

A NOVEL DESIGN OF PERISTALTIC CARBON NANO PUMP AND AN ANALYSIS OF HELIUM FLOW

NOV DIZAJN PERISTALTIČNE NANOKARBONSKE ČRPALKE IN ANALIZA PRETOKA HELIJA

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A novel nano-scale pump that can transport atoms or small molecules with a peristaltic motion is designed. It is proven by molecular-dynamics simulations that the introduced nano-pump design works properly. The designed nano-pump consists of one main carbon nanotube named the flow tube and two rotors where multi-walled carbon nanotubes are attached. The pumping of helium atoms by the designed peristaltic carbon nano-pump is investigated by molecular-dynamics simulations. For varying rotor speeds and blade counts, time-averaged velocity, temperature, and pressure results of pumped helium atoms are calculated, and relationships between them are modeled as polynomial surfaces. The results showed that rotor frequency increases the velocity of helium linearly and the temperature and pressure of helium non-linearly. Furthermore, the blade count of the proposed mechanism does not substantially affect the velocity as per the previous studies in the literature.

Keywords: carbon nanotubes, molecular dynamics, nano pump, helium, peristaltic motion

Avtorja sta konstruirala novo nano črpalko, ki omogoča transport atomov ali malih molekul na osnovi principa peristaltike. S pomočjo simulacij molekularne dinamike sta dokazala, da je konstrukcija in delovanje razvite nano črpalke ustrezna. Črpalka vsebuje eno glavno oglikovo nanoceevčico imenovano pretočna cevin dva rotorja na katera je pripeto večje število večstenskih nano- cevčic. S pomočjo simulacij molekularne dinamike dizajnirane nano črpalke sta avtorja preiskovala črpanje helijevih (He) atomov. Pri različnih hitrostih rotorjev in različnem številu lopatic rotorjev sta ugotavljala rezultirajočo povprečno hitrost, temperaturo in tlak črpanja He atomov ter določila povezave z modeliranjem v obliki polinomskih površinskih funkcij. Rezultati analiz so pokazali, da frekvenca rotorja linearno poveča hitrost He ter nelinearno poveča njegovi temperaturo in tlak. Nadalje avtorja ugotavljata, da število lopatic rotorjev predlaganega mehanizma ne vpliva bistveno na hitrost, kot nakazujejo v znanstveni literaturi predhodno objavljene raziskave.

Gljučne besede: oglikove nanoceevčice, molekularna dinamika, nano črpalka, helij, peristaltično gibanje

1 INTRODUCTION

Carbon nanotubes and graphenes are among the most investigated materials for nano-scale applications. Recently, these materials attracted researchers and the industrial community due to their promising mechanical, thermal, and electrical properties. Despite many studies having been carried out on carbon nanotubes, their potential has not been fully resolved. Hence, they can still offer new designs of nano-scale systems such as nano-propellers and nano-pumps.

Carbon nano-propellers and carbon nano-pumps are innovative nano-mechanisms that allow atoms or small molecules to be transported by carbon nanotube or graphene structures. Even though currently most of the studies on nano-propellers and nano-pumps are theoretical or conceptual studies that are carried out by computational simulations, these kinds of studies prepare the groundwork for future biological, medical, chemical and several other nano-scale applications.

The main challenges of designing a nano-propeller or nano-pump are to find the stable nanostructure and the right mechanical, thermal, or electro-magnetic behavior to sustain the transportation of molecules or atoms. There are several designs in the literature that are inspired by the macro propeller and pump mechanisms. Also, there are other designs that depend on the behaviors occurring only at the atomic or nano scale.

Some of the recent studies, where pumping is based on the mechanical behavior of the structure, are mentioned as follows. Wang and Kral¹ adapted a classic propeller geometry to the nano scale by using carbon nanotubes as the rotor, and pyrene molecules as the propeller blades. They also investigated the effect of the chemical properties of the blades on the water flow. Similarly, Lohrasebi² developed a nano-pump with angled graphene blades attached to a rotating carbon nanotube to push helium and neon atoms. In addition, Qui³ showed that vibrating cantilever carbon nanotubes can drive water molecules inside the tube from a fixed tip to a free tip by centrifugal forces.

Besides mechanical systems, there are nano-pump designs based on electric charges, fields, or currents ap-

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plied to the carbon nanotubes. Gong et al.⁴ imitated cellular aquaporins and simulated the pumping of water molecules through carbon nanotubes using positive charges. Wang et al.⁵ investigated the transportation of water molecules through carbon nanotubes by applying a gradient electric field to carbon nanotubes attached between two graphene membranes. Kou et al.⁶ demonstrated the flow of water molecules by vibrating electric charges applied to carbon nanotubes having an asymmetric surface energy. In a similar setup, Zhou et al.⁷ investigated the relationship between the transportation of water molecules and the deformation of carbon nanotubes. Li et al.⁸ studied the flow of water molecules inside carbon nanotubes that are exposed to rotating electric and magnetic fields. Xiao et al.⁹ imposed a rotating electric charge on a curved carbon nanotube and investigated the relationship between the water flow and the angular speed of the rotating charge. As inspired by a biomolecular motor named ATP synthase, Lohrasebi and Feshanjerdi¹⁰ designed an ion pump based on a rotating carbon nanotube with electric charges attached to it.

The thermal behavior of the nanostructures, especially thermophoretic effects, are also used to transport the atoms or small molecules through carbon nanotubes in the literature. When a temperature gradient is applied between the tips of the carbon nanotubes, thermophoretic effects cause the atoms or molecules encapsulated inside carbon nanotubes to move through from the hot tip to the cold tip. By using thermophoretic effects, Schoen et al.¹¹ simulated the motion of solid-gold nanoparticles inside carbon nanotubes. Using similar methods, Zambrano et al.¹² studied water molecules, Rurali and Hernández¹³ and Wei et al.¹⁴ fullerene clusters, and Zhang et al.¹⁵ mercury atoms. Oyarzua et al.¹⁶ showed that the Brownian motion of water molecules is rectified by the thermal oscillations of carbon nanotubes, driving the flow to the desired direction. Oyarzua et al.¹⁷ also investigated the relationship between thermophoretic motion and frictional forces. Kou et al.¹⁸ studied the transportation of water molecules by applying a surface-energy gradient to carbon nanotubes instead of a thermal gradient.

Physical deformation and subsequently occurring Van der Waals interactions are also used to transport the atoms or small molecules inside carbon nanotubes. Chang¹⁹ showed that the collapsing of carbon nanotubes can be used to accelerate the molecules inside the tube. Wang²⁰ applied torsion to carbon nanotubes and was able to simulate the transportation of helium atoms by kink propagation. Duan and Wang²¹ used a similar method to study the motion of water molecules.

Apart from the mechanisms mentioned above, some unique studies can also be found in the literature. Král and Tománek²² studied the excitation of carbon nanotubes by laser pulses to control the movement of single atoms inside the carbon nanotube. Feng et al.²³ showed that rotating chiral carbon nanotubes placed between two graphene membranes can transport water molecules.

Similarly, Mistry et al.²⁴ used coaxially rotating carbon nanotubes to pump water molecules.

In this study, a novel nano-pump mechanism consists of carbon nanotubes that can continuously transport atoms or small molecules by a peristaltic motion. The testing of the introduced peristaltic carbon nano-pump design and the simulation of helium flow within the nano-pump is performed by molecular-dynamics simulations. It is clear that the designed nano-pump works as expected. Velocity, temperature, and pressure of the transported helium atoms are calculated and their characteristics are discussed.

2 DESIGN OF PERISTALTIC CARBON NANO PUMP

The nano pump is designed by taking advantage of the flexibility and chemical stability of carbon nanotubes to transport atoms or small molecules inside the tube. The geometry and dimensions of the peristaltic carbon nano-pump are illustrated in **Figure 1**. The nano pump is composed of two main components. The first one is a single-walled carbon nanotube named the flow tube, containing the atoms or molecules to be transported. The second component consists of two rotors made of nickel atoms and four multi-walled carbon-nanotube blades attached to each of them. The flow tube is fixed from the top and bottom as indicated by the orange color in the figures. The rest of the flow tube can deform freely. The rotors rotate synchronously, and they are located at a specific distance from the flow tube to squeeze and sweep it as they rotate. In particular, the distance in the y-axis is carefully selected to be tight enough to prevent the backflow of the atoms and also wide enough not to damage the structure. The designed pump is considered to be a peristaltic pump, due to the periodic sweeping action of the rotor blades over the flow tube and considered as a nano pump because of its size.

The dimensions of the peristaltic carbon nano-pump are expressed as follows: D_{rot} is the diameter of the rotor

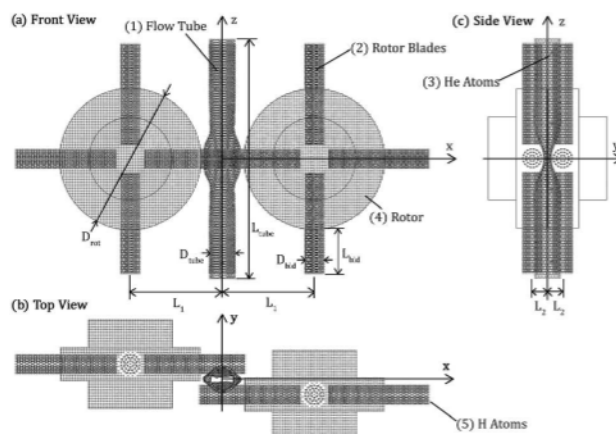


Figure 1: Dimensions of the peristaltic carbon nano-pump: a) front view, b) top view, and c) side view

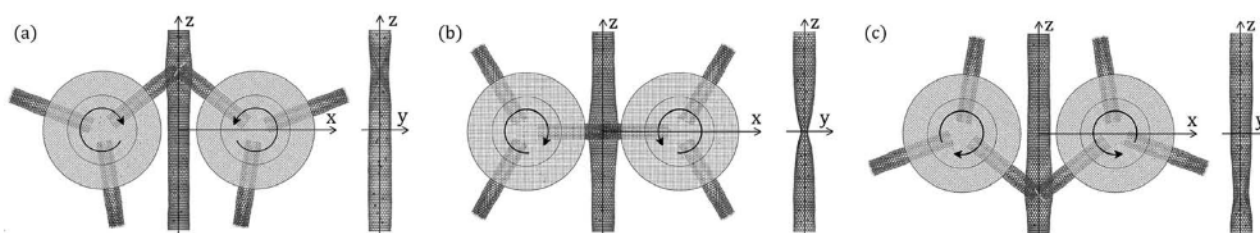


Figure 2: Interaction of the rotor blades with the flow tube: a) engaging, b) middle, and c) disengaging stage

holding the multi-walled carbon nanotube blades and transmitting the input torque. L_{tube} and D_{tube} are the length and diameter of the flow tube. L_{bld} and D_{bld} are the length and diameter of the rotor blades measured from outside of the rotor. L_1 and L_2 are the distances between the centerline of the flow tube and the centres of the rotors in the x and y axes, respectively.

The peristaltic carbon nano pump contains carbon, nickel, and hydrogen atoms in the structural components. Carbon atoms construct the carbon nanotubes. Nickel atoms are known to stick carbon nanotubes well.²⁵ Hence, they are used in the rotors to hold the blades in place. Additionally, at the free tip of rotor blades carbon atoms having two bonds are stabilized by bonding them with hydrogen atoms.

In Figure 2, the interaction of the rotor blades with the flow tube in a peristaltic carbon nano pump with three-bladed rotors is shown. At the engaging stage, the rotor blades squeeze the top of the flow tube, as seen in Figure 2a. Then the rotor blades sweep the squeezed region down as the rotors rotate, as illustrated in Figure 2b. Finally, they disengage from the flow tube, as shown in Figure 2c. Since the rotor blades are selected as multi-walled carbon nanotubes, they can withstand mechanical forces occurring during the squeezing and sweeping action. The squeezed region does not allow the transported atoms to pass through. As the squeezed region moves down, it pushes the atoms inside the flow tube. Squeezing and sweeping actions repeat periodically as the rotors rotate synchronously; hence, it leads to the flow of atoms. The arrangement of the synchronous movement and power transmission of the rotors are not discussed thoroughly in this study. It is assumed that the rotors and the carbon-nanotube blades are properly rotating as desired.

3 MOLECULAR-DYNAMICS SIMULATIONS

There are many analytical and numerical methods in the literature to investigate the behavior of nanostructures. Among them, molecular dynamics simulations are the most preferred method for studying the complex behaviors of nanostructures. They allow researchers to test their concepts without conducting expensive experimental studies. Furthermore, they provide an opportunity to calculate the mechanical and thermal properties of nano-scaled structures and mechanisms. For these reasons, molecular-dynamics simulations were employed to

investigate the introduced peristaltic carbon nano pump in this study.

In molecular-dynamics simulations, the movements and interactions of atoms or molecules are considered as bond stretching, bond-angle bending, out-of-plane torsion, dihedral angle torsion and Van der Waals interactions. A potential field formulation is developed to express each of these interatomic behaviors. Then, the equations of motion of the whole system are constructed, grounded on Newton's laws of motion with the help of potential field formulations. Finally, the equations of motion of the system are solved numerically for small timesteps to reveal the dynamics of the system by using algorithms such as velocity-Verlet integration and reversible reference system propagator algorithm.

In all the calculations the interactions between the C-C, C-H, and H-H pairs are defined with the Airebo potential field.²⁶ The Airebo potential field formulation is given as follows:

$$E^{\text{Airebo}} = \frac{1}{2} \sum_i \sum_{j \neq i} [E_{ij}^{\text{Rebo}} + E_{ij}^{\text{LJ}}] + \sum_{k \neq i} \sum_{l \neq i, j, k} [E_{ijkl}^{\text{Tor}}] \quad (1)$$

Where E_{ij}^{Rebo} is the Rebo potential that controls the bond forming or breaking between two atoms. E_{ij}^{LJ} is the Lennard-Jones potential defining the long-range interactions between non-bonded atoms. E_{ijkl}^{Tor} is the dihedral torsional potential representing the torsional behavior between four atoms.

The Beck potential field, which is particularly developed for the interactions of helium, is used for the pumped helium atoms at the simulations. The basic formulation of the Beck potential field²⁷ is presented below:

$$E^{\text{Beck}}(r) = Ae^{(-\alpha r - \beta r^6)} - \frac{B}{(r^2 + a^2)^3} \cdot \left(1 + \frac{2.709 + 3a^2}{r^2 + a^2}\right) \quad r < r_c \quad (2)$$

Where r is the distance between helium atom pairs. Their interaction is ignored to reduce the computational load if the distance between atom pairs exceeds the cut-off distance (r_c). A , α , β and a are the parameters of the Beck formulation. The parameters of the Beck potential field are chosen as follows: $A = 399.672$ eV, $B = 8.57 \times 10^{-9}$ eV·nm, $a = 43.901$ nm⁻¹, $\beta = 375$ nm⁻¹, $a = 0.0675$ nm and $r_c = 0.750$ nm.

The interactions between Ni-C pairs and Ni-Ni pairs are represented by using the Morse potential field²⁸, as it

is generally preferred in the literature for Ni-C interactions. The formulation of the Morse potential field is given below:

$$E^{\text{Morse}}(r) = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \quad r < r_c \quad (3)$$

Here, D_0 and α are constants, r_0 is the equilibrium bond distance. The parameters of the Ni-C pairs and Ni-Ni pairs are given in **Table 1**.

Table 1: Morse potential field parameters for Ni-C and Ni-Ni pairs

Pair	D_0/eV	$a/(\text{nm}^{-1})$	r_0/nm	r_c/nm
Ni-C ²⁹	0.4330	32.440	0.232	0.425
Ni-Ni ²⁹	0.4205	14.199	0.278	0.425

Finally, the interactions between the C-He pairs and H-He pairs are defined using the well-known 12/6 Lennard-Jones potential field.

$$E^{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad r < r_c \quad (4)$$

The ϵ and σ parameters of the C-He and H-He pairs are calculated using the Waldman-Hagler combining rule.³⁰ The Lennard-Jones parameters of C-C, H-H, He-He, C-He and H-He pairs are listed in **Table 2**, respectively.

Table 2: Lennard-Jones potential parameters

Pair	ϵ/eV	σ/nm	r_c/nm
C-C ³¹	8.6177×10^{-3}	0.300	—
H-H ³¹	3.4471×10^{-3}	0.260	—
He-He ³²	0.8807×10^{-3}	0.255	—
C-He	2.7377×10^{-3}	0.294	0.425
H-He	1.6582×10^{-3}	0.276	0.425

4 NUMERICAL RESULTS AND DISCUSSION

Peristaltic carbon nano pumps were investigated for three configurations with three, four, and six blades for each rotor. The output of the flow tube is coupled to the input by applying a periodic boundary condition. Time-averaged velocities, temperatures, and pressures of the pumped helium atoms are calculated for various cases having different helium atom counts (6; 12; 24; 36; 48) in the flow tube and having different rotor frequencies (0.5–50 GHz). Open-source LAMMPS³³ software is used to perform the molecular-dynamics simulations. All the simulations are executed at 300 K with 1 fs time steps by using the potential fields and parameters described in the previous section.

The rotor blades are chosen as three-walled carbon nanotubes with (18; 12; 6) chiralities. The chirality of the flow tube is selected as 25. The other dimensions of the simulated peristaltic carbon nano-pumps are given in **Table 3**.

The rotor frequency is increased from 0.5 GHz to 50 GHz, and the variation of time-averaged velocity of helium atoms along the flow tube is given in **Figure 3** for (6; 12; 24; 36; 48) helium atom cases. In **Figure 3f**, all the cases are plotted together. A linear relation is observed between the helium velocity and the rotor frequency. The helium velocity decreases slightly with the increase of helium atoms inside the flow tube. As can be inferred from the plots, the number of rotor blades does not have a significant effect on the helium velocity. This situation has also been stated in a similar nano-pump study.²

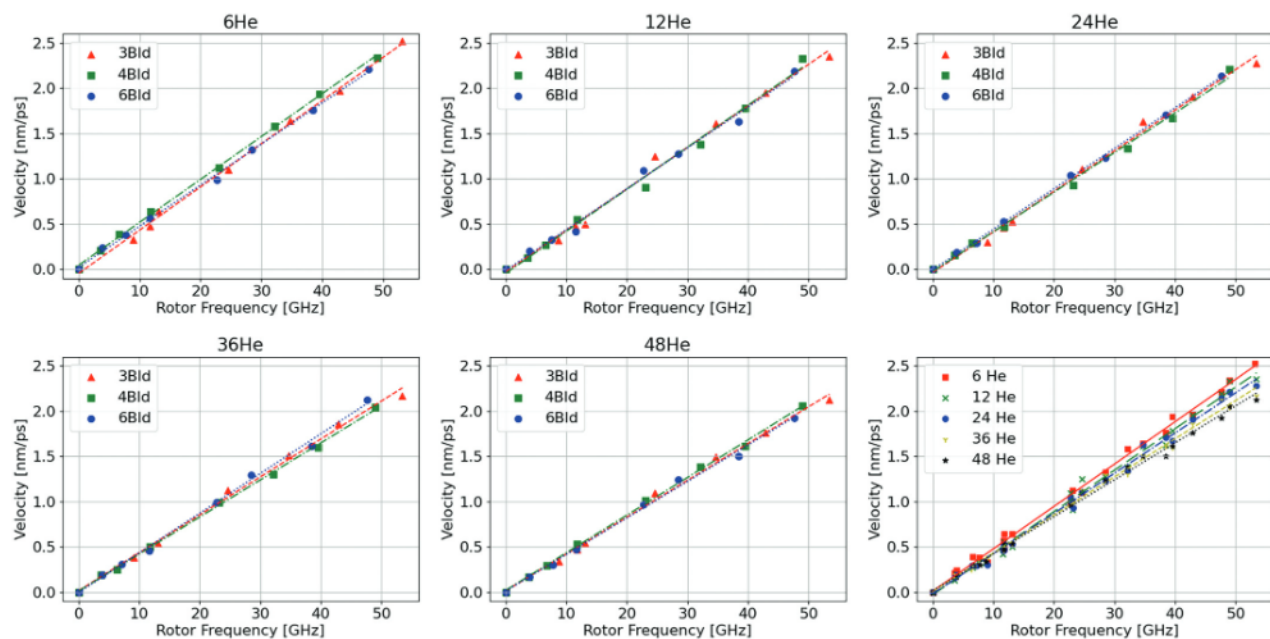


Figure 3: Variation of the helium velocity with the rotor frequency

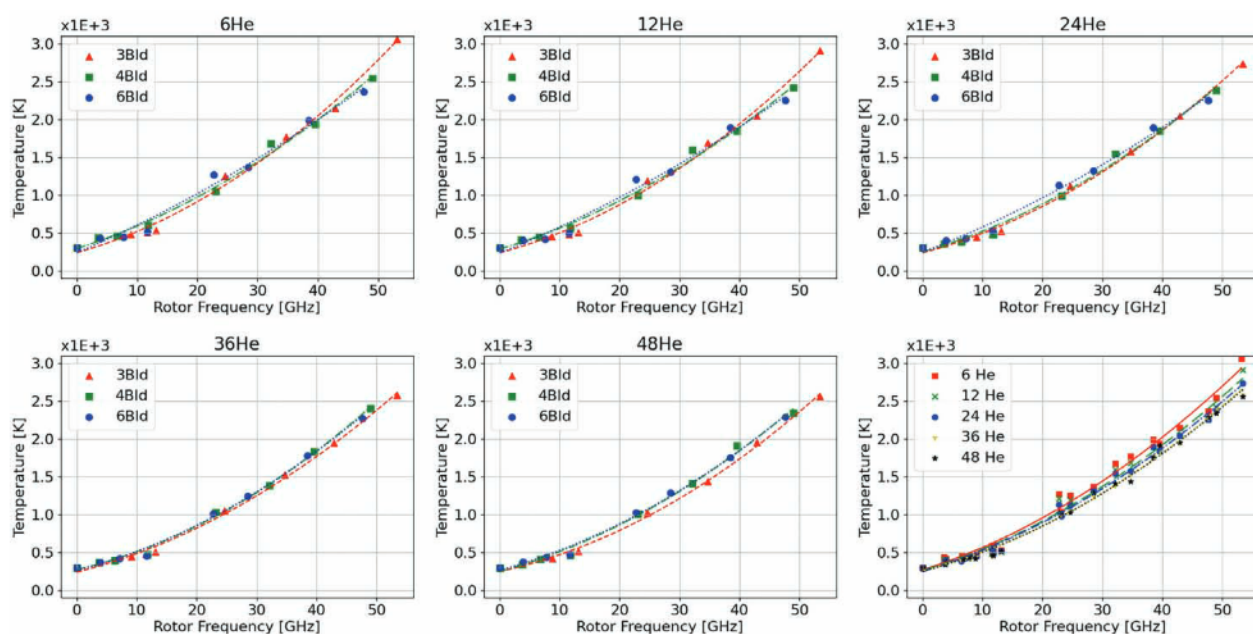


Figure 4: Variation of the helium temperature with the rotor frequency

Table 3: Dimensions of the peristaltic carbon nano-pumps used

Parameter	Value (nm)
D_{tube}	1.946
L_{tube}	18.181
D_{bld}	1.410
L_{bld}	3.519
D_{rot}	10.688
L_1	7.000
L_2	1.165

In Figure 4, the variation of temperature with the rotor frequency is plotted for (6; 12; 24; 36; 48) helium atom cases. Helium temperature and the rotor frequency have a non-linear relationship. Similar to the relationship between rotor frequency and velocity, it is observed that the helium temperature slightly decreases with the increase of the helium atom count, and the number of rotor blades does not have a meaningful effect on the temperature of the helium atoms.

The variation of the helium pressure with the rotor frequency can be seen in Figure 5 for (6; 12; 24; 36; 48)

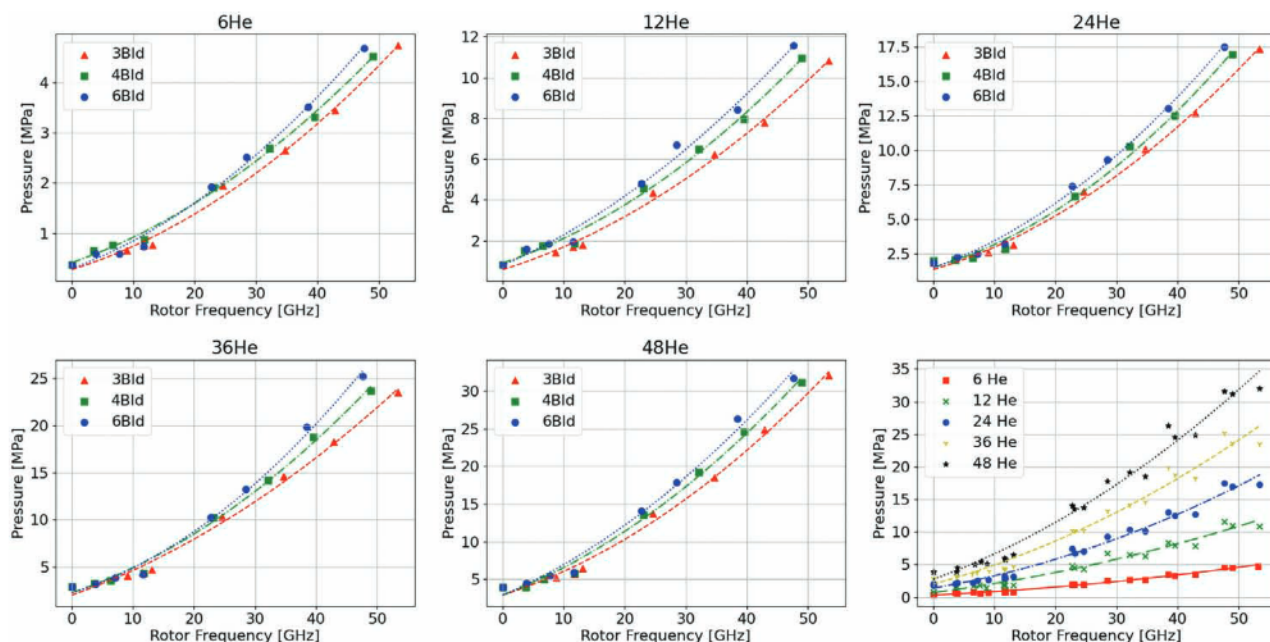


Figure 5: Variation of the helium pressure with the rotor frequency

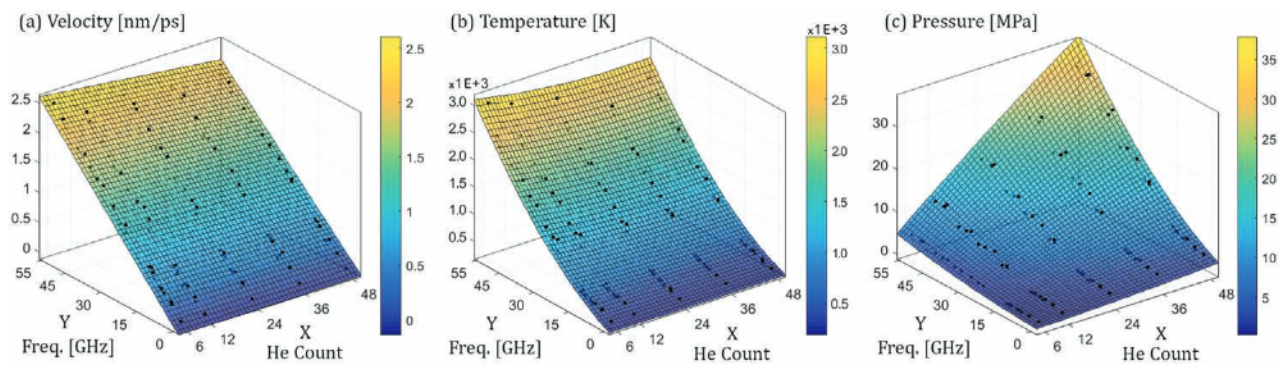


Figure 6: Surface plots for pumped helium: a) velocity, b) temperature, c) pressure

helium atom cases. The relationship between the pressure and the rotor frequency is non-linear, similar to the relationship between rotor frequency and temperature. However, for the pressure, the number of rotor blades affects the helium pressure where the pressure increases with the blade count. In addition, it is seen that the helium pressure significantly increases as the helium-atom count inside the flow tube increases.

The relation between rotor frequency and helium atom count with the helium velocity is modelled as a linear surface, as described in Equation (5a), by using the results of the molecular-dynamics simulations. Similarly, the variation of helium temperature and pressure depending on the rotor frequency and helium-atom count are modelled as polynomial surfaces, as defined in Equation (5b).

$$z(x, y) = c_1 + c_2x + c_3y + c_4xy \quad (5a)$$

$$z(x, y) = c_1 + c_2x + c_3y + c_4xy + c_5x^2 + c_6y^2 + c_7x^2y + c_8xy^2 \quad (5b)$$

where x and y represent the helium-atom count and the rotor frequency, respectively, and z is the result of the model. The coefficients c_i of the model and the coefficients of determination R^2 are presented for velocity, temperature, and pressure in Table 4.

The surface plots showing the variation of helium velocity, temperature, and pressure with the rotor frequency and helium-atom count are given in Figure 6a, 6b, and 6c, respectively. The plotted surfaces are in good agreement with the simulation results represented by the black points in Figure 7.

Table 4: Coefficients of surface models

Coef.	Velocity	Temperature	Pressure
c_1	-1.99×10^{-2}	264.1	1.439×10^{-1}
c_2	5.63×10^{-4}	-6.056×10^{-1}	$3.927e \times 10^{-2}$
c_3	4.77×10^{-2}	27.34	2.734×10^{-3}
c_4	-1.45×10^{-4}	-3.024×10^{-1}	8.213×10^{-3}
c_5	-	6.295×10^{-3}	3.424×10^{-4}
c_6	-	4.479×10^{-1}	4.577×10^{-4}
c_7	-	3.358×10^{-1}	-3.249×10^{-5}
c_8	-	2.135×10^{-4}	9.639×10^{-5}
R^2	0.99	0.99	0.98

5 CONCLUSION

A novel peristaltic carbon nano pump has been modelled and simulated by molecular dynamics. It is proven that the new pump design can successfully convey atoms through the carbon nanotubes by squeezing and sweeping the flow tube. The following conclusions can be drawn after the analyses of the helium flow for various values of the pertinent parameters:

- With the increase of the rotor frequency, the velocity of the helium increases linearly, while the temperature and pressure of the helium show a non-linear behavior.
- The number of blades does not significantly affect the velocity and temperature of helium, as shown in previous studies. Nevertheless, it increases the pressure of the helium.
- The helium-atom count in the flow tube decreases the velocity and temperature slightly, while significantly increasing the pressure.
- The dependences of the helium velocity, temperature, and pressure on the rotor frequency and the number of helium atoms were modelled as polynomial surfaces.
- Similar pumping mechanisms can be adapted to micro- and macro-scale applications by using proper materials.
- It is believed that in the near future, similar nano-pump designs can be perfected with the help of developing nano-scale manufacturing methods and can be used in biological, medical, chemical and many other technological applications.

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