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Numerical Study of the Passage of Natural Gas Components through C₆₀ Fullerite in the Low-Temperature Phase

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Abstract: The movement of natural gas components through a crystalline fragment of C₆₀ fullerite in a simple cubic phase is numerically investigated. The methods of classical molecular physics, the Monte Carlo and Euler approaches, and a step-by-step numerical method of a high order of accuracy are used to study the effects arising from the passage of the particles through the C₆₀ fullerite. The influence of the characteristics of incoming particles on the permeability of fullerite was analyzed using the results of the performed calculations. The application of the fast integral approach based on the smoothed spherical potential is discussed and compared with the Monte Carlo method.

Keywords: rotating fullerene; natural gas; permeability; fullerite crystal; low temperature phase; Monte Carlo method



Citation: Borodin, V.I.; Bubenchikov, A.M.; Bubenchikov, M.A.; Ovchinnikov, V.A.; Chelnokova, A.S. Numerical Study of the Passage of Natural Gas Components through C₆₀ Fullerite in the Low-Temperature Phase. *Crystals* **2022**, *12*, 1653. <https://doi.org/10.3390/cryst12111653>

Academic Editor: Philip Lightfoot

Received: 30 October 2022

Accepted: 15 November 2022

Published: 17 November 2022

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1. Introduction

Since their discovery in 1985, fullerenes have been of great interest to researchers [1]. This is due to a wide range of unique properties (increased strength, hardness, high tribological properties, high fire and chemical resistance, durability, thermal stability, etc.) of fullerene-containing materials [2–11]. These properties make fullerenes interesting as a building block for creating structural materials with new properties [12–14]. Fullerenes are closed molecules consisting of 20 or more atoms located at the vertices of a polyhedron [15]. The most common fullerene is C₆₀, a truncated icosahedron built from 20 hexagons and 12 pentagons. At room temperature, these fullerenes form into a fullerite crystal, with a face-centered cubic (fcc) structure with a lattice parameter of 14.154 Å [16]. At temperatures below 260 K, the fullerite crystal transforms into a simple cubic (sc) phase with a lattice parameter of 14.111 Å [16]. In the range from 252–257 K, the fullerite structure is in a transitional phase, combining the fcc and sc phases [16]. In the fcc and sc phases, fullerenes perform rotational motions with frequency in the gigahertz range [17,18]. In the fcc phase, the centers of fullerene molecules are at a distance of 1.002 nm from each other [16]. This significantly complicates the movement of particles through the existing voids between fullerenes compared to the sc phase. Thus, a change in temperature makes it possible to radically change the permeability of C₆₀ fullerite for incoming particles.

Natural gas mainly (70–98%) consists of methane (CH₄) and contains other heavy hydrocarbon gases (ethane, propane, butane, etc.) to a lesser extent. In natural gas, there is a fairly high content of rare inert monatomic gases such as helium, xenon, and others (many orders of magnitude higher than Earth's atmosphere). Helium (He) is the lightest noble gas and has a number of unique properties, such as chemical and radiological inertness, low density, high heat capacity and thermal conductivity, the lowest boiling point, etc. Xenon (Xe) is the heaviest noble gas and is used in spacecraft ion thrusters and as an effective and

safe general anesthetic agent, but its high cost limits its use. In this regard, the possibility of separating these components from natural gas is of interest.

In this work, we numerically simulate the motion of incoming particles (components of natural gas) in a crystalline fragment of C_{60} fullerite in the sc phase. The numerical study is carried out using classical molecular dynamics methods [19–24] and the Monte Carlo method [25–27]. The Monte Carlo approach is a way to solve a problem numerically based on random statistical trials. This method is based on using a probabilistic model of the interaction of nano-objects and allows us to find effects that are difficult to identify using measurements. The additive and integral approaches are used to model incoming particles' interaction and fullerenes [19,23]. A comparative study of the influence of the characteristics of incident particles (helium, methane, ethane, xenon) and the parameters of the pair interaction potential on the permeability of fullerite is carried out.

2. Physical Statement of the Problem

The study of xenon atom motion in C_{60} fullerite is of the greatest interest since it has the lowest thermal velocity, which limits the probability of xenon atoms passing through fullerite compared to other natural gas components. The C_{60} fullerenes, depending on the temperature, can form sc and fcc structures. The fcc structures have the highest packing density of identical non-overlapping spheres in three-dimensional space. Therefore, the space unoccupied by C_{60} fullerenes will be minimal in the fcc lattice. The distance between the centers of the nearest fullerenes in the fcc fullerite (which is formed at temperatures above 260 K) is 1.002 nm, and this distance in the sc lattice (below 260 K) is 1.4111 nm. At the same time, the fcc lattice does not have straight tunnels, in contrast to the sc lattice shown in Figure 1. Taking into account the radius of C_{60} fullerene ($a = 354$ pm), as well as the van der Waals radii of the xenon atom (216 pm) and the carbon atom (170 pm), the passage of xenon atoms through the fcc structure of C_{60} fullerite has a very low probability, in contrast to fullerite in the sc phase.

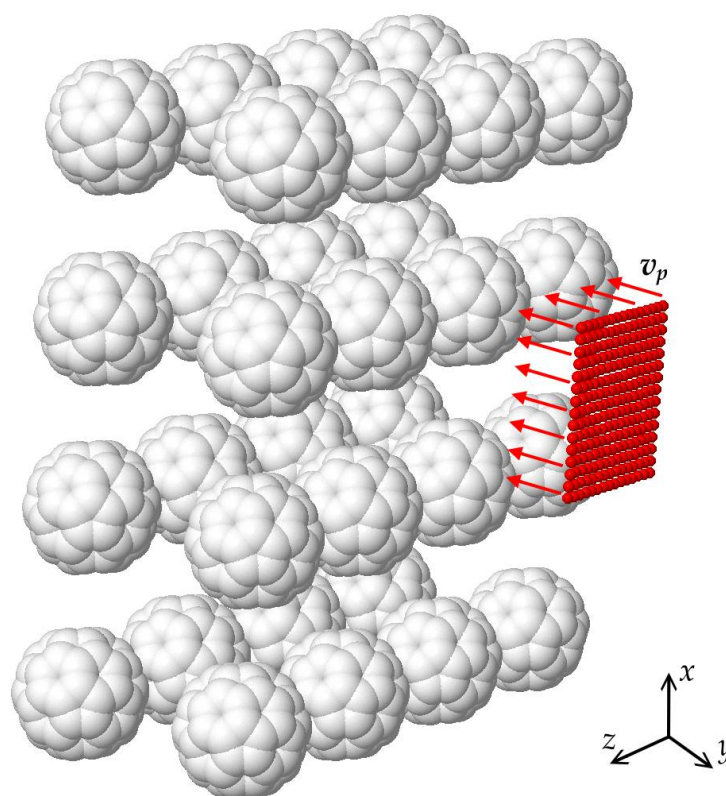


Figure 1. Scheme of the interaction of incoming particles (red color) with a group of rotating C_{60} molecules (grey color).

We consider a crystalline fragment of C_{60} fullerite, consisting of 32 fullerene molecules, as shown in Figure 1. The C_{60} molecules are located at the nodes of an sc lattice and interact with the incoming components of natural gas (helium, methane, ethane, xenon) (see Figure 1).

Each fullerene molecule is initially considered as an icosahedral structure consisting of sixty carbon atoms (additive approach) or as a particle with a spherical interaction potential (integral approach) [23]. The rotational motion of a fullerene is determined by the nature of the interaction of its carbon atoms with the surrounding fullerenes and is described using the Euler approach presented in papers [19,21,23]. The centers of mass of the nearest rotating C_{60} molecules are at a distance of $a_0 = 1.4111$ nm [16], corresponding to an sc phase of fullerite. The conditional beam of independent particles moves in the direction of the fullerite fragment. The interaction of carbon atoms of individual fullerenes with natural gas components is described based on the additive potential 12-6 repulsion attraction or the interaction potential in the surface-integral form.

3. Mathematical Statement of the Problem

Let us introduce some absolute (fixed) system of Cartesian coordinates (xyz), whose origin will be placed at the center of a series of fullerenes closest to the incoming particles. Cartesian coordinate systems ($\xi_i\eta_i\zeta_i$, $i = \overline{1,32}$) are rigidly connected with rotating fullerenes and their centers of mass.

If fullerenes are considered as structures consisting of 60 carbon atoms, the interaction of a particular carbon atom with an incoming particle or atoms of neighboring fullerenes is determined using the potential: 12-6 repulsion–attraction (additive approach)

$$U_{LJ}(\rho_{pik}) = 4\varepsilon \left[\left(\frac{\sigma}{\rho_{pik}} \right)^{12} - \left(\frac{\sigma}{\rho_{pik}} \right)^6 \right], \quad (1)$$

where ρ_{pik} is the distance between the p th incoming particle and the k th atom of the i th fullerene, $i = \overline{1,S}$, $p = \overline{1,N}$, $k = \overline{1,K}$; $S = 32$ is the number of fullerenes of the crystalline fragment of fullerite; $K = 60$ is the number of carbon atoms in C_{60} fullerene; $N = 225$ is the number of incident particles of the conditional beam; ε , σ are the Lennard-Jones parameters [28].

If fullerenes are considered as spherical particles of radius a (integral approach), then the interaction potential between the i th fullerene and the p th incoming particle is determined by the following formula [19,23,29–31]

$$U_{sph}(\rho_{pi}) = \frac{4\varepsilon a\pi}{\rho_{pi}A_1} \left[\frac{\sigma^{12}}{5} \left((\rho_{pi} - a)^{-10} - (\rho_{pi} + a)^{-10} \right) - \frac{\sigma^6}{2} \left((\rho_{pi} - a)^{-4} - (\rho_{pi} + a)^{-4} \right) \right], \quad (2)$$

where $A_1 = A/K$, where $A = 4\pi a^2$ is the area of a sphere of radius a ; ρ_{pi} is the distance between the center of the i th fullerene and the p th incoming particle. Potential (2) is based on the Lennard-Jones potential (1) uniformly distributed over the area of the sphere.

The rotational motion of the i th fullerene molecule around its center of mass is described using the Euler dynamic equations in the following form [21,23]

$$J_1 \frac{dp_i}{dt} + (J_3 - J_2)q_i r_i = M_{\xi i}, \quad (3)$$

$$J_2 \frac{dq_i}{dt} + (J_1 - J_3)r_i p_i = M_{\eta i}, \quad (4)$$

$$J_3 \frac{dr_i}{dt} + (J_2 - J_1)p_i q_i = M_{\zeta i}. \quad (5)$$

here p_i , q_i , r_i are the components of the angular velocity relative to the principal axes; J_1 , J_2 , J_3 are the principal moments of inertia of the C_{60} molecule for its center of mass; $M_{\xi i}$, $M_{\eta i}$,

M_{ξ_i} are the projections of the moments of external forces on the ξ -, η - and ζ -axes associated with the i th fullerene and determined according to the paper [23].

The components of the angular velocity of the i th fullerene molecule, written in terms of the Euler angles φ , ψ , θ , have the following form:

$$p_i = \dot{\psi}_i \sin \theta_i \sin \phi_i + \dot{\theta}_i \cos \phi_i, \quad (6)$$

$$q_i = \dot{\psi}_i \sin \theta_i \cos \phi_i - \dot{\theta}_i \sin \phi_i, \quad (7)$$

$$r_i = \dot{\psi}_i \cos \phi_i + \dot{\phi}_i, \quad (8)$$

where the dot above the function name indicate a derivative taken with respect to time.

The motion of the center of mass of the p th incoming particle when using the additive approach is determined by the law

$$m_p \frac{d\mathbf{v}_p}{dt} = \sum_{i=1}^S \sum_{k=1}^K \text{grad} U_{LJ}(\rho_{pik}), \quad \mathbf{v}_p = \frac{d\boldsymbol{\rho}_p}{dt}, \quad (9)$$

and for integral approach

$$m_p \frac{d\mathbf{v}_p}{dt} = \sum_{i=1}^S \text{grad} U_{sph}(\rho_{pi}), \quad \mathbf{v}_p = \frac{d\boldsymbol{\rho}_p}{dt}. \quad (10)$$

here m_p is the mass of the p th incoming particle; $\boldsymbol{\rho}_p$ is the position vector of the p th incoming particle. Note that since Equation (10) has one summation, the numerical solution of the problem will be much faster than Equation (9).

The initial conditions for solving the system of differential Equations (3)–(10) are given in the following form

$$t = 0 : \psi_i = \psi_i^0, \theta_i = \theta_i^0, \phi_i = \phi_i^0; p_i = p_i^0, q_i = q_i^0, r_i = r_i^0, \quad (11)$$

$$\mathbf{v}_p = \mathbf{v}_p^0, \quad \boldsymbol{\rho}_p = \boldsymbol{\rho}_p^0, \quad (12)$$

The system of differential Equations (3)–(10) with initial conditions (11), (12) is solved using a high-order step-by-step time integration scheme [32,33], which makes it possible to determine the spatial trajectories of the incoming particle and each atom of the central fullerene.

4. Results and Discussion

Consider a fragment of fullerite consisting of $4 \times 4 \times 2 = 32$ fullerene molecules (see Figure 1), the initial orientation of which is set randomly (Monte Carlo method). We apply the Monte Carlo method only with an additive approach. The first row of 16 fullerenes is in position $y = 0.0$ nm; the second row is in position $y = -a_0 = -1.4111$ nm, where a_0 is the crystal lattice parameter. Incoming particles in the amount of $15 \times 15 = 225$ at the initial moment of time are in positions corresponding to $y = 4.0$ nm and have an initial velocity directed along the y -axis (Figure 1). In this paper, the initial velocity of the incoming particles is assumed to be equal to the value of the thermal velocity for the temperature $T = 260$ K, determined by the formula

$$v_p^0 = \sqrt{\frac{3k_B T}{m_p}}, \quad (13)$$

where k_B is the Boltzmann constant.

Figure 2 shows the mutual arrangement of fullerenes and a conditional beam of incident particles in the xy -plane. This number of particles makes it possible to estimate the fraction of transmitted particles with a step of $\sim 0.44\%$. The conditional particle beam is

located opposite four central fullerenes. This arrangement of incoming particles relative to fullerenes makes it possible to extend the obtained results to large scales. However, it should be taken into account that filling with incident particles with a similar step, for example, the space between the centers of $4 \times 4 = 16$ fullerenes, will require 43×43 particles, and not 9×225 . This suggests that among the 225 selected particles, there is a small fraction of particles (~10%) that belong to neighboring regions. Therefore, it is necessary to apply appropriate coefficients when extending the results of calculations to large scales.

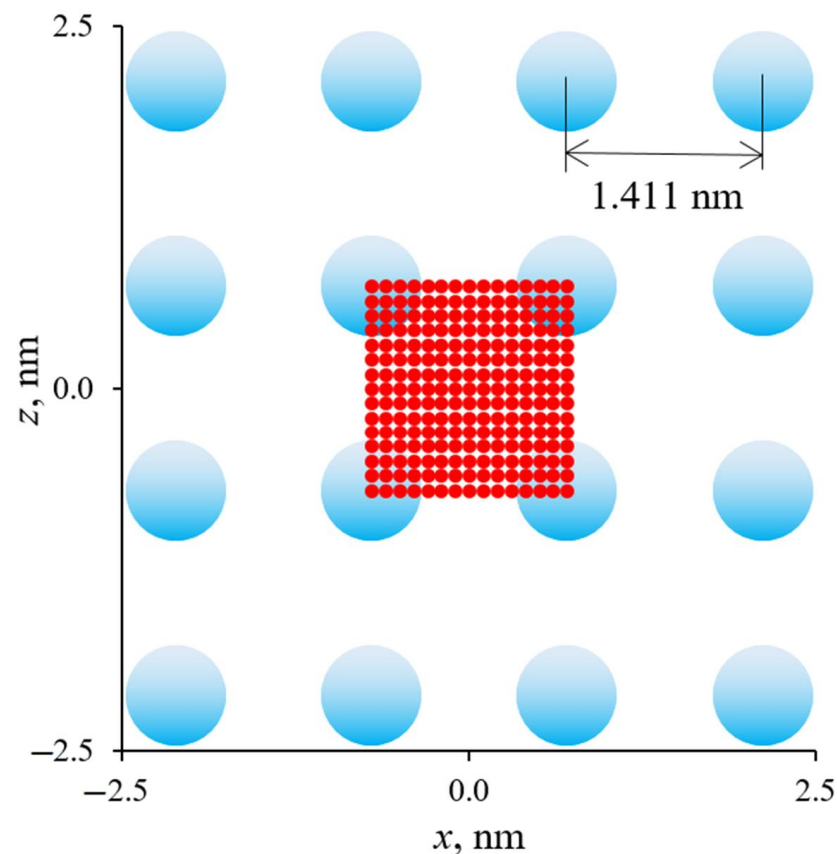


Figure 2. The initial position of the conditional beam of incoming particles (red color) relative to the considered C_{60} fullerite (blue color) in projection on the xz -plane.

Figure 3 shows a comparison of the additive ($U_{\Sigma} \times \varepsilon^{-1}$) and integral ($U_{sph} \times \varepsilon^{-1}$) dimensionless functions of the potential on the distance ρ_{pi} between the centers of the incoming particle and the center of the fullerene. The integral function of the potential U_{sph} is determined by Formula (2). The additive function of the Lennard-Jones potential U_{Σ} is determined by the following formula

$$U_{\Sigma}(\rho_{pi}) = \sum_{k=1}^K U_{LJ}(\rho_{pik}), \quad (14)$$

The potential integral function approximates the Lennard-Jones additive function well with an error of less than 1% at a distance between the particle and fullerene centers $\rho_{pi} > 0.705$ nm. The error increases significantly as the incoming particle and fullerene approach each other. The depth of the potential well differs by 4.5%.

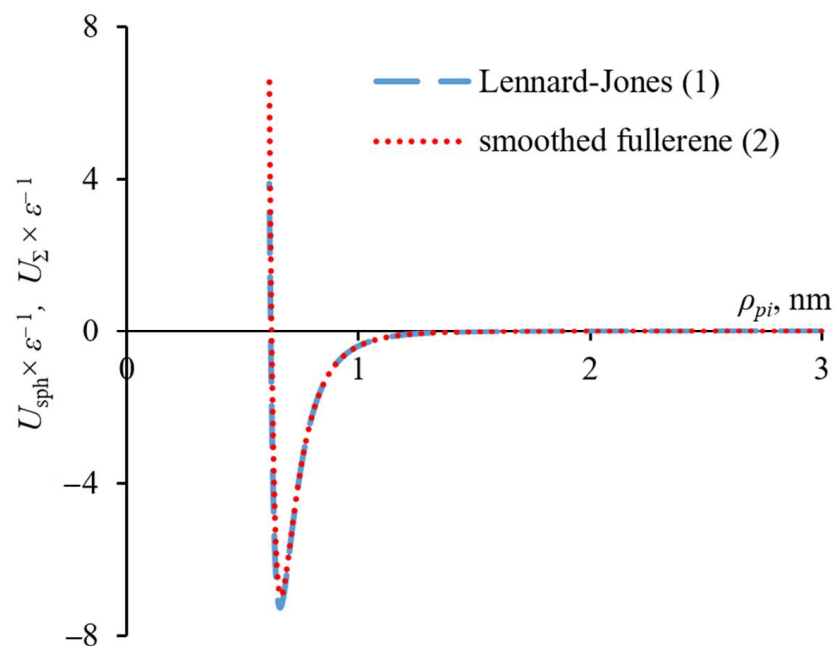


Figure 3. Dependences of relative potential energies for interaction between the C_{60} fullerene and single helium atom on the distance between the centers of mass.

4.1. Thermal Motion of Natural Gas Components

Let us consider when the initial velocities of incident particles (helium, methane, ethane, xenon) are equal to their thermal velocity. Using this assumption, we simulate the motion of particles near the surface of fullerite at a temperature of 260 K due to chaotic thermal motion (“thermal mode”). We will calculate up to the time $t_z = 0.02$ ns. Figure 4 shows that the sample size (200) is sufficient to determine the average value of the fraction of passing helium, methane, ethane, and xenon atoms.

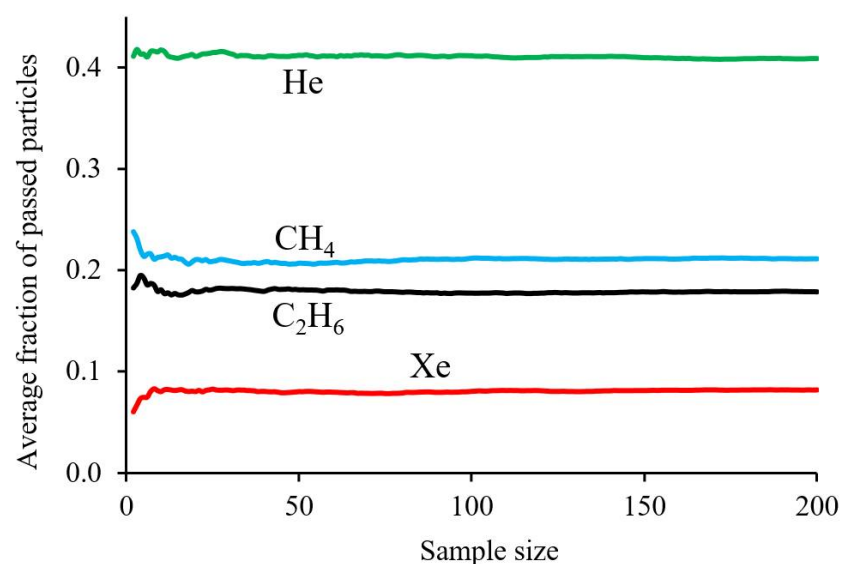


Figure 4. Dependence of the average value of the fraction of passed particles on the sample size.

Figure 5 shows the probability density function of the fraction of helium atoms that have passed through the fullerite fragment. The circles correspond to the calculations

performed using the additive approach. The solid line shows the normal distribution obtained from the formula

$$\Phi(f) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{f-\mu}{\sigma}\right)^2\right), \quad (15)$$

where the parameter μ is the mathematical expectation (mean), and σ is the standard deviation of the normal distribution.

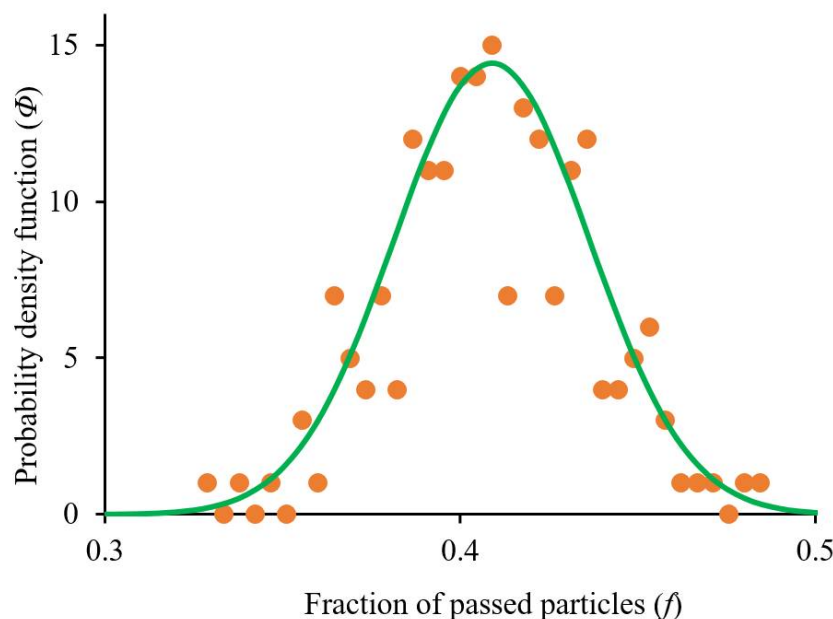


Figure 5. Probability density function for helium atoms. Orange color corresponds to calculations (additive approach). Green color corresponds to the normal distribution (15).

For the results presented in Figure 5, the mathematical expectation $\mu = 0.4089$, and the standard deviation $\sigma = 0.0276$. As can be seen from Figure 5, the distribution of random variables obeys the normal distribution law.

The normal distributions (Figure 6) are similarly constructed for the other particles under consideration. Table 1 shows the interaction potential parameters ε and σ , obtained using the Lorentz-Berthelot mixing rules and used in Formulas (2) and (3). As can be seen from Figure 6, the larger the particle mass (Table 1), the less likely they are to pass through the fullerite crystalline fragment. Note that the time $t_z = 0.02$ ns is chosen so that all helium atoms leave the region occupied by fullerenes. However, according to (13), the initial velocity of other particles is significantly less than that of helium, so not all particles (methane, ethane, xenon) have time to leave the region occupied by fullerenes in the time interval $[0, t_z]$. This shows that helium has a significantly greater ability to overcome the crystalline fragment, unlike other particles. Note that xenon and helium atoms have the minimum and maximum thermal motion velocities, respectively. At the same time, the minimum and maximum fullerite permeability is observed for xenon and helium atoms, respectively. This suggests that the permeability of fullerite directly depends on the initial velocity of the particles (helium, methane, ethane, xenon) in thermal motion.

The dashed lines show the results of calculations obtained using the integral approach. As we can see, the integral approach to some extent, qualitatively reflects the relative pattern of permeability for different particles.

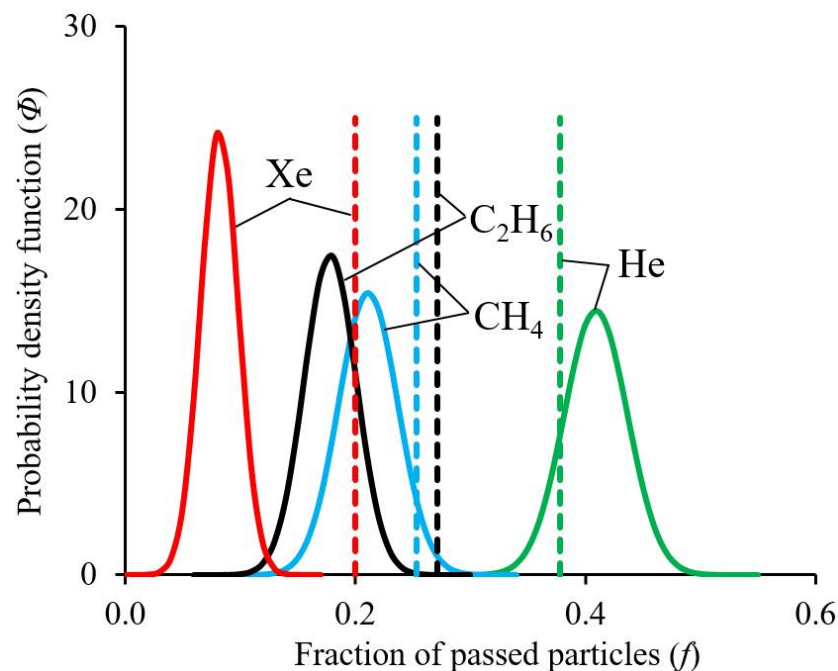


Figure 6. Probability density functions for particles moving with thermal velocity (13) corresponding to a temperature of 260 K.

Table 1. Lennard-Jones parameters for the mixture (particle-carbon) and particle mass.

Parameters	Mixture			
	He-C	CH ₄ -C	C ₂ H ₆ -C	Xe-C
ϵ/k_b	22.875	87.05	109.15	108.28
σ , nm	0.3102	0.3727	0.4024	0.3854
m_p , Da	4	16	30	131

4.2. Velocity Effect on the Permeability of Fullerite

In addition, we will analyze the permeability of fullerite under conditions of equal initial velocity, which is taken to be the thermal velocity of helium (see Figure 7). This assumption allows us to model the convective mode of movement of incoming particles near the fullerite surface. The average values of the fraction of passing atoms, determined using models using the additive and integral function of the potential, are presented in Table 1. As can be seen from Table 1, the best agreement between the methods was obtained for xenon (relative error $\delta = 2.7\%$) and the worst for methane and ethane ($\delta = 15.6\text{--}16.8\%$). At the same time, both methods show that helium and xenon give the largest number of passing particles, while methane and ethane give the smallest number. At the same time, it can be seen from Figure 7 and Table 2 that the probabilities of passage through fullerite, determined by the additive method, for helium and xenon turned out to be almost the same. However, calculations for helium showed large deviations from the average permeability compared to xenon. With the exception of xenon, a qualitative picture of the relative position of the distributions in Figures 6 and 7 has been preserved.

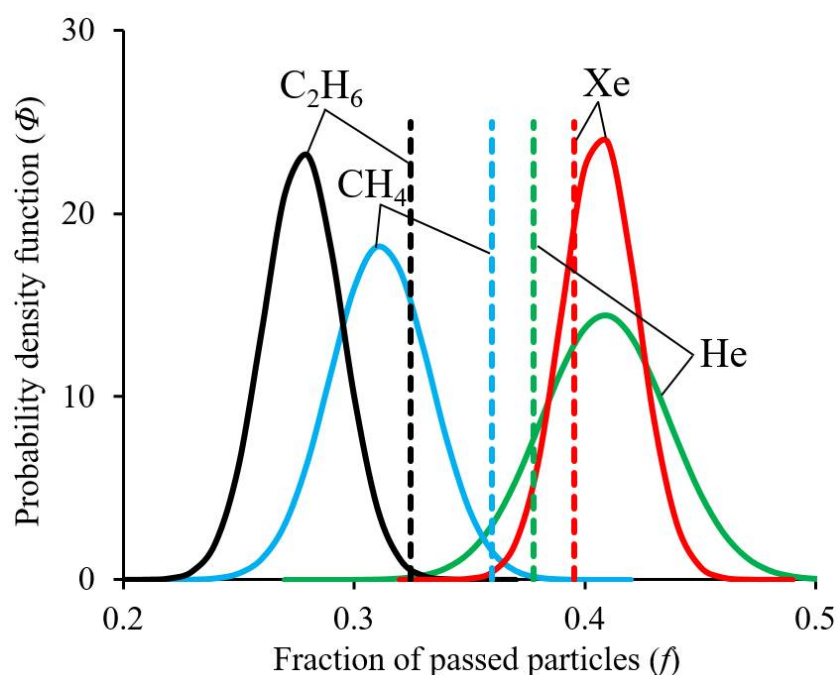


Figure 7. Probability density functions for particles moving with the same initial velocity v_p^0 .

Table 2. Average values of the fraction of passed particles (f) calculated by the integral and additive methods.

Mean Values	Particles			
	He	CH ₄	C ₂ H ₆	Xe
f_{sph}	0.3778	0.36	0.3244	0.3956
f_{Σ}	0.4089	0.3115	0.2778	0.4067
δ	7.6%	15.6%	16.8%	2.7%

As can be seen from Table 1, the xenon atom, according to the Lennard-Jones parameters ϵ and σ , is between CH₄ and C₂H₆, i.e., not much different from them. At the same time, the fraction of passed xenon atoms is much larger than that of methane and ethane. This is due to the significantly larger mass of the xenon atom compared to methane and ethane.

The results of the calculations presented in Figures 6 and 7 show that with the convective movement of a natural gas substance near the fullerite, it is possible to significantly increase the probability of the passage of xenon atoms through the fullerite in the PS phase. The average probability of passage of xenon atoms increases from 8.22% (thermal mode) to 40.67% (convective mode). At the same time, changing the regime also increases the permeability of fullerite for methane (from 21.1% to 31.1%) and ethane (from 17.84% to 27.78%), but to a lesser extent. To assess the change in the concentration of a substance, one can analyze the selective release factor, which is defined as the ratio of the fractions of particles that have passed through fullerite. Based on the calculations obtained, the average selective xenon release factor with respect to methane (the main component of natural gas) in the thermal mode of particle motion near fullerite is 0.39. Therefore, fullerite will represent a barrier for xenon atoms and lead to a decrease in the concentration of xenon atoms. At the same time, this factor in the convective mode of movement of particles near fullerite is 1.31, which causes an increase in the concentration of xenon atoms after passing through the fullerite. This procedure must be carried out repeatedly to significantly increase the concentration of xenon atoms. As a result, this effect makes it possible to separate helium and xenon from natural gas using a fullerite crystal in the sc phase.

5. Conclusions

Classical molecular dynamics simulations were carried out to investigate the passage of natural gas components through the C₆₀ fullerite in a simple cubic phase using the Monte Carlo method. The calculation results showed that natural gas components have different abilities to pass through fullerite. The analysis using the Monte Carlo method showed that helium atoms have the highest probability of passing through the fullerite barrier with a thermal velocity, and xenon atoms have the smallest one. However, at the same initial speed of movement, xenon atoms achieve a similar permeability of helium atoms. In addition, helium atoms have the smallest deviation from the average value of the fraction of the passed atoms. An increase in the initial velocity made it possible to significantly increase the permeability of fullerite for xenon. This effect can be used to increase the concentration of noble gases. It is shown that the method based on the integral potential makes it possible to quickly obtain a qualitatively correct overall picture of presented effects and the distribution of the average values of fullerite permeability for incoming particles.

Author Contributions: Conceptualization, A.M.B.; data curation, V.I.B.; formal analysis, M.A.B.; funding acquisition, M.A.B.; investigation, M.A.B. and V.A.O.; methodology, A.M.B.; project administration, M.A.B.; software, V.A.O. and A.S.C.; supervision, V.I.B.; visualization, V.A.O.; writing—original draft, V.A.O.; writing—review and editing, V.A.O. and A.M.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Russian Federation President Grant, grant number MD-4273.2022.1.1.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

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