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Permeability of the Regular Structure from Spherical Nanoparticles

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Abstract. This paper presents a theoretical study on permeability of a regular structure composed of twenty spherical nanoparticles of the same size. The numerical solution is constructed using turn-based schemes of higher-order accuracy. The interaction between structure elements and moving molecules is determined by the V.Y. Rudyak and S.L. Krasnolutsky potential. It was found, that the tested model structure has the helium permeability to four times more than for methane.

INTRODUCTION

Compacted materials are used for the separation of gases and water treatment, as catalysts in chemical processes and are promising for use in modern high-tech processes. The variety of particles shapes and methods of its compounding make the investigation of materials permeability extremely difficult. Many aspects of the membranes work from compacted nanomaterials are similar to the work of biological membranes [1]. The movement of molecules and non-ionized atoms in the nanopores occurs in a gradient field of Van der Waals forces, unlike of the free neutral particles motion through the pores of large size. The differential permeability of a nanoporous structure with respect to individual components of a mixture forms the ground for development of passive gas separation technologies based on creation of membranes of the specific structure. When constructing the membrane it is important to pay attention to the original substance constituting the structure or the mixture of these substances. Experimental developments in this direction go on the adaptation way of a specific material to problems of gas separation. At the same time, computer simulation allows us to pose the question about the theoretical development of nanoporous membranes having specified properties. Since the penetration of substance through the nanoporous structure refers to the problems of classical mechanics, then to study the permeability of the ultrathin nanoporous layer, are applied the relevant methods and models of classical mechanics. Using the methods of molecular dynamics, are studied the penetration of the atoms and molecules of gas mixtures through the nanoporous structures. In this case, the problem is multiparameter. A large number of parameters of the initial position and the state of molecules, which penetrate through the structure is stochastically, result in necessary to accumulate of large amounts of data on performing molecular ballistic tests. To reduce the number of statistical data there is a method of the equivalent homogeneous layer, in which the scatter in the initial position is eliminated by movement symmetry, and the difference in rate of motion is taken into account by the Maxwell distribution.

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In this paper, using theoretical methods, we study the penetration of molecules through a regular structure from ideal spherical nanoparticles. The aim of the research is the study of differential permeability of the spherical nanoparticles layer with respect to the helium atoms and methane molecules.

MATHEMATICAL MODEL

The structure under consideration consists of spherical nanoparticles of the same size, whose centres lie in one plane. The "nanoparticle–molecule" interaction potential [2–8] was used for these particles:

$$ {}^{3}_{9}U(\rho_j) = {}_9U(\rho_j) - {}_3U(\rho_j), \tag{1} $$

where ρ_j is the distance from the centre of the jth particle of the porous structure to the test molecule (atom),

$$ {}_9U(\rho) = C_9\left\{\left[\frac{1}{(\rho-\rho_p)^9}-\frac{1}{(\rho+\rho_p)^9}\right]-\frac{9}{8\rho}\left[\frac{1}{(\rho-\rho_p)^8}-\frac{1}{(\rho+\rho_p)^8}\right]\right\}, \tag{2} $$

$$ {}_3U(\rho) = C_3\left\{\left[\frac{1}{(\rho-\rho_p)^3}-\frac{1}{(\rho+\rho_p)^3}\right]-\frac{3}{2\rho}\left[\frac{1}{(\rho-\rho_p)^2}-\frac{1}{(\rho+\rho_p)^2}\right]\right\}, \tag{3} $$

where ρ_p is the radius of the nanoparticle, $C_3 = 2\pi\varepsilon_{12}\sigma_{12}^6/(3V)$, $C_9 = 4\pi\varepsilon_{12}\sigma_{12}^{12}/(45V)$ and V is the volume per one carbon atom in the diamond structure.

The system of 20 diamond nanoparticles with radius r = 4 nm, each of which consists of 6.4×10^4 carbon atoms forming the four tunnels for the moving particle seen as a porous member. The particles are supposed to be stationary and the movement of the molecule (atom) occurs in the total Van der Waals field of twenty nanoparticles which follow the basic equation of Newton's dynamics. The force impact of each nanoparticle is determined by potential gradient (1)–(3). The equation of the moving particle dynamics is integrated using the fourth-order Runge-Kutta method. A similar approach is used in [9, 10] for the study of permeability of molecular structures and nanostructures.

CALCULATION RESULTS AND ANALYSIS

When constructing the layer, we used a tunnel packing of particles, with small gaps between particles in the column. The arrangement of particles in the layer is shown in Fig. 1.

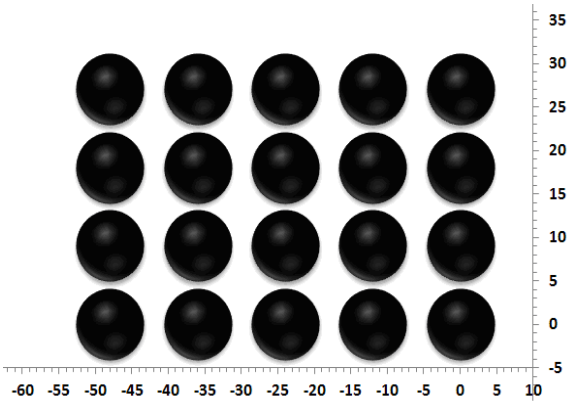


FIGURE 1. Structure of porous element

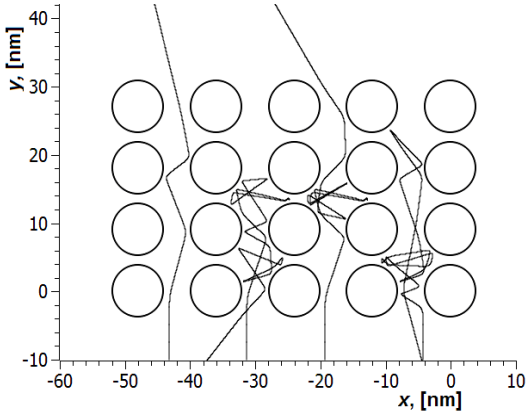
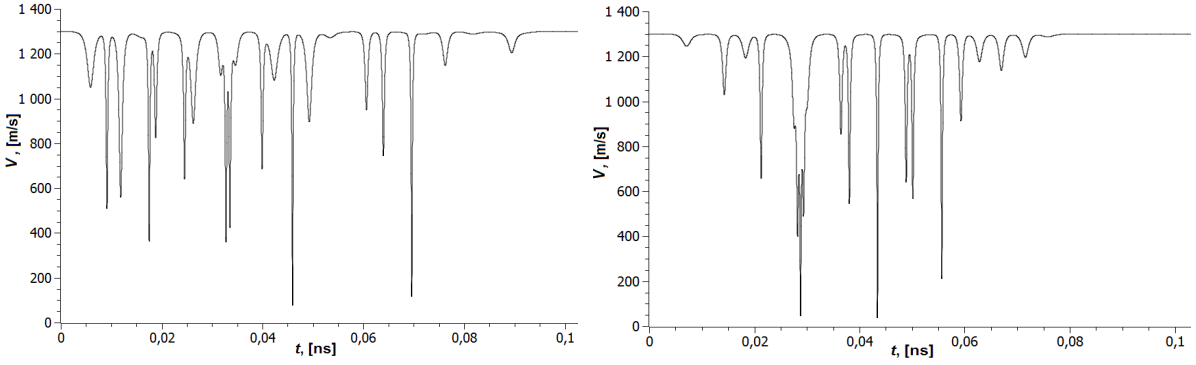


FIGURE 2. Trajectories of helium atoms



(a) (b)

FIGURE 3. (a) Velocity graph for He $x_0 = -4.2$ nm; (b) velocity graph for He $x_0 = -19.3$ nm

The origin of coordinates is placed at the centre of the bottom particle in the right column. Test molecules will move with a mean velocity of 1300 m/s in the positive direction of the *OY*-axis from the distance of 10 nm, and their initial coordinates along the *OX*-axis will be –4.2, –19.3, –31.3, –43.2 nm, respectively. The resulting motion trajectory for helium atoms is shown in Fig. 2.

Figure 3 shows the velocity curves of helium atoms motion, which were send up with the positions of –4.2 nm and –19.3 nm with respect to the *OX*-axis. As can be seen from the figures below, helium atoms actively use the porous space and approach close enough to the surface of the nanoparticles. This is due to the relatively lower energy of interaction in the system "helium–nanoparticle" compared with the case of "methane–nanoparticle". The calculations have shown that the helium permeability of the filter element is about 68%.

Figure 4 shows motion trajectories for test molecules of methane, started up from the positions of –4.9, –17.8, –30.8, –41.8 nm along the *OX*-axis at the speed of 650 m/s (the average thermal velocity of methane molecules movement under normal conditions). A higher energy of interaction between a methane molecule and a nanoparticle, which is realized in the form of repulsive forces, allows its movement only in the axial zone of the tunnel composed of spherical nanoparticles. The calculations showed that permeability of the considered layer fragment on methane is about 16%.

Figure 5 shows the velocity curves of methane molecule motion which were send up with position: –17.8 nm and –30.8 nm.

As can be seen from the graphs (see Fig. 5), in the case of the methane molecule motion, penetrating through the considered tunnel structure, it is possible to find the oscillation frequency of the velocity value, which is determined by the character of the nanoparticles packing in the tunnel.

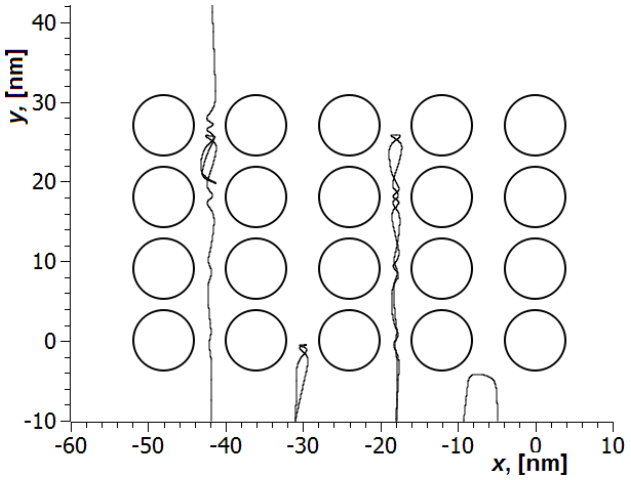


FIGURE 4. Trajectories of methane molecules

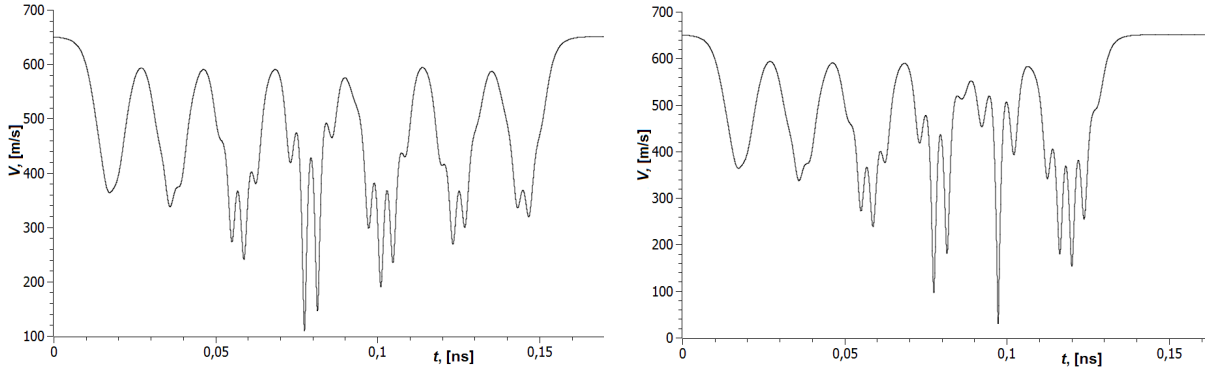


FIGURE 5. (a) Velocity graph for methane molecule $x_0 = -17.8$ nm; (b) velocity graph for methane molecule $x_0 = -30.8$ nm

CONCLUSION

The use of ideal spherical nanoparticles as components of the layer compaction, as well as the application of a tunnel packing these elements, allows us to construct a rigorous mathematical model of process of molecular penetration through the layer of the nanoporous structure. The interaction of nanoparticles with molecular components of the gas environment has a Van der Waals nature. In contrast to gravitational interactions, where the force has a definite direction, Van der Waals forces are both attractive and repulsive. Usually, attractive forces are long-range, while repulsive forces are of greater values and are manifested at short distances. As shown by the calculations, in the case of methane molecules movement, repulsive forces are more potent as compared with the case of helium atoms motion. Therefore, helium atoms move closer to the particles of the diamond structure. In addition, they show a better penetration through the compacted layer of nanoparticles. As a result, we get a helium permeability coefficient equal to 68% compared to 16% for methane.

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