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FEATURES OF NEAR-SURFACE LAYER AT MONOMOLECULAR ISOTROPIC ADSORPTION: NONEQUILIBRIUM MOLECULAR DYNAMICS SIMULATION

Processes running in the gas phase near a solid surface have been analyzed in the framework of nonequilibrium dynamics and by simulating the irreversible monomolecular isotropic adsorption. Their influence on the adsorption kinetics is analyzed. A complicated spatial organization of particles in the near-surface layer, where the particle concentration and energy vary in time, is revealed,. It is found that the local particle concentration can either decrease (down to about 60% of the initial value) or increase with the distance from the surface, depending on the system concerned. The obtained results can be used to analyze and to predict processes running in the near-surface layer of elements for the sensor and electronic engineering, gas dynamics, and other areas, where the ballistic character and the kinematics of motion dominate and govern the functional properties of the system.

Keywords: molecular dynamics, isotropic adsorption, adsorption kinetics, near-surface concentration.

1. Introduction

Nowadays, the concept of molecular dynamics is one of the most efficient ways for studying and predicting the physico-chemical characteristics of statistical ensembles composed of particles of different origin [1]. These are the structure of organic molecules and their complexes, the conformation of protein ensembles, the distribution of particles in nanopores and capillaries, and so forth [2]. The majority of the applied approaches were developed to analyze the equilibrium states of multiparticle systems, in which the interaction between individual particles is governed, in many cases, by statistical regularities [3].

At the same time, the little attention was paid to the kinematics of particle ensembles, in which particle trajectories have a stochastic character. However, these are the processes of microscopic motion that play the role of driving forces for the gradients of those physical quantities, which are responsible for the macroscopical changes in parameters of a system. Really, these are the transport processes that determine the efficiency of technological procedures (thermal sputtering [4], laser ablation [5], plasma stability [6], *etc.*) and the functioning of technical devices (radio-electronic tubes [7], particle beams in accelerators [8], sensors [9], and so on) in many cases.

A distinctive feature of the processes mentioned above is a ballistic character of the motion of particles, when the particles move without collisions over distances that are many-fold larger than their characteristic dimensions. Really, the mean free path of particles in a gas amounts to about 100 nm under the atmospheric pressure, but it increases to approximately 0.5 mm already at a pressure of 0.1 mm Hg. Furthermore, the mean free paths of electrons and ions in plasma are often many times longer than the mean free paths of molecules in gases under the ordinary conditions (about 10^{-6} cm) [10]. A similar type of trajectories is observed at adsorption processes in the immediate proximity of a sensor surface [9, 11], when the mass of macromolecular analyte (for instance, a protein molecule) exceeds the mass of individual particles in a medium by many times. In all those cases, a typical model of the process describes a translational ballistic motion of an ensemble of non-interacting particles, which more or less compete for free sites on the surface.

When considering such processes, in particular, of adsorption, the features in the course of reactions taking place at the phase interface are mostly associated only with surface peculiarities, although the formation of surface-coupled complexes is actually affected by various processes at the interface, in which the surface itself, molecules adsorbed near the surface, clusters of those molecules, and free particles on the surface (with regard for the gradient of their concentration) participate. As a result, the adsorption is described by a complicated function of numerous variables. In effect, this function not only describes processes running at the adsorption surface, but it is a result of the self-consistent behavior of the ensemble of adsorbed particles on the surface and particles that freely move in the near-surface layer. Unfortunately, the processes of motion of particles near the surface are not considered, as a rule, when analyzing the adsorption processes.

Why the consideration of mentioned processes is a matter of interest can be easily understood if we consider the mainly elastic-scattering character of the molecular motion at the microscopic level for gas mixtures at the normal pressure, diluted solutions, and particles in plasma. Only a small number of surface collisions results in the formation of bound states, whereas the overwhelming majority of them forms a flow directed from the surface. As a result, specific dynamic states can be formed in the near-surface layer, which can considerably affect the processes in gas-dynamic systems [12], the processes taking place on the surface of biochemical sensors [9, 11, 13], and so forth.

Various models and algorithms of their simulation have been developed to describe the adsorption processes, by considering, to a greater or less extent, the driving forces and the specific features of the system concerned at the phase interface. First of all, these are phenomenological models based on the extraction of a certain dominating process "averaged" over the macrosystem (e.g., surface filling, diffusion, reduction of the particle concentration in bulk, and others), which can usually be well described by relevant differential equations [14, 15].

Typical examples of computer-assisted simulations are "cellular automata" algorithms, which have played a considerable role in the development of the statistical mechanics of surface processes [16]. The main shortcoming of those models consists in that they consider processes taking place exclusively on the surface and omit the processes occurring in the volume near the surface (the system is described making no allowance for the dynamics of changes in the particle concentration in the near-surface layer). Therefore, the effects arising owing to the features in the trajectories of particles moving near the surface are not taken into consideration. Unfortunately, a substantially restricted character of conditions, for which they were predicted, considerably reduces the importance of corresponding conclusions obtained, while analyzing experimental results. All the aforesaid determined the aim of this work: to find specific features in the spatial distribution of particles and their energies at the interface between a gas and a solid surface, which arise during the processes of monomolecular isotropic adsorption.

In order to elucidate the features of processes running in the near-surface layer, it is necessary to compare time variations of the particle concentration and energy in this layer with features of the adsorption kinetics. This task can be fulfilled, if the particle motion in the bulk phase is taken into account, and the common particle dynamics is adequately visualized by monitoring the variations of particle concentration gradients in bulk. As a result, the adsorption kinetics will change. The principles of this approach applied in some cases of anisotropic cooperative and anticooperative adsorption were considered in our previous works [17, 18].

2. Algorithm of Computer Simulation

The algorithm developed by us is based on the concept of nonequilibrium molecular dynamics, which consists in the account for the boundary conditions at the surface, which change in the course of adsorption

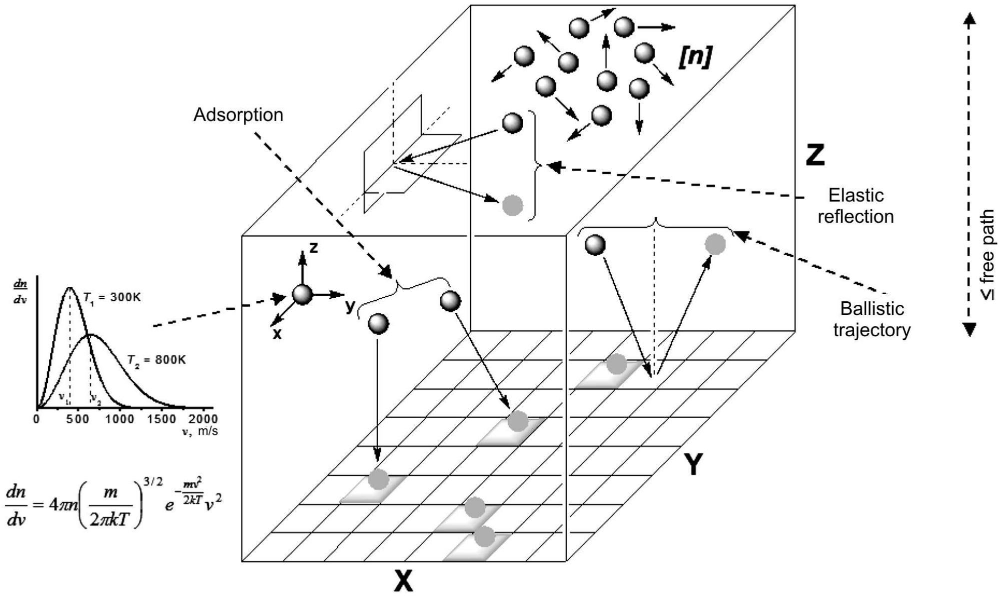


Fig. 1. General idea of the computer simulation algorithm and typical parameters of the virtual model of reaction space

[17]. The simulated system consists of an ensemble of identical particles at the temperature T. The particles are in a confined volume and in contact with a thermostat. The motion of point-like particles, every possessing the mass m, is described by the classical equations of Newton mechanics with the parameters specific to each separate particle. The particles do not interact in bulk and do not collide with one another. The interaction of particles with the walls confining the volume is absolutely elastic (Fig. 1).

In this work, we consider the isotropic type of irreversible monomolecular adsorption, for which the probability of the binding of particles on the surface is constant and does not depend on the short-range effects from particles adsorbed earlier. In order to elucidate the features in the spatial structuring of the near-surface layer, we consider the following variants:

1) *a variant with a finite number of particles in the ensemble:* new particles did not enter the volume; the number of particles in the volume decreases during the adsorption;

2) *a variant with an infinite particle source:* particles are added onto the upper face from a quasiinfinite space, which is the doubled volume of the cell, to compensate the adsorption; the number of particles in the volume did not change during the adsorption;

3) *a variant with the particle "agitation" in the volume* after their addition: after every adsorption event, the system is reinitialized, i.e. the particles are stochastically agitated in the volume; this variant simulates momentum fluctuations of particles at their random collisions with one another.

The computing experiments were carried out as follows. At the initial stage, the system was initialized by an arbitrary distribution of particles in the space and a given distribution of their velocities (the Maxwell distribution, if not specified differently). A new position of each particle was calculated at every time step Δt. If the particle was found to be behind the upper or side walls, its new position was calculated according to the elastic reflection law. If the particle crossed the adsorbing surface, one of the following scenarios was implemented:

1) if the particle binding center on the surface had already been occupied by a particle adsorbed earlier, the particle was elastically reflected from the surface;

2) if the binding center was free, the particle was adsorbed (the irreversible binding of the particle on the surface);

3) if the particle was adsorbed on the surface in the "infinite source" regime, a new particle was added at an arbitrary site of the upper face of the double-volume cell; the velocity of a new particle was equal

to that of the particle adsorbed on the surface; the direction of the velocity vector for the added particle was selected arbitrarily. In such a way, the number of particles in the volume and their total kinetic energy were maintained to be constant. The addition of new particles at the upper face was regarded as their supply from a quasiinfinite source located over the upper boundary.

The simulation was carried out for the temperature $T_0 = 300$ K, the number of particles $N = 2.5 \times 10^6$ in the volume $V = 1 \times 1 \times 1$ m^3 (the concentration $C_0 = 2.5 \times 10^6$ m^{-3}), and the particle mass $m = 5.3 \times 10^{-23}$ kg (32 Da). The number of particle binding centers on the surface amounted to $A = 2.5 \times 10$, and the time step was $\Delta t = 10^{-5}$ s.

The spatial dimensions of elements of the system that were used in this work were selected from the viewpoint of convenience, when representing the final results, provided that the SI system is used for the quantities typical of the Maxwell equations. The choice of those quantities is arbitrary, because the geometrical sizes of the reaction space are determined by the average particle velocity and the time step in the computation procedure; the latter can be varied in a wide interval. Both the particles and the binding centers are material points having no physical size. The specific values of model parameters do not affect the general character of the results obtained, because the calculated dependences are governed by relative particle velocities and the ratio between the number of the centers of particle binding on the surface and the number of particles in the reaction volume, $N/A = 10$.

According to the simulation result, we plotted the time dependence of the surface filling degree, $S(t)$, and approximated it, by using the stretched exponential function [19–21],

$$S(t) = A\left(1 - e^{-\left(\frac{t-t_0}{\tau}\right)^{\beta}}\right). \qquad (1)$$

Here, A is the number of particle binding centers on the surface, τ a scaling coefficient with the time dimensionality, and β the stretching parameter depending on the distribution of elementary processes at the phase interface [21].

The spatial distribution of particles in the volume was determined, by calculating the concentration profile, i.e. the ratio between the number of particles C in the elementary volume dV to the value of this volume ($dV = V/20$), in the direction normal to the adsorption plane. The results of simulating the processes taking place in the near-surface layer of the bulk phase are presented as the following dimensionless parameters:

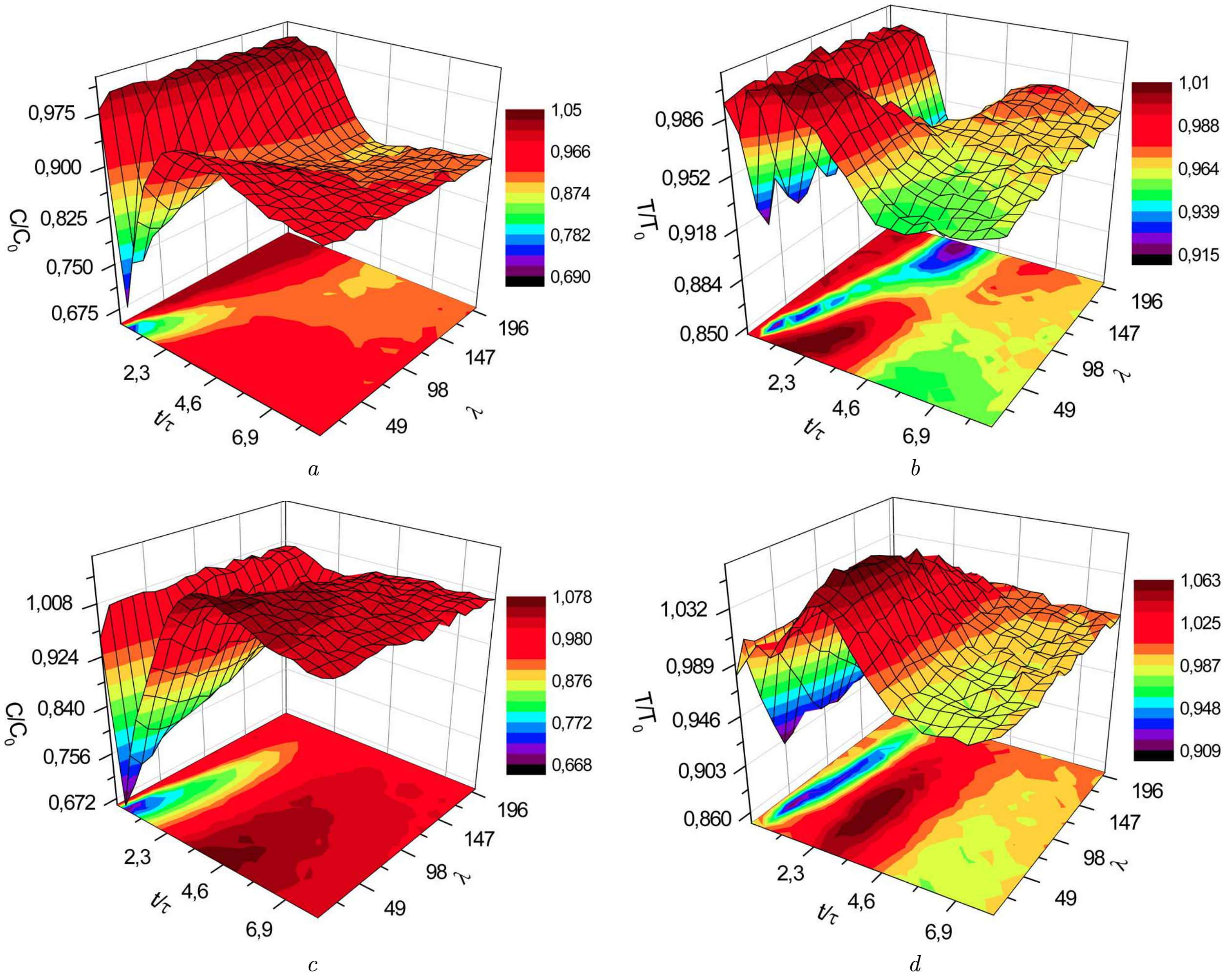
- the relative particle concentration C/C_0, i.e. the ratio between the number of particles in an elementary volume dV and the total number of particles in the volume ($C_0 = 2.5 \times 10^6$ m^{-3});
- the relative temperature T/T_0, i.e. the ratio between the temperature in an elementary volume dV and the average temperature over the ensemble ($T_0 = 300$ K);
- the relative free path λ, i.e. the ratio between the path of a particle moving at the average velocity over the ensemble for the time interval Δt and the capture depth (the height of the volume, in which particles move ballistically);
- the relative adsorption time t/τ, i.e. the ratio between the adsorption time and the characteristic adsorption time obtained from approximation (1).

The algorithm was implemented in the programming environment Delphi, and it can be used in the OS Microsoft Windows. The efficiency of the used mathematical algorithm allowed a computing experiment to be terminated after about 30 to 120 min, depending on the initial conditions, if the computations were carried out on a PC with a clock frequency of 2.3 GHz.

3. Adsorption Simulation Results

The surface breaks the translational invariance of the space and, accordingly, changes the concentration of particles and the distributions of their velocities and vectors of motion near the interface. Typical features of the surface film growth (the adsorption mechanism) is actually governed by the features of a transient layer separating the surface and the isotropic "gas" phase (the "topographical adsorption" model [21]). Hence, there must exist general dependences for the "structure" and "composition", which determine the dynamic state of the transient inhomogeneous layer on the basis of the interaction features between analyte particles and surface adsorption centers, type of particle source, influence of a medium, and so forth.

In the molecular dynamics framework, the most interesting issue concerns the time dependence of



a *b* *c* *d*

Fig. 2. Dynamic dependences of the particle concentration (*a* and *c*) and temperature (*b* and *d*) variations in the bulk phase along the normal to the adsorption surface for the regimes with a finite number of particles (*a* and *b*) and with an infinite particle source (*c* and *d*)

the microscopic particle distribution in the transient layer, which describes a variety of particle transport processes near the surface in the generalized form. In the course of surface filling, particle fluxes arise in both directions: toward the surface and backward. Therefore, the near-surface layer is an immanently dynamic object. Let us consider the simulation results obtained for various types of particle sources in more details.

In Fig. 2, the dynamic dependences of the particle concentration and temperature changes in the bulk phase along the normal to the adsorption surface are depicted. They testify that the near-surface layer has a complicated dynamic structure. The concentration gradients in it differ not only by value; they also change their direction in time. In the regime with a restricted particle source, when no new particles are added into the bulk after every adsorption event (Figs. 2, *a* and *b*), the equilibrium state of the system corresponds to a smaller number of particles in the bulk. After the system has been initialized, a drastic drop in the near-surface bulk concentration of particles is observed at the initial time moment, because the empty surface does not restrict the binding process. As a result, the bulk concentration of particles gradually decreases to the upper limit. As the time goes by, the bulk concentration along the normal to the surface becomes more uniform, and its

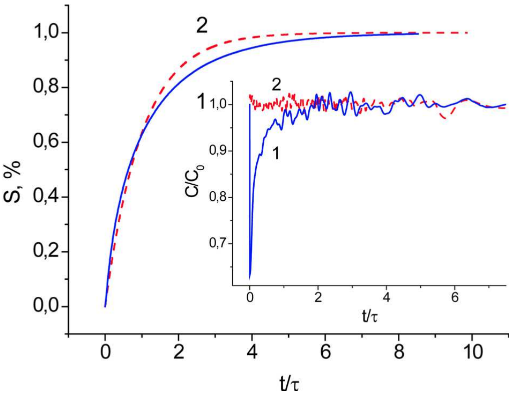


Fig. 3. Kinetic dependences of the adsorption surface filling by particles in the regime, when particles are added at the upper boundary of the volume (*1*) and in the "agitation" regime (*2*). The corresponding kinetic dependences for the particle concentration near the adsorption surface are shown in the inset

value diminishes in comparison with the initial one by the number of adsorbed particles. The kinetic dependence of the adsorption is well described by Eq. (1) with the parameter β close to 1.0 and $\tau \approx 8.7\times10^{-4}$ s.

Variations in the local temperature distribution for an ensemble of particles differ from those of their concentration. In particular, at the initial time moment, the temperature in the near-surface layer quickly drops (similarly to a change of the bulk concentration) and afterward drastically grows, which is connected with a reduction in the number of high-energy particles near the surface, which could come closer to it more quickly. As the time goes by, the temperature in the bulk becomes more uniform and lower than the initial one due to the dominating adsorption of "hot" particles on the surface.

In the scenario with an infinite source, particles analogous to those that have just been adsorbed on the surface are introduced at the upper boundary of the doubled volume. As one can see from Figs. 2, *c* and *d*, the variation dynamics of the bulk concentration in whole is similar to the previous regime. But in the case of infinite particle source, an insignificant reduction of the particle concentration near the upper boundary is observed. This reduction takes place due a constant "supply" of particles from the "upper volume", which plays the role of a damper between the transient layer and the infinite source at the upper boundary. However, even in the presence of such a damper, the concentration gradient extends far into the bulk.

This is also true for the temperature dynamics in the bulk that is observed in this regime. As a whole, the temperature value is higher in comparison with the case of limited source and reaches a maximum farther from the surface. This can be explained by a "slower" particle supply from the quasiinfinite volume. The kinetic dependence of the adsorption, as was in the previous regime, is described by Eq. (1) with similar parameters, which is illustrated by a similar dynamics of concentration variations in the near-surface layer in the both cases.

As was shown above, the presence of the ballistic regime gives rise to the appearance of concentration anomalies in the near-surface region. However, those anomalies can probably be cancelled under the influence of the stochastic noncorrelated motion of particles in the medium. To verify this statement, we made a simulation in the scenario where the particles are agitated in bulk. In this case, the near-surface particle concentration and the temperature remain constant irrespective of the particle source type. Figure 3 demonstrates the kinetic dependences for the filling of the adsorption surface by particles obtained in the model with a constant concentration: "without agitation" (the ballistic regime) (curve *1*) and "with agitation" (curve *2*). The kinetic dependences describing a variation of the ratio between the concentration of particles near the surface and the total concentration of particles in bulk are shown in the inset. One can see that the kinetic dependences of the adsorption are different in those regimes. The regime "with agitation" is characterized by that the near-surface concentration of particles does not change during the whole adsorption process (Fig. 3, curve *2* in the inset). This behavior corresponds to classical algorithms and describes the adsorption processes on the basis of cellular automata that account for only the surface binding [15, 16]. The rate of particle supply at the surface remains constant in the "agitation" regime, which results in a higher rate of surface filling at the initial stage of the irreversible adsorption process. At the same time, the dynamics in the regime, when particles are added at the upper boundary, which is driven by a change of the particle concentration in the near-surface layer, seems to be more adequate to the actual processes in the system. The difference between those approaches can be directly seen, in particular, from the kinetic dependences: a drastic reduction of the particle concentration in the near-surface layer (Fig. 3, curve *1* in the inset) leads to a reduction of the adsorption rate at the initial stage (Fig. 3, curve *1*).

It should be noted that all examined regimes of monomolecular isotropic adsorption do not result in the formation of any ordered organized structures or separate clusters on the surface (Fig. 4, the inset), which are formed in the presence of cooperative interactions [17].

In order to demonstrate the capabilities of the analysis of the features in the behavior of various dynamic systems, we considered other scenarios of computing experiments. The results of corresponding simulations are summarized in Table. Those scenarios differ from each other by different combinations of the particle velocity distribution in the ensemble and the procedure of particle addition into bulk after the adsorption event. The absolute values of particle velocities in bulk were given according to the Maxwell distribution. Alternatively, the particles were ascribed to have constant velocities (e.g., as in particle accelerators before the target bombardment). Concerning the procedure of particle addition after every adsorption event, the particles were added either at the lower volume limit or uniformly in bulk with the velocity component $v_z > 0$.

The visualization of the dynamic system state in various scenarios of the computing experiment showed that specific oscillations of the bulk particle concentration arose in some cases. Their frequency and amplitude strongly depended on the particle velocity distribution and the procedure of particle addition to the volume. For example, in Fig. 4, the kinetic dependences of concentration variations near the adsorption surface are depicted for various velocity regimes. Curve *1* corresponds to the Maxwell distribution of the absolute values of velocities at $T = 300$ K, and curve *2* was obtained for the identical velocity of all particles (484.3 m/s, which corresponds to the average particle velocity over the ensemble with the Maxwell distribution, $v_{av} = (3kT/m)^{1/2}$. One can see that, unlike curve *1*, curve 2 demonstrates a polymodal character. This result testifies that stable spatial modes are not formed in a statistical ensemble consisting of noninteracting particles that are located in a confined space volume and move at velocities characterized by the Maxwell distribution. At the same time, for the case of ballistic motion of particles at a constant velocity, the formation of quasiperiodic concentration modes is a consequence of the confinement of the volume containing the ensemble.

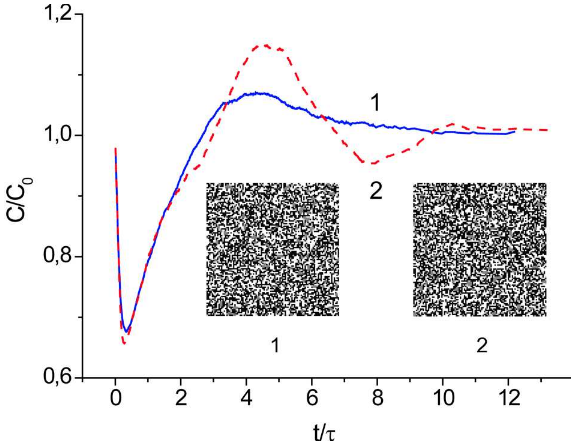
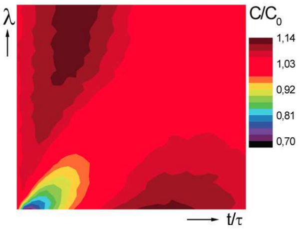
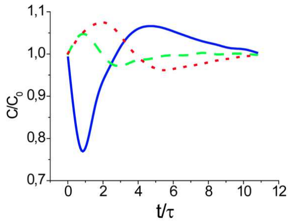
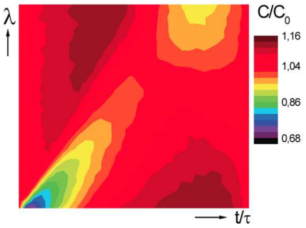
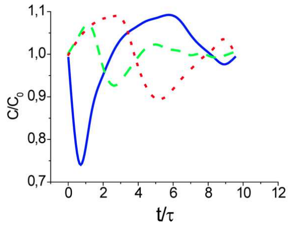
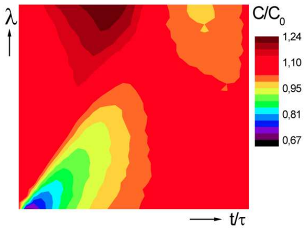
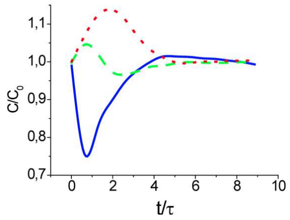
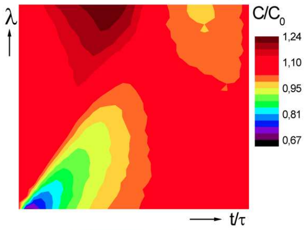
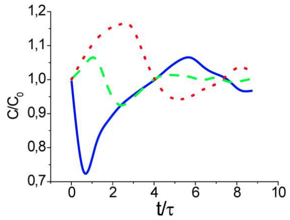
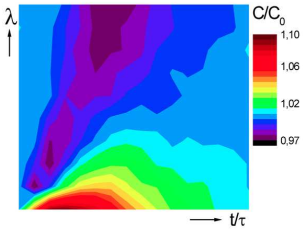
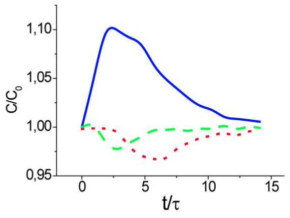
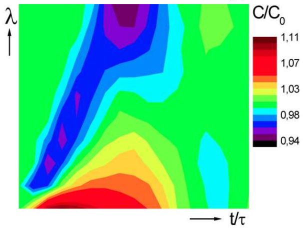
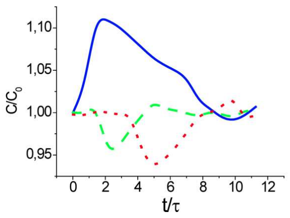


Fig. 4. Dynamic dependences for the particle concentration variation near the adsorption surface in the cases (*1*) when the absolute values of the particle velocities are distributed according to the Maxwell distrbution and (*2*) when all particles have the same velocity. The corresponding fragments of the surface at monomolecular isotropic adsorption are shown in the inset

The result obtained is a consequence of the form selected to simulate the distribution of molecules over the absolute values of their velocities. Really, in the case of Maxwell distribution, the distribution of velocity projections of gas molecules onto an arbitrary direction in the space is described by the normal Gaussian distribution [22]. This means that, for any direction, any correlations between particle velocities (in particular, if the velocities are directed along the same straight line) are absent. Hence, the formation of the correlated concentration regions is also impossible, because particles in a gas always move.

Nevertheless, this trivial result allows some important conclusions to be drawn. First of all, it should be noted that, according to M.M. Pyrogov, the distribution law for gas molecules over their velocities at their chaotic motion including mutual collisions is valid only in the case where the gas occupies an infinitely large volume [22]. Therefore, the examined variant of ballistic motion can be useful while considering the control problems of a gas flow in a confined volume (e.g., jet nozzles), where

Concentration distribution diagrams and concentration profiles obtained in various scenarios of the computing experiment. Solid curves correspond to concentration profiles near the lower boundary of the volume, dashed curves to concentration profiles in bulk, and dotted curves to concentration profiles near the upper boundary of the volume

Scenario	Concentration distribution diagrams	Concentration profiles
Particles are added uniformly into bulk. Maxwell distribution for particle velocities. Bulk association model		
Particles are added uniformly into bulk. Particles have the same velocity. Bulk association model		
Particles are added uniformly into bulk. The vector component $v_z > 0$. Maxwell distribution for particle velocities. Bulk association and sedimentation model		
Particles are added uniformly into bulk. The vector component $v_z > 0$. Particles have the same velocity. Bulk association and sedimentation model		
Particles are added at the lower boundary of the volume. Maxwell distribution for particle velocities. Laser ablation model		
Particles are added at the lower boundary of the volume. Particles have the same velocity. Laser ablation model		

the processes of collision with walls dominate. In this case, the formation of oscillatory modes with critical high-temperature regions can be prevented, if technical facilities allow the Maxwell distribution of particle velocities to be maintained. Furthermore, it should be noted that the result obtained by means of the computer simulation confirms the conclusion that, in the case of ideal gas, the specific features of its behavior near the gas–solid interface are completely determined by the form of the gas molecule distribution function over the velocities.

To summarize, the simulation of the process of irreversible monomolecular isotropic adsorption and the analysis of the results obtained enable us to demonstrate the necessity to consider the dynamic processes that run not only on the surface, but also in the near-surface layer. It is shown that the processes taking place in this region can stimulate a number of secondary processes such as a local heating of walls, stable oscillations of particle concentration, distinctions in the adsorption dynamics and adsorbate structure, and so forth. The results obtained can be used to analyze and to predict features for the processes running in the near-surface layers of various elements and devices of sensor and electronic engineering, gas dynamics, and other domains, where the ballistic character and the particle motion kinematics dominate and govern the functional properties of the system.

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ОСОБЛИВОСТІ ПРИПОВЕРХНЕВОГО ШАРУ ПРИ МОНОМОЛЕКУЛЯРНІЙ ІЗОТРОПНІЙ АДСОРБЦІЇ: МОДЕЛЮВАННЯ В РАМКАХ НЕРІВНОВАЖНОЇ МОЛЕКУЛЯРНОЇ ДИНАМІКИ

Резюме

У рамках підходу нерівноважної динаміки з використанням алгоритму моделювання незворотної мономолекулярної ізотропної адсорбції проаналізовані процеси, які відбуваються біля межі об'ємної газової фази та твердої поверхні. Проаналізовано їх вплив на кінетику адсорбції. Виявлена складна просторова організація приповерхневого шару частинок, концентрація та кінетична енергія яких змінюється з часом. Встановлено, що локальна концентрація частинок може як зменшуватися (до $\sim 60\%$ від початкової), так і збільшуватися на різній відстані від поверхні залежно від особливостей системи та часу, які розглядаються. Одержані результати можуть бути використані для аналізу і передбачення особливостей процесів у приповерхневих шарах елементів сенсорної та електронної техніки, газодинаміки та інших областей, де балістичний характер і сама кінематика руху є домінуючим процесом, що визначає функціональні властивості системи.