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Simple Energy Barrier for Component Mixture of Natural Gases

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Abstract. This paper investigates the ability of a test molecule to overcome the energy barrier being in the gap between spherical nanoparticles. Three particles make a primitive structural element of composite porous material. The ability of molecules to converge with nanoparticles and then to move through more powerful repulsion field defines the filtration properties of porous materials. This paper presents the investigation of carbon nanoparticles and molecules of helium and methane bombarding them. Calculations proved that methane molecules can not get through three particles if the gap equals to 3.5 nm. For helium molecules this value makes 1.02 nm. These gaps remain the same when the size of nanoparticles increases. Therefore filters for helium separated from natural gas are to have nanopores within the range from 1.02 nm to 3.5 nm.

INTRODUCTION

Carbon filters can be obtained though pressing of char coal or powder of high-molecular carbon received in MW plazmatron. In any case nanoparticles of extremely small size will be the main filler for the realized filtering element. Naturally the pores of carbon filters will be of nanosize. The article [1] refers to the ability of functionalized graphene nanopores to effectively generate methane from air. In [2], using molecular-dynamic simulation, it is shown that porous graphene can efficiently separate gases according to their molecular sizes. The work [3] presents a study of gas molecules penetration through nanoporous graphene membranes using molecular-dynamic simulation. In [4], on the basis of the experiment [5] as the result of which micrometer-sized pores are created in graphene by means of UV-induced oxidative etching, the authors use membranes as molecular sieves. The aim of the study is to establish a quantitative relationship between the measured leakage rate and the simulated gas permeability. In the paper [6] activated graphene-based carbon showing excellent gas storage properties with an exceptionally high performance is considered. In [7] the experimental data on gas sorption which showed significant opportunities of hierarchical porous graphene-based carbons (HPGCs) for CO2 и H2 adsorption are given. In order to simulate the movement of molecules in porous space spherical nanoparticles have been converged to the distance of one or several nanometers and the ability of test molecules to get through this gap has been investigated. Should the velocity vector of the molecule be within the plane of centers of nanoparticles and molecule, then the task of the molecule convergence with the particle will be two-dimensional. Examples presented in this article belong to plane problem for the features of molecules' convergence with the particles to be investigated with more detail. However, the numerical model presented in this paper describes the three dimensional case. And it is true for any fairly numerous quantity of N_p particles. Moreover the particles can be polydisperse and be randomly dispersed in the space as it happens in real situations. The problem of the joint impact of a molecule within the structure on the movement of surrounding molecules has been already investigated in [8, 9].

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THE BARRIER ENERGY

This paper investigates the system of three carbon nanoparticles as a porous element generating the barrier for a moving molecule (see Fig. 1).

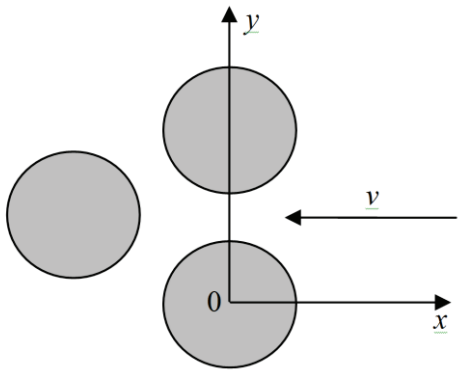

FIGURE 1. System of three spherical nanoparticles

The porous body is the assembly of spherical nanoparticles, which have the interaction potential between the nanoparticle and molecule [10]:

$$ {}_3^9\Phi\left(\rho_j\right) = {}^9\Phi\left(\rho_j\right) - {}_3\Phi\left(\rho_j\right). \tag{1} $$

Where ρ_j – distance from the j-th particle of porous structure to the test molecule, ρ_p – radius of nanoparticle,

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

$$ {}_3\Phi\left(\rho\right) = C_3\left\{\left[\frac{1}{\left(\rho-\rho_p\right)^3} - \frac{1}{\left(\rho+\rho_p\right)^3}\right] - \frac{3}{2\rho}\left[\frac{1}{\left(\rho-\rho_p\right)^2} - \frac{1}{\left(\rho+\rho_p\right)^2}\right]\right\}. \tag{3} $$

Equations (2) and (3) define the repulsion potential and attraction potential respectively.

Here $c_9 = \frac{4\pi\varepsilon_{12}\sigma_{12}^{12}}{45V}$, $c_3 = \frac{2\pi\varepsilon_{12}\sigma_{12}^{6}}{3V}$, V – volume of the solid carbon body, falling within one molecule. Potential (1) was obtained by integration of double Lennard-Jones potentials as per nanoparticle volume.

TABLE 1. The values of ε and σ constants of the Lennard-Jones potentials for some couples of substances

Interacting molecules		Relative depth of potential well	Radius of interaction potential
C – C	(1)	ε/k = 51.2 K	σ = 0.335 nm
He – He	(2)	ε/k = 10.2 K	σ = 0.228 nm
CH_4 – CH_4	(3)	ε/k = 148 K	σ = 0.228 nm

In Table 1 k is Botlzmann constant.

Should the investigated system consist of dissimilar molecules (atoms) then the following Lorentz-Berthelot mixing rule is true for ε and σ parameters.

$$\sigma_{12} = \frac{\sigma_{11} + \sigma_{22}}{2}, \quad \varepsilon_{12} = \left(\varepsilon_{11} \cdot \varepsilon_{22}\right)^{1/2}. \tag{4}$$

THE BASELINE DATA AND THE NUMERICAL METHOD

Here this impact is defined by three nanoparticles of radius ρ_p = 10 nm, each of them contains $1.5 \cdot 10^6$ carbon molecules.

The gap between double particles is defined by Δ. Let the point of reference be located in the center of one of the particles, as it is shown on Fig. 1, therefore $x_1^0 = 0$, $y_1^0 = 0$, $z_1^0 = 0$. And let 0*x* axis be directed perpendicular towards the line between particles centers. After this it is easy to define the coordinates of the center of the second nanoparticle: $x_2^0 = 0$, $y_2^0 = 2\rho_p + \Delta$, $z_2^0 = 0$. The coordinates of the center of the third nanoparticle: $x_3^0 = \left(\rho_p + \frac{\Delta}{2}\right)\sqrt{3}$, $y_3^0 = \rho_p + \frac{\Delta}{2}$, $z_3^0 = 0$. Dynamic equations for molecule movement are numerically integrated using step-by-step techniques exploiting the enumeration idea to enhance the accuracy of calculations. And for each step respective time and even in each point of enumeration within this step one should know the distance from the center of the test molecule to the center of each nanoparticle, which defined by the regular way:

$$\rho_j = \sqrt{\left(x - x_j^0\right)^2 + \left(y - y_j^0\right)^2 + \left(z - z_j^0\right)^2}, \tag{5}$$

where *x*, *y*, *z* – coordinates of the moving molecule; x_j^0, y_j^0, z_j^0 (j=1, 3) – coordinates of the center of carbon spheres (nanoparticles).

RESULTS OF THE CALCULATIONS

Figures 2-4 present the result of molecular ballistics calculations for methane and helium molecules, interacting with three nanoparticles. Calculations proved that Δ gap for methane molecules when molecules can not get through three particles makes 3.5 nm. For helium molecules this value makes 1.02 nm. These gaps remain the same when the size of nanoparticles increases. Therefore, filters for helium separated from natural gas are to have nano pores within the range from 1.02 nm to 3.5 nm.

Figure 2 shows a methane molecule going through the space between nanoparticles.

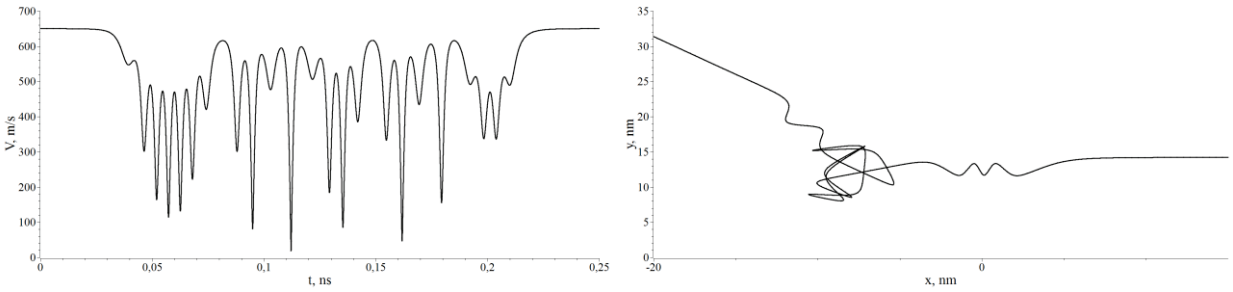

FIGURE 2. Velocity and trajectory of a methane molecule forwarded perpendicular the line between centers of nanoparticles from *y* position = 14.2 nm. The gap between nanoparticles makes 5 nm

Figure 3 shows a methane molecule being unable to get through the gap Δ and coming back almost along the same trajectory.

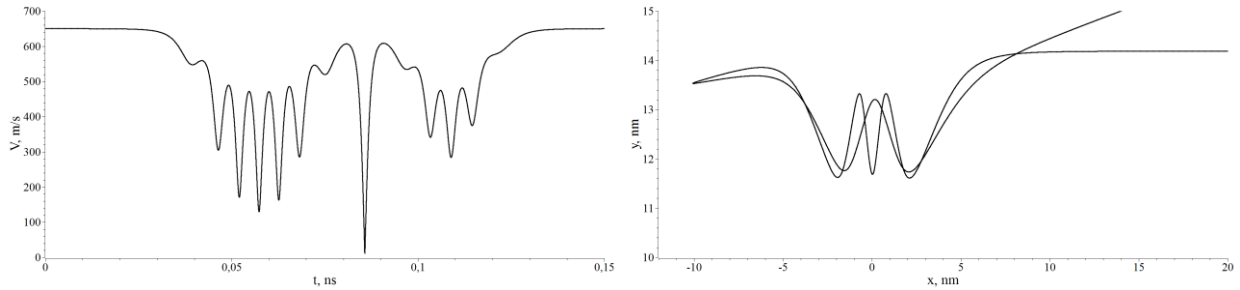

FIGURE 3. Velocity and trajectory of a methane molecule forwarded perpendicular the line between centers of nanoparticles from *y* position = 14.185 nm. The gap between nanoparticles makes 5 nm

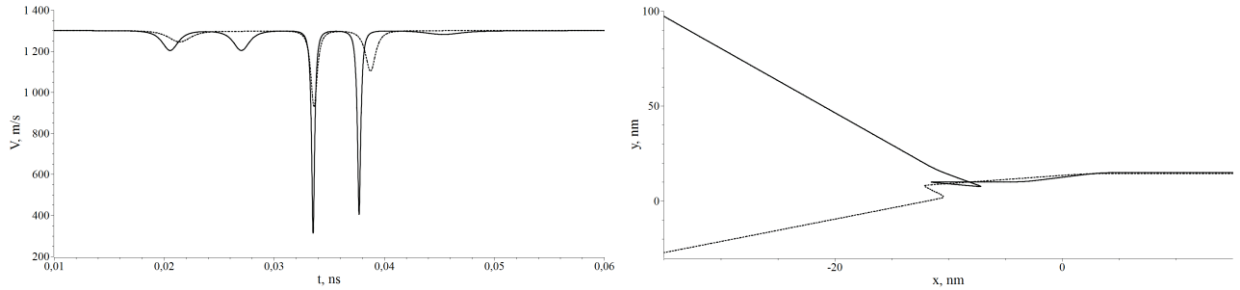

FIGURE 4. Velocity and trajectory of a helium molecule forwarded perpendicular the line between centers of nanoparticles from *y* position = 15 nm – the solid line, *y* position = 14.5 nm – the dashed line. The gap between nanoparticles makes 5 nm

Figure 4 shows helium molecules easily getting through the gap of the given size even in the case when the straight line continuing the initial trajectory of the molecule touches one of the nanoparticles.

Thus the size of pores of nano porous material was calculated for provision of free pass of helium molecules while bigger molecules of methane, nitrogen and other gases fail to get through.

CONCLUSION

The approach described in the paper allows studying the permeability of systems composed of homogeneous spherical nanoparticles. The particles may have different sizes and may be made of different materials. However, in the present paper, for reasons of simplicity, we studied a system of three identical carbon spheres. Calculations defined the size of the gap ensuring passage of helium atoms and preventing that of methane molecules.

REFERENCES

1. A.W. Hauser, P. Schwerdtfeger, Phys. Chem. Chem. Phys., **14**, 13292-13298 (2012).
2. H. Liu, Z. Chen, S. Dai, D. Jiang, J.Solid State Chem., **224**, 2-6 (2015).
3. C. Sun, M. S. H. Boutilier, H. Au, P. Poesio, B. Bai, R. Karnik, N.G. Hadjiconstantinou, Langmuir, **30**, 675–682 (2014).
4. S.P. Koenig, L. Wang, J. Pellegrino, J.S. Bunch, Nat. Nanotech., 7, 728–732 (2012).
5. H. Liu, S. Dai, D. Jiang, Solid. State Commun., **175–176**, 101-105 (2013).
6. A. Ganesan, M.M. Shaijumon, Micropor. Mesopor. Mat., **220**, 21-27 (2016).
7. K. Xia, X. Tian, S. Fei, K. You, Int. J. Hydrogen Energ., **39**, 11047-11054 (2014).
8. M.A. Bubenchikov, A.I. Potekaev and A.M. Bubenchikov, Appl. Mech. and Materials, **698**, 525–528 (2015).
9. M.A. Bubenchikov, A.I. Potekaev and A.M. Bubenchikov, Appl. Mech. and Materials, **698**, 627–630 (2015).
10. V. Y. Rudyak and S.L. Krasnolutskii, J. Aerosol Science **34** (1), 579–580 (2003).