Helium passage through homogeneous ultra-fine hydrocarbon layers

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Abstract. The present paper deals with the problem of helium atoms and methane molecules moving through a hydrocarbon layer of evenly distributed energy sources. A computational technique for integrating the Schrödinger equation based on formulation of two fundamental numerical solutions to the problem of waves passing through a barrier is suggested. A linear combination of these solutions defines the required wave function, while cross-linking with asymptotic boundary conditions allows determining the coefficients of transmission and particle reflection from the potential layer barrier.

1 Introduction

Fluid motions in nanochannels [1-3], diffusion of nanoparticles in gas [4-6], deformations of crystalline and diamond-like phases [7-12], as well as permeability of ultra-thin films [12-18], are the subject of modern nanomechanics. In this paper, we conduct theoretical research of permeability for nanoscale layers, which have a fibrous structure and are created on a polymer basis. Threads of such structures are fragments of polymer chains. The formula of a polymer molecule can be written as follows: $CH_4-(CH_2)_n, n=50\div100$.

Under these values of *n,* it can be approximately assumed that a polymer thread contains twice as many hydrogen atoms as compared to carbon atoms. With no further consideration of $C-H$ linkages and the character of spatial arrangements of threads, we will analyze helium atoms passing through a layer with evenly distributed carbon and hydrogen atoms.

2 Numerical model

To study the problem of particles with the mass *m* and the energy *E* passing through a potential barrier, one can solve the one-dimensional stationary Schrödinger equation.

The classical Schrödinger equation is [19-21]:

$$-\frac{\hbar^2}{2m}\Delta\psi+U\psi=i\hbar\frac{\partial\psi}{\partial t}. \quad (1)$$

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Here ψ is the wave function, $\hbar = h(2\pi)^{-1}$, h is the Planck's constant, U is the potential energy, i is the imaginary unit. Knowing the function ψ from solving equation (1), we can find the density of particle distribution: $\rho=|\psi|^2$. If the potential energy U does not depend on time, the solution of equation (1) is found in the form of: $\psi = \Psi\exp(-iEt/\hbar)$. Then, for the function Ψ we get the stationary Schrödinger equation:

$$\frac{\partial^2\Psi}{\partial z^2} + \frac{2m}{\hbar^2}\left(E - U(z)\right)\Psi = 0\,. \tag{2}$$

In problems related to molecular passage through nanoporous layers, the Schrödinger equation is used, ultimately, to find the density of moving particles experiencing elastic interactions with the porous frame. Therefore, instead of the Planck's constant, it is advisable to take a value which is proportional to the size of the layer $\hbar = l\sqrt{m\varepsilon}$, where l is the transverse dimension of the layer; ε is the depth of the potential well within the interaction between molecules of the layer structure and the filtered component, m is the mass of the particle passing through the layer. Thus, equation (2) can be written as follows:

$$\frac{\partial^2\Psi}{\partial z^2} + \left(K^2 - \tilde{U}(z)\right)\Psi = 0, \text{ here } K^2 = \frac{2m}{\hbar^2}E, \;\; \tilde{U}(z) = \frac{2m}{\hbar^2}U(z)\,. \tag{3}$$

If we assume, that $\tilde{U}(z) = 0$, the particular solutions of equation (3) will be the functions e^{iKz} and e^{-iKz}, the first private function being the wave which falls on the barrier and the second one being reflected. Their combination should provide the necessary physical result, including the case of the barrier being present, however at a distance. Therefore, as mathematical boundary conditions for the function Ψ(z) we can write:

$$\Psi(z) = e^{iKz} + be^{-iKz}, \;\; \Psi(z) = ae^{iKz}, \;\; |z| \approx l\,. \tag{4}$$

These conditions can be called asymptotic because they must be carried out away from the barrier. The first function in (4) determines the value of the density of probability that particles are located to the left of the barrier, and the second one – to the right. The coefficients a and b are complex values that define the character of the transmission and reflection in the z-axis direction. To find them, we approximate the second derivative in equation (3) by symmetric differences:

$$\frac{\Psi_{j-1} - 2\Psi_j + \Psi_{j+1}}{\Delta z^2} + K^2\Psi_j - \tilde{U}_j\Psi_j = 0, \;\; j = 1,\ldots,N-1. \tag{5}$$

By changing values of the index j, we obtain a system of algebraic equations with a tridiagonal matrix for finding the wave function at the nodes of the difference grid.

By removing any two rows of the main matrix of coefficients and applying the resulting function **null()** of the MATLAB package [22] to the matrix, we find two independent numerical solutions $\Psi_1(z)$ and $\Psi_2(z)$ to the system of equations (5). Therefore, the required wave function Ψ(z) is a superposition of these solutions: $\Psi(z) = C_1\Psi_1(z) + C_2\Psi_2(z), \;\; \Psi'(z) = C_1\Psi_1'(z) + C_2\Psi_2'(z).$ Equating the value of the function Ψ(z) and its derivative Ψ′(z) on the borders of the area under consideration and the asymptotic values (4), we obtain a system of four algebraic equations for finding the 4 un-

known coefficients C_1, C_2, a and b. In general, all the values resulting from this system are complex. Then, the physical transmission coefficient is $D=|a|^2$.

3 Calculation results

Figure 1 shows the dependence of a layer's permeability on the value of a helium particle's energy E/k for a fixed barrier height U/k=300 K, as well as the form of the respective barrier. Here k is the Boltzmann's constant. A rectangular barrier of about 10 nm in width was selected for the study. As can be seen from Fig. 1, the resulting solution is close to analytical.

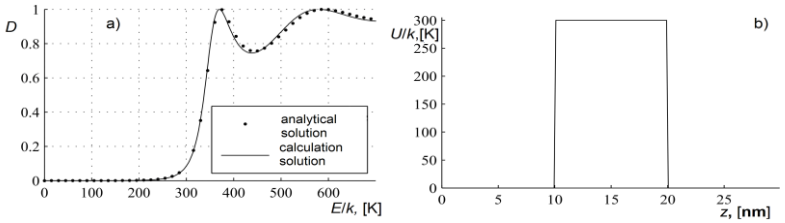

Fig. 1 Comparison of analytical [21] and calculated solutions for rectangular barrier (a) and barrier form (b).

As calculations show, the dependence of the layer's permeability on its thickness is negligible. Figure 2 presents a graph of this relation for a rectangular barrier with the height of U/k=200 K.

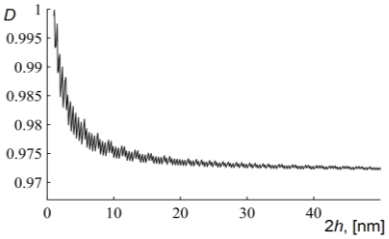

Fig. 2 Dependence of layer's permeability on its thickness at U/k=200 K for rectangular barrier.

Let us find the value of the barrier, which is defined by the resistance of carbon atoms $U_C(z)$. The potential energy, in case of uniform distribution of field sources in an infinite layer with the thickness of $2h$, is [23, 24]:

$$U_C(z) = 2\pi q \int_0^{\infty} r dr \int_{-h}^{h} \Pi_C\left(\sqrt{r^2+(z-c)^2}\right) dc \,. \qquad (7)$$

Here q is the number of carbon atoms per cubic nanometre of the layer material, $\Pi_C(\rho) = 4\varepsilon_C(\sigma_C/\rho)\,\mathrm{th}\left((\sigma_C/\rho)^{11} - (\sigma_C/\rho)^5\right)$ – is the modified potential of pair molecular interactions built on the basis of the classical LJ-potential. σ_C and ε_C are the parameters of this potential which are defined as the average values of the relevant parameters of monomolecular interactions for carbon, helium and methane. The depth of the potential well ε in the expression for $\hbar$ is defined as follows: $\varepsilon = 0.333\cdot\varepsilon_C + 0.666\cdot\varepsilon_H$, where ε_C and ε_H are geometric mean values of the corresponding values for monomolecular interactions. Let us consider a hydrocarbon layer with the thickness of 10 nm consisting of evenly distributed C and H atoms. The movement of helium atoms and methane molecules occurs in the positive direction of the Oz-axis perpendicular to the layer (Fig. 3). Then, for helium atoms and

methane molecules the interaction energy from the ultra-thin layer having a polymer base is equal to the sum of potentials $U(z) = U_C(z) + U_H(z)$. In Fig. 4 we show the dependence of a layer's permeability on density of packing with carbon atoms q. It can be seen that a layer becomes impermeable for methane molecules already at q=20 nm^{-3}, while helium atoms pass through it without any difficulty. The layer permeability of about 50%, as shown in Fig. 4, is achieved when q=60 nm^{-3}, which corresponds to compacted polyethylene. Layers with the thickness of 100 nm were investigated.

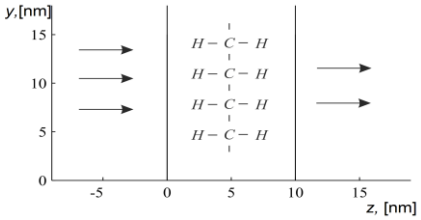

Fig. 3 Dependence of layer's permeability on its thickness at U/k=200 K.

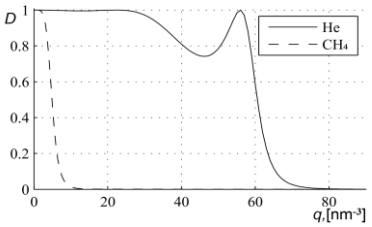

Fig. 4 Dependence of layer's permeability on density.

4 Summary

To sum up, if it is possible to create a plastic layer with the thickness of $50 \div 100$ nm, it may well be used as a passive filter for separation of methane-helium mixtures.

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