Mathematical modeling of the interaction of a model water molecule with a membrane based on cells of double-walled open carbon nanotubes

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Abstract. In this work, the process of interaction of a cell of four double-walled nanotubes with a water molecule was numerically simulated. The simulation results show that under normal conditions, water molecules pass through a cell of nanotubes in a plane parallel to the length of the tubes, and in a plane perpendicular to the length, the structure for such molecules is not passable.

1. Introduction

As a result of industrial development and increased energy demand, there is a rapid diminution of fresh potable water reserves and generation of large amount of wastewater, which leads to the need of developing methods to treat the contaminated water. Nanoporous materials are successfully used for both ion and molecular nanofiltration. Nanofiltration technology has shown promising application in purification of water contaminated with pathogenic bacteria, viruses, and protozoa [1]. Reverse osmosis is also an effective multi-stage method of water filtration. Nanofiltration and reverse osmosis processes are very similar in that they are designed to remove dissolved chemical contaminants including salts. Both require high hydraulic pressures and utilize similar membrane materials [2]. In work [3] studies the manufacturing techniques for the synthesis of porous carbon spheres with high compressive strength. It was found that magnetically functionalized activated surfaces of porous coals can lead to contactless remote control or manipulation using external magnetic fields. So, they have great potential for applications as adsorbents for purification of water.

Nanoporous materials have insufficient strength over large areas and tend to change properties over time, so improved hybrid nanomembranes are being developed. An ultra-thin, large-area hybrid membrane has been developed for highly efficient water treatment. Such membranes can address the trade-off between water permeability and solute rejection in conventional desalination membranes [4]. In additional, it was proposed a novel all-carbon nanofiltration membrane that consists of multi-walled carbon nanotubes interposed between graphene oxide nanosheets. The as-prepared membrane has nanochannels that can physically sieve antibiotic molecules through electrostatic interaction [5].

The work [6] presents the results of numerical simulations of the interaction of a unit cell of a membrane composed of four open nanotubes and water vapor molecules based on the Lenard-Jones potential. The simulation results show that during the rotation of the unit cell of the membrane, it is possible to change the modes of passage of the membrane in relation to water vapor. These results can be used in creation of various filter materials. This paper compared a commercial polyester nanofiltration membrane and a polypropylene hollowfiber membrane distillation module for their ability

to remove fluoride ions from water in the presence of hardness ions and organic fouling agents. The nanofiltration membrane can offer more than 10 times higher water productivity than membrane distillation, under realistic gradients of temperature and pressure, respectively. However, these two processes are based on different mechanisms of permeation and selectivity, and thus they show different performances during concentration of fluoride-contaminated water [7]. The purpose of this study was to investigate the behavior of a model water molecule when describing its interaction with a nanostructure using only the Lennard-Jones potential.

2. Materials and research methods

In this work, we describe the process of interaction between a model water molecule and a carbon nanostructure, represented by 4 double-walled open nanotubes. These nanotubes form a square cell, which is studied for the permeability of water molecules at different speeds. We will build the model using the concepts of classical mechanics and molecular dynamics. The physical model is a description of the movement of a water molecule using Newton's second law in the field of forces caused by the intermolecular interaction of the molecule and the structure. Potential forces using the Lennard-Jones ability formalism, but the potential form has been modified to eliminate the features at zero. The system of equations of motion will be represented below:

$$\frac{du}{dt}=\sum_{j=1}^{N}a_j\frac{x-x_j}{\rho_j},\frac{dv}{dt}=\sum_{j=1}^{N}a_j\frac{y-y_j}{\rho_j},\frac{dw}{dt}=\sum_{j=1}^{N}a_j\frac{z-z_j}{\rho_j}.$$

Here $a_j=24\frac{\varepsilon}{\rho_j m}\left(\frac{\sigma}{\rho_j}\right)^6\left[2\left(\frac{\sigma}{\rho_j}\right)^6-1\right]$ is the acceleration, determined by the j^{th} atom of the nanostructure.

3. Modeling and Results

This problem was solved numerically by the Runge-Kutta method of the fourth-order of accuracy; the implementation of the numerical solution was carried out in the author's program written in the FORTRAN programming language.

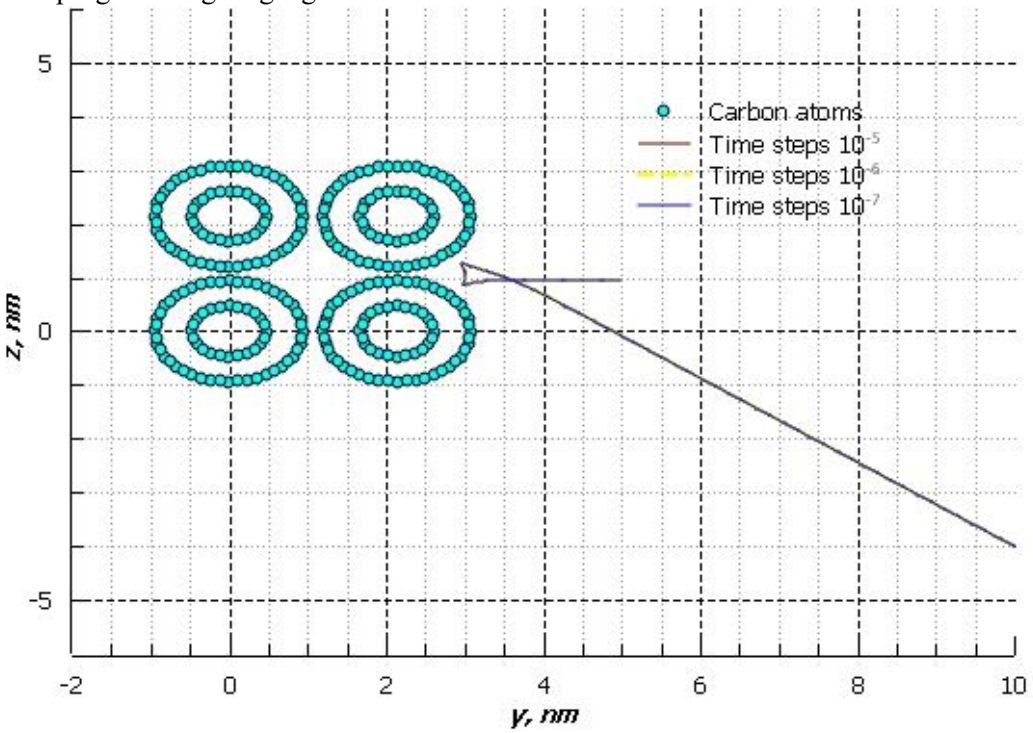

Figure 1. Grid convergence for numerical solution by the Runge-Kutta method.

To assess the convergence on the time grid, the simulation results were built on three grids – with a time step of 10^{-5}, with a step of 10^{-6} and a step of 10^{-7} seconds. The results of evaluating the grid convergence are shown in Figure 1. It can be seen that, in all three cases, the trajectory of the water molecule remains the same, which makes it possible to select a variant of the grid with a step of 10^{-6} seconds. After evaluating the convergence, the interaction effects of the selected structure of 4 double-walled open carbon nanotubes and a model water molecule were modeled. In Figure 2, you can see the areas in which the movement of low-energy water molecules is concentrated. By such molecules, we mean molecules with a speed of movement of 50 m/s or less, under normal conditions.

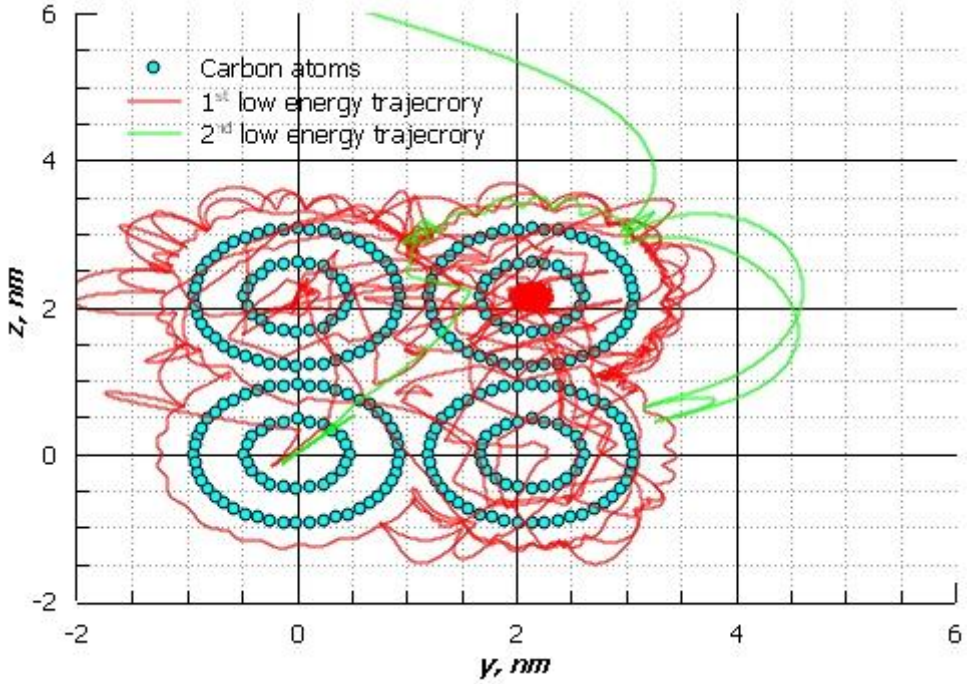

Figure 2. Low energy molecules motion.

Figures 3 and 4 show the results of modeling the interaction of water molecules with velocities of 450 m/s and a system of double-walled open nanotubes. Results are presented in XY and YZ planes.

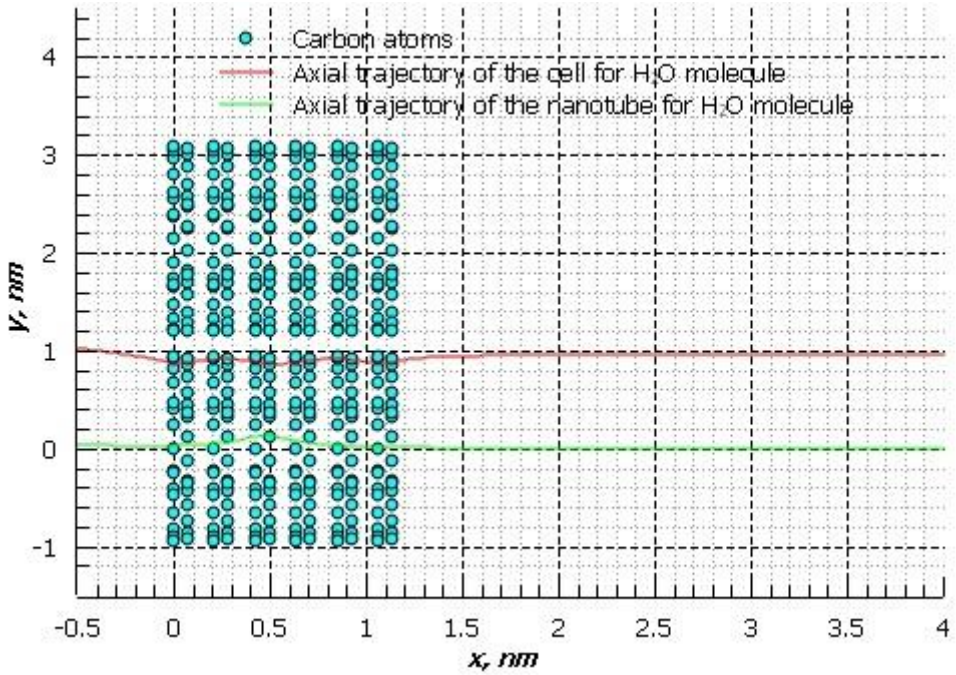

Figure 3. Trajectories of motion of water molecules in a system of 4 double-walled nanotubes at a speed of 450 m / s in the XY plane.

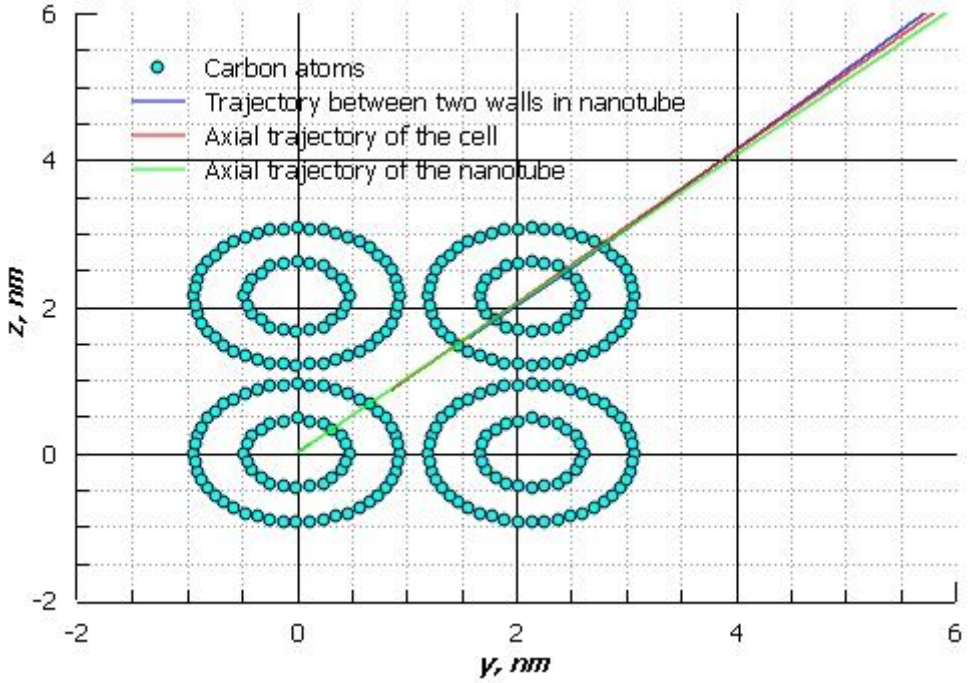

Figure 4. Trajectories of motion of water molecules in a system of 4 double-walled nanotubes at a speed of 450 m / s in the YZ plane.

In this configuration of a system of 4 nanotubes and the starting position of the test water molecule, the results show that water molecules with an average thermal (according to the Maxwell distribution) speed of motion for normal conditions quietly pass both the area inside an nanotube and the area in the center of the cell.

Figure 5 shows a variant of interaction in which the initial point of motion of the test molecule was displaced so that the structure was rotated at an angle of 90 degrees relative to the length of the nanotubes.

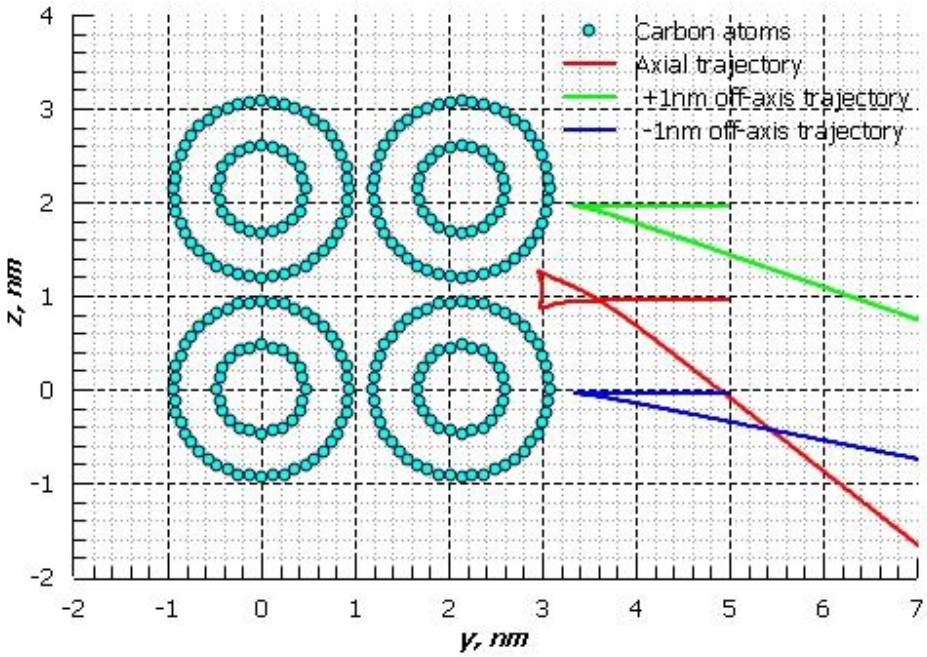

Figure 5. Three trajectories of motion of water molecules: axial, +1nm off-axis and -1nm off-axis variant

It can be seen that in the case of a rotation of the structure, it becomes impenetrable for molecules with speeds of motion of 450 m / s, regardless of whether the initial trajectory of motion lies on the axis of symmetry of the system or not.

4. Conclusion

The simulation results show that if molecules move along the coordinate corresponding to the length of the nanotubes, this cell allows water molecules to pass through. And in the case when the trajectory of motion lies perpendicular to the structure, this structure does not allow water molecules moving at an average thermal speed.

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