces obtained in present work can be used as lift and drag forces exerted on rotating nanotube.

3.3. Effect of rotation on streamlines

In order to investigate the effect of nanotube rotation on argon flow, the streamlines of the flow are plotted. For capturing the streamlines, the simulation domain in *yz* plane is divided by a 50×60 mesh that is a total of 3000 bins which are extended across the *x* direction [14]. The local velocity is calculated in each bin.
Using the *y* and *z* components of the local velocities, the streamlines are plotted and presented in Fig. 7, for stationary and rotating nanotube.

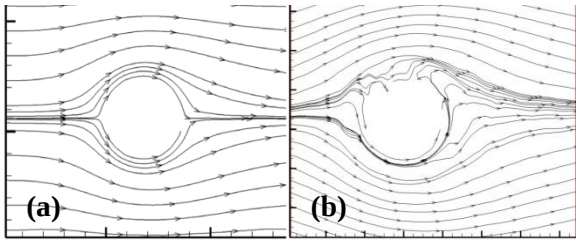

Fig. 7.Streamlines for uniform flow past, (a) Stationary, and (b) Rotating with α=1

As it can be seen in Fig. 7, in the case of stationary nanotube, streamlines are symmetric. The rotation of nanotube causes asymmetricity, more in the back and in front of the nanotube, and less in the top and bottom and far from the nanotube.

3.4. Effect of rotation rate on drag and lift coefficients

In order to investigate the effect of rotation rate on drag and lift coefficients, simulations with different rotation rates in the range of 0-5 is performed. Rotation rates of 0, 0.1, 0.5, 1, 1.5, 2, 2.5, 3, 4 and 5 are considered for different cases. The drag coefficient C_D is calculated as follows:

$$C_D = \frac{D_{ave}}{\frac{1}{2}\rho U_0 A} \qquad (6)$$

Where $A = L_x \times d$, L_x and d are the length and the diameter of carbon nanotube, respectively. The results for drag and lift are shown in Fig. 8, And Fig. 9.
As it can be seen in Fig. 8, maximum drag coefficient is obtained when nanotube is stationary and the rotation causes a reduction in drag coefficient. Under the rotation rate of 3.0 as rotation rate is increased the C_D is decreased more. Above the rotation rate of 3.0, increment

in rotation rate does not have a remarkable effect on drag coefficient, and the drag coefficient is almost constant after rotation rate of 3.0.

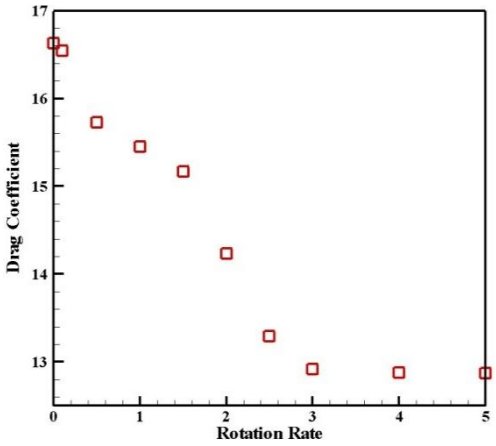

Fig. 8. Drag coefficients in different rotation rates from 0 to 5

The reduction percentage of drag coefficient is calculated and showed in Table 6. Increasing the rotation rate from 0 to 5 causes a decrement in drag coefficient from 16.63 to 12.87, corresponding to 22.6% reduction in drag coefficient.

Table 6
Lift and drag coefficients in different rotation rates from 0 to 5

α	C_l	C_D	C_D Reduction Percentage
0	**0.13**	**16.63**	
0.1	**-0.22**	**16.54**	**0.51%**
0.5	**-0.61**	**15.73**	**5.42%**
1	**-0.33**	**15.45**	**7.10%**
1.5	**-0.24**	**15.17**	**8.76%**
2	**-0.62**	**14.23**	**14.44%**
2.5	**-0.76**	**13.29**	**20.10%**
3	**-0.74**	**12.92**	**22.31%**
4	**-0.29**	**12.88**	**22.54%**
5	**-0.26**	**12.87**	**22.60%**

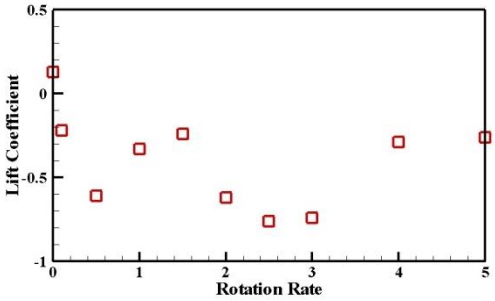

Fig. 9. Lift coefficients in different rotation rates from 0 to 5

As it can be seen in Fig. 8, in stationary nanotube the lift coefficient is positive and about 0.15. With a low amount of rotation α=0.1, the lift coefficient changes to 0.22 below the zero. Since the rotation is counter clockwise the lift force is expected to be downward and the results confirm this fact, but the amount of lift coefficients are negligible compared with drag coefficients and also increase in rotation rate does not have a significant effect on lift coefficient. It was seen before in section 3.3 that the rotation of nanotube has a little influence on the streamlines at top and bottom of the nanotube.

4. CONCLUSION

Liquid argon flow over a stationary and a rotating carbon nanotube was simulated using molecular dynamics simulation. The flow was driven by rescaling particle velocities at the inlet. Drag and lift forces on the nanotube calculated using direct summation of forces. The results show that under the rotation rate of 3.0, rotation of the nanotube causes a significant reduction in drag force exerted on the nanotube. At rotation rate of 3.0 the drag coefficient is reduced to 78% of stationary nanotube drag coefficient. Above the rotation rate of 3.0 drag coefficient is almost constant. Rotation of nanotube has a little influence on lift

coefficient. Clockwise rotation of nanotube causes a negative/downward lift force, but the value of lift coefficient is not comparable with drag coefficient, and the change of rotation rate does not have a significant effect on lift coefficients.

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