# COMPUTER MODELING OF PARTICLES TRANSPORT STATIONARY PROCESS IN OPEN NANOSYSTEMS

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By far, the analysis of particles heat and mass transfer in open nanosystems is of noticeable importance both in theoretical and practical researches. Due to a slotted and cylindrical systems resort we have been able to carry out some essential experimental investigations as well as provide new theoretical computations.

The distinctive feature of nanosystems gas particles transport research is connected with the fact that particles collisions with the walls of the nanosystems prevail over those in gas phase. The process of particle transport in such systems runs in a free-molecular regime. (Kn>>1). At this point the importance of the ratio between particles sizes and nanosystems geometry rises noticeably.

The use of Boltzmann equation would not lead to a practical result in the analysis of gas transport in such systems due to the leap of particles gas density fluctuations as well as gas – surface nonequilibrium condition toughening.

The work represents the analysis of neutral particles heat and mass transfer process in slotted and cylindrical open nanosystems by direct Monte-Carlo method in a free-molecular regime. Every computer experiment models over 10,000,000 particles trajectories, designates the flows of particles out of the systems in compliance with the sizes of the particles as well as dimensionless parameter r = U / kT - the ratio of the particles cohesive energy with the walls of the systems U value and system temperature T alongside with systems geometry.

The basis of the model used to describe the interaction of gas particles and systems walls surfaces refers to the assumption of the partial loss of the kinetic energy by the particles escaping out of condensed phase or system walls surface. The above energy amounts to a potential barrier U value and is spent on intermolecular gravity forces surmount.

## COMPUTER SIMULATION OF EVAPORATION PROCESS INTO THE VACUUM

### INTRODUCTION

One of the important problems of a gas dynamics is a question of interaction of gas molecules with the surface of a condensed phase[1]. Near the surface of a gas phase the molecules also collide with the molecules reflected from the surface. Near the surface there is a Knudsen's layer, in which practically there are no collisions of the molecules with each other [2,3]. The value of this layer is equal to the length of a free molecule run of the gas phase. Thus, there are two independent flows of molecules in the Knudsen's layer - one flow of molecules, flying to the surface from the gas phase, and the other from the surface into the gas phase. The difficulty of obtaining a distribution function of molecule speeds in the Knudsen's layer is that the process of molecule interaction with the surface is non-equilibrium and the function of the distribution of such molecules differs from that of equilibrium.

While calculating the heat and mass transfer processes the molecules that have left the surface are supposed to have the Maxwell function of the distribution in speeds with the temperature of the condensed phase[4]. In case of a hydrodynamic mode of the flow there are jumps of the temperature and the density on the surface and in the gas phase[5]. In case of a gasdynamic mode of the flow it is necessary to use the Boltzmann equation or model equations. The above-mentioned assumptions are used for setting boundary conditions in describing the gas medium movement near the surface.

The process of evaporation from the surface of the condensed phase into the vacuum is a more simple case (Overcoming by the molecules of a potential barrier on the surface of the condensed

phase). In case of the evaporation of a monoatomic condensed phase there will be no back flow of the atoms. The back flow will be observed in case of the evaporation of a multicomponent condensed phase or molecules, as well as in an intensive evaporation of the monoatomic condensed phase when multiatomic collisions are becoming important.

When a substance is evaporated from the surface of the condensed phase the temperature lowers. To maintain the constant temperature of the condensed phase surface it is necessary to bring to it the amount of the heat, which depends on the temperature of the condensed phase and the value of the potential barrier. The form of the potential barrier curve, in this case, does not play any role, since only those molecules are considered which have overcome the potential barrier.

However, we consider the evaporation process as not enough justified. Some experimental data cannot be explained within the framework of the existing theory of the heat and mass transfer during the evaporation. So, for example, in Stern's experiments on the evaporation of metal from the furnace into the vacuum, the deficit of the atoms with small speeds is observed, which shows a discrepancy of the distribution function of the departed particles from the Maxwell function[6]. It is interpreted by a deviation from the model of the dot particles and their collisions near a hole when they are leaving the furnace. The experimental data on the evaporation of the uranium melt given in [7], do not correspond to the theoretical ones.

The analysis of published articles has shown, that the regularities connecting the parameters of the condensed phase characteristics of the molecules flow which have overcome the potential barrier on the surface of the condensed phase have not been defined yet.

## BASIC PRINCIPLES OF CALCULATIONS

As a result of fluctuations within the part of the molecules of the condensed phase the speed can be sufficient for overcoming the potential barrier on the surface of the condensed phase. These molecules leaving the surface of the condensed phase into the vacuum or gas phase. The molecules, leaving the surface of the condensed phase, some part of the kinetic energy spent for overcoming the potential barrier. Therefore, only those molecules which posses a larger kinetic energy than the value of the potential barrier can escape. The potential barrier on the surface of the condensed phase is a peculiar filter separating slow molecules from fast ones.

In the contributed paper the approach for finding the distribution functions of atoms on speeds and energies in the Knudsen's layer depending on the atoms mass $m$, the temperature $T$ of the condensed phase and the value of the potential barrier $U$ is offered. The paper describes the case of evaporation of the monoatomic condensed phase into the vacuum and the Maxwell distribution of atoms in speeds in the condensed phase.

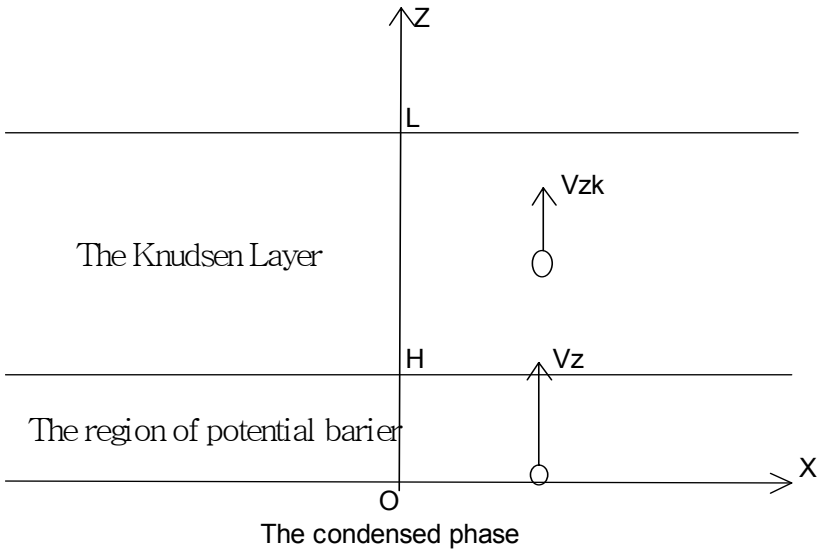


**Figure 1** - The general picture.

We shall assume that the condensed phase occupies half-space $z \leq 0$. The forces of interaction between the escaping atoms and the atoms on the surface of the condensed phase become negligibly small at the distance of H. Let us suppose that H is the constant value that is considerably smaller than the length of the free run of the escaped atoms (The Knudsen's layer value is L) $H << L$.

By computer simulations of the evaporation process, due to the principle of independent motion, we can consider only the change of z - component of the atoms speed. A part of the kinetic energy of every escaped atom is spent for overcoming the interaction forces with the atoms of the condensed phase. It follows from the energy conservation law:

$$\frac{mv_{zk}^2}{2} = \frac{mv_z^2}{2} - U, \qquad (1)$$

where $v_z$ and $v_{zk}$ are the components of atoms speed on the surface of the condensed phase and in the Knudsen's layer, accordingly.

Algorithms, described in [8] were used as random number generators for the definition of atoms speeds on the surface of the condensed phase. The following technique for obtaining distribution functions of atoms energies in the Knudsen's layer was used. The components of atoms speeds on the surface of the condensed phase were defined with the help of the generator of normally distributed casual values. Then the value of atom kinetic energy in the Knudsen's layer was determined from the equation (1) and the conclusion was made about its possible appearance in the Knudsen's layer. The simulation of 10,000,000 atoms escape was made for definite parameters.

## RESULTS AND DISCUSSION

Fig. 2 shows the schedules of dependencies of the normalized average speeds $\nu_n(r)$ and energies $e_n(r)$ in the Knudsen's layer on the dimensionless parameter $r = U / kT$ (where $k$ is Boltzmann's constant).

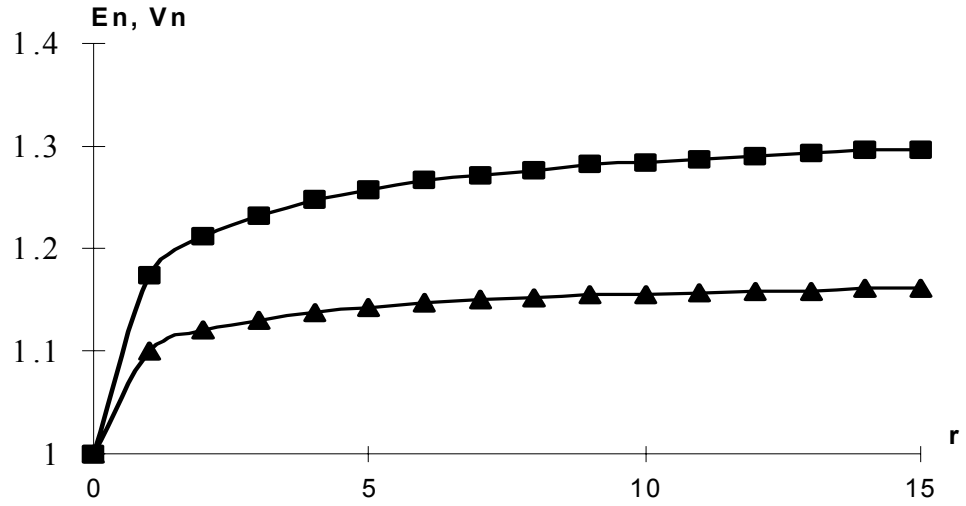


**Figure 2** - The dependensies of the normalized speeds $\nu_n(r)$ ■ and energies $e_n$ ▲.

The normalization was made by dividing the appropriate value by the value, when $r = 0$ ($\nu_n(r) = \nu_a(r) / \nu_a(0)$, $e_n(r) = e_a(r) / e_a(0)$). The analysis of computer simulation showed that masses of atoms and the temperature of condensed phase do not influence the dependencies of the normalized average speeds and atoms energies. Statistical deviations did not exceed 1%. The curves growth slows down after meaning $r$ = 2, which is characteristic for both regularities. The question of the existence of asymptotic meanings for the curves distributions is open. The existence of the potential barrier on the surface of the condensed phase leads not only to a simple division of slow and fast atoms, but to such paradox phenomenon that average speeds and atoms energies in the Knudsen's layer exceed similar values in the condensed phase.

Fig, 3 shows normalized z distributions - component atoms energies in the Knudsen's layer for different meanings of $r$. The distributions maxima are when $e$ = 0. The maxima values decrease with the increase of $r$. Within the increase of $r$, parts of slow atoms decrease and parts of fast atoms increase.

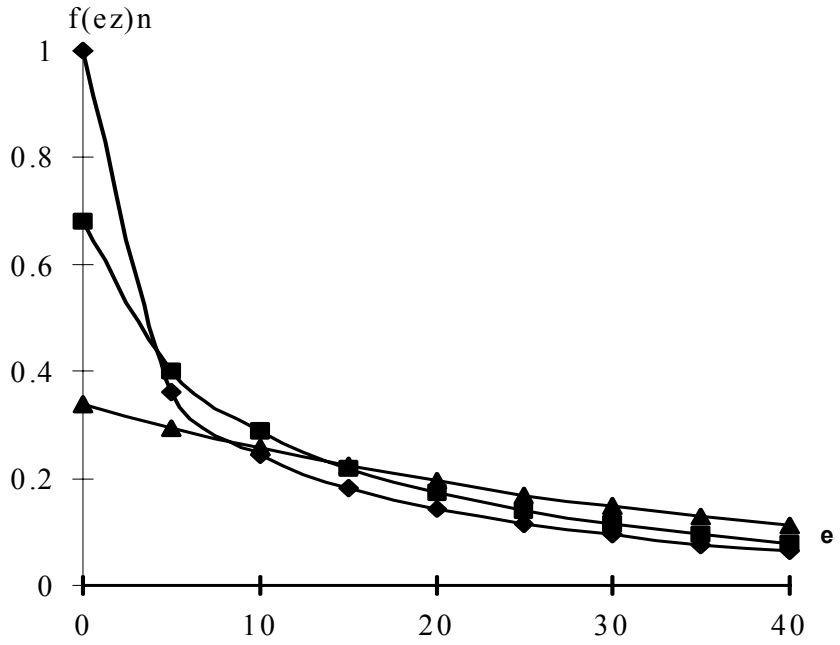


**Figure 3** - The normalized distributions z – component atoms energies. ♦ $r$=0, ■ r=0.1, ▲ $r$=5.

The distribution functions of atoms in energy in the Knudsen's layer are shown in Fig. 4. The distributions curves look the same for all meanings of $r$. With the increase of $r$ the maxima decreases in height and displaces to the side of larger energies.

The results obtained enable to understand the role of the potential barrier on the surface of the condensed phase and explain a divergence of theoretical results with experimental data, for example in Stern's experiments.

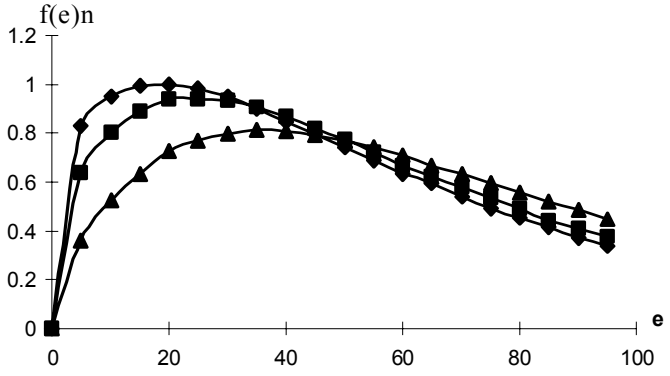


**Figure 4** - The energy distribution functions of atoms. ♦ $r$=0, ■ $r$=0.1, ▲ $r$=5.

The analysis of the computer simulation showed that the probability of atoms escape from the condensed phase into the Knudsen's layer decreases with the increase in the condensed phase, i.e. with the increase of $r$. It happened that the probability of atoms escape from the condensed phase into the Knudsen's layer is determined by the function:

$$P(r) = 1 - F(\sqrt{r}), \qquad (2)$$

where $F(x)$ is the integrated Laplace function.

The greatest interest, from the practical point of view, are the results of power calculation for the redundant heat flow from the surface of the condensed phase:

$$G(r) = P(r)(\varepsilon_a(r) - \varepsilon_a(0)) \qquad (3)$$

The schedule of $G(r)$ function is shown in Fig. 5.

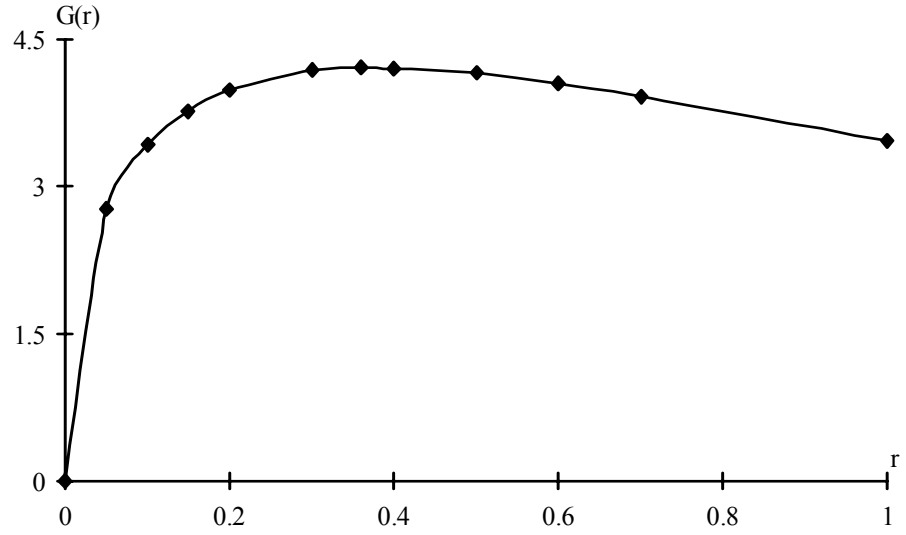


**Figure 5** - The schedule of $G(r)$ function.

When $r \to 0$, the function $G(r) \to 0$, because $P(r) \to 1$ and $\varepsilon_a(r) \to \varepsilon_a(0)$. When $r$ ($r \to \infty$) are large, the calculation results showed, that $G(r) \to 0$. Computer simulations have given an interval estimation of the maxima position for $G(r)$ rmax $\in$ (0,35; 0,37). The practical interest of the results obtained is that a maximum flow of heat can be retracted near maximum $G$(rmax) irrespective of the temperature of the condensed phase (if an appropriate substance is chosen) and minimum when $r \to 0$ or $r \to \infty$ in evaporation processes.

The importance of computer simulations made is that they enabled to look at the evaporation process in a new way from a microscopic point of view. It is shown that the escaping atoms sp end energy not only for overcoming the potential barrier during the evaporation of the substance into the Knudsen's layer, but due to the escape of much faster atoms an additional kinetic energy is carried away, which can be interpreted as overcoming of the higher potential barrier.

The suggested problem solution of evaporation can be transferred, by analogy, to other physical processes connected with overcoming potential barriers, for example, ions escape from melts, electron thermoemission, particles escape from relativistic space objects, etc.

The practical significance of the obtained results lies in the possibility on their basis to create qualitatively new and to modify known methods of substance division. Selecting appropriate substances and the temperatures it is possible to create optimum modes of the heat and mass exchange in installations.

#### MODELING OF STATIONARY HEAT AND MASS TRANSFER IN OPEN NANOSYSTEMS BY MONTE CARLO METHOD

*Computer experiments being run include estimations of particles escapes probabilities out of the w1(H,r)-systems, condensed phase hit probabilities of particles collided with w3(H,r)-systems walls, angular distributions of escaped particles p4(H,r) and particles dispensing over the surfaces sprayed on p5(H,r). The aforesaid probabilities and distributions have been made for various size systems and quantities of particles collisions with systems walls.*

*The results of the analysis and research made show both minor fluctuations of particles escapes probabilities out of the systems and their distribution laws depending on the r>4 parameter changes. Maximum distinction has not exceeded 0.1 %.*

*In spite of a simple geometry of the systems analyzed, they may be applied in a number of technical devices. The nanosystems scrutinized are of big potential to be used in electric nanoappliences cooling. Moreover, considering the fact of a free-molecular assumption of tiny and medium aerosol particles and viruses motion in air, it is possible to use these nanosystems as filters of their capture.*

The process of particles heat-and-mass transmission in open nano-systems appears to be of essential importance for theoretical and practical researches. The use of simple systems for the transfer process analysis allows conduct both abovementioned researches. The main feature of gas particles process transfer in nanosystems is that collisions of particles with the walls of the systems prevail over those in a gas phase between the particles themselves. The process of particles transfer in such systems is carried out in a free molecular mode (Kn >> 1). The correlation between the geometry of a system and that one of gas particles is to be strictly observed in the calculations. It is impossible to use Boltzmann equation when analyzing gas transfer in such systems, which has been used to describe the equilibrium gas particles transfer. The density of gas particles fluctuations alongside with the condition of nonequilibrium gas-surface interaction is also very important in those systems.

The direct Monte Carlo method describes the process of monatomic particles heat and mass transfer into the open systems of slotted and cylindrical type. It was assumed that particles had moved into the system without any collisions with each other, but could have run against the walls of the system. The trajectories of 10,000,000 particles were modeled in every computer experiment. The streams of particles outcomes out of the system turning back into a condensed phase depend on the dimensionless parameter r = U / kT, the ratio of particles and system walls liaison energy U, the temperature of the system T and the geometry of the system. We've used a special realistic model to depict the interaction between gas particles and system walls. The model is based on an assertion that particles when escaping the surface of the condensed phase or walls of the system spent some part of their kinetic energy equal to the potential barrier U on overcoming the intermolecular forces. Conducted computer experiments determined the probabilities of particles flights out of the system, probabilities of particles turns back into the condensed phase after collisions with the walls of the system, particles dissemination heightwise the system walls, angular distribution of escaping particles. These probabilities and distributions are determined by various geometries of the systems examined and the number of particles collisions with the walls of the systems. The amount of heat has been calculated which is taken away by particles escaping the systems.

The results of particles flights out probabilities calculations W1 (s, 0) out of the systems after all possible collisions of particles with walls of the systems are presented on fig.1 , which

reveals that particles could escape out of the systems either without collisions, or after a one, the two, etc. collisions with the walls. The number of such particles has been counted up and divided on a total amount of all examined particles. According to the results it has been possible to consider, that relative frequencies of outcomes are practically equal to the probabilities of the corresponding outcomes. The data received for r=0 parameter shows that particles escape the surface of the condensed phase out of the systems bottom and walls are equiprobable. The use of 's' symbol means that all particles escaping the systems have been counted up afer all possible collisions with system walls. The parameter 'a' defines the distance between the walls of a system. The radius of particles in all experiments, was assumed equal to $2 \cdot 10^{-10}$ m. Symbol 'H' goes for the comparative system walls height and is defined as a ratio of system wall height to its width.

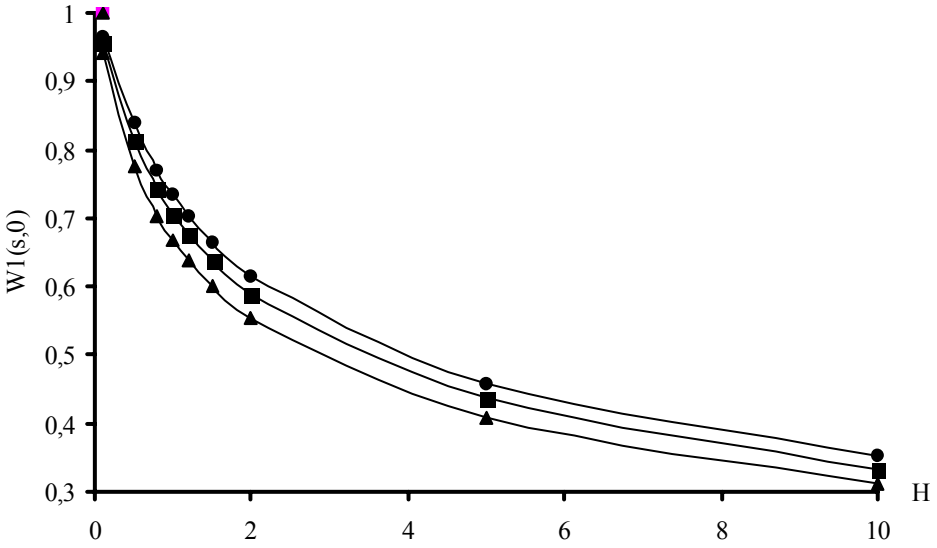


Figure 6 - Particles slotted systems escapes probabilities. N=s. r=0. ▲- a = $2 \cdot 10^{-8}$ m, ■ –a = $0.25 \cdot 10^{-8}$ m, ● – a = $0.125 \cdot 10^{-8}$ m.

The limiting case for parameter r = 0 has been considered. The probabilities of particles escapes slightly differ in compliance with various distances between walls of systems for relevant small system heights H. With increase in height of systems walls distinction becomes greater. For value of parameter a = $2 \bullet 10^{-10}$ m, results coincide with calculations for dot particles.

Figure 7 shows the results of calculations for the same systems, although the ratio between the energy of particles interaction with walls of the system and system temperature this time is r = 0.5. The distributions of probabilities of particles escapes out of the system in this case appear to be similar to those for parameter r = 0. In comparison with results for r = 0, there observed more significant distinctions in probabilities of flights in the area of greater heights systems. It shows that in the second case the particles escape the system without any collisions. For value of parameter r, distinct from zero value the increase in number of the particles escaping the system without collisions with walls is marked, the law of particles escapes differs from equiprobable one. When r approaches infinity this law tends to cosine law.

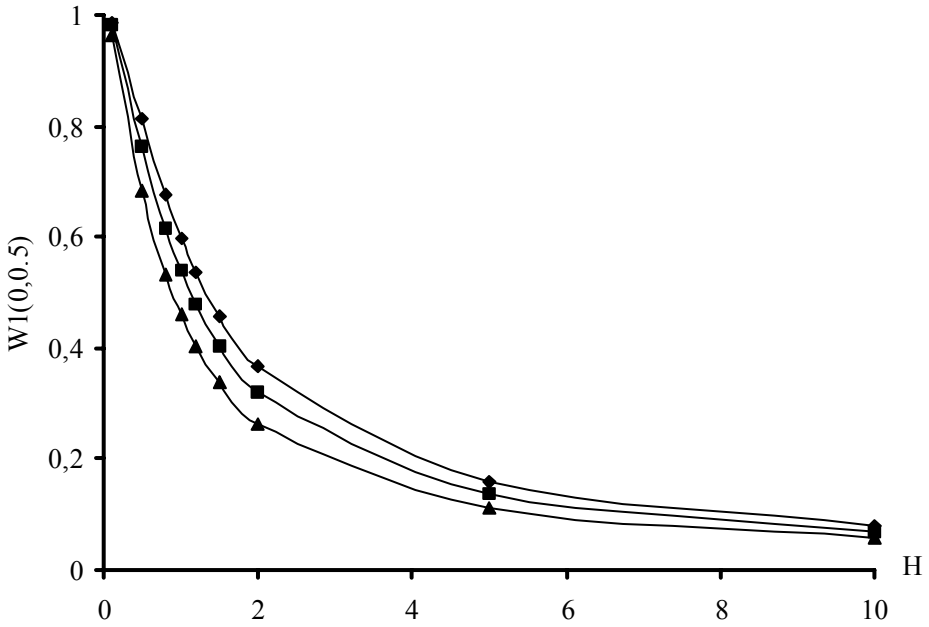


Figure 7 - Particles slotted systems escapes probabilities. N=0. r=0.5 ▲- a = $2 \cdot 10^{-8}$ m, ■ –a = $0.25 \cdot 10^{-8}$ m, ● – a = $0.125 \cdot 10^{-8}$ m.

Figure 8 represents the calculations of particles system escapes probabilities W1 (s) after all collisions with the walls, according to various r parameter values and depending on the distance between system walls. The data presented proves that with the increase in energy of particles interaction with surface of the condensed phase and walls of systems the probability of particles escapes from systems inclines.

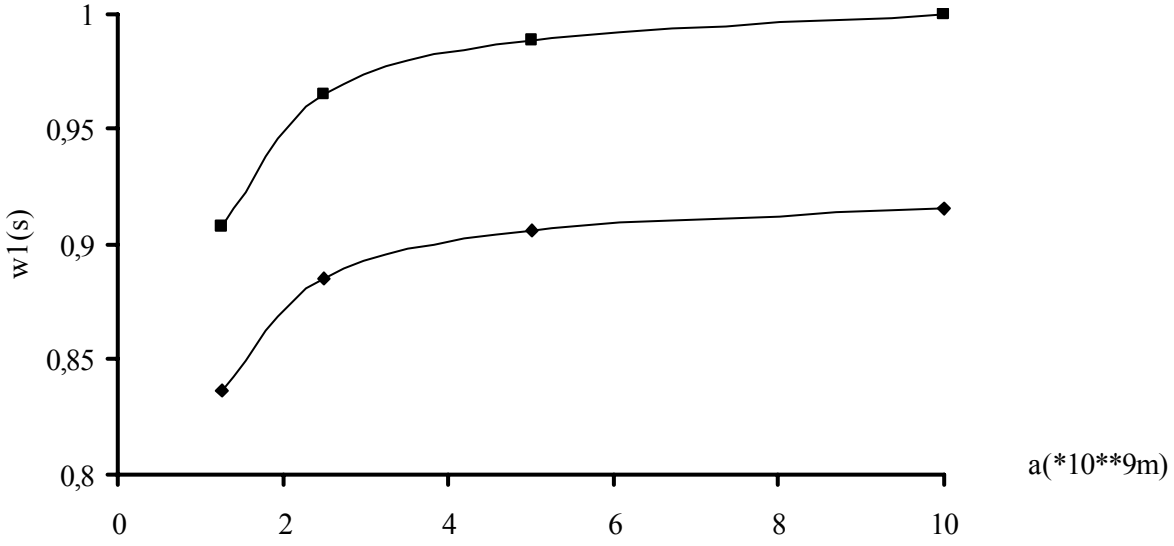


Figure 8 - Particles slotted systems escapes probabilities. H = 1. N = s. ♦ – r = 0, ● – r = 0.5.

Figures 9 and 10 show the results of calculations of particles dissemination density p2 heightwise the walls of systems H=1, which have been carried out for those particles escaped the condensed phase surface (N=0). For values of parameter r = 0 and r = 0.5 those disseminations have noticeably different behavior in the area close to the bottom of the condensed phase. For each certain value of r parameter the curves of disseminations have an identical appearance. The

difference of shapes of the curves defines the difference of particles speeds distributions subject to different values of r parameter at a flight-out start from a surface of the condensed phase.

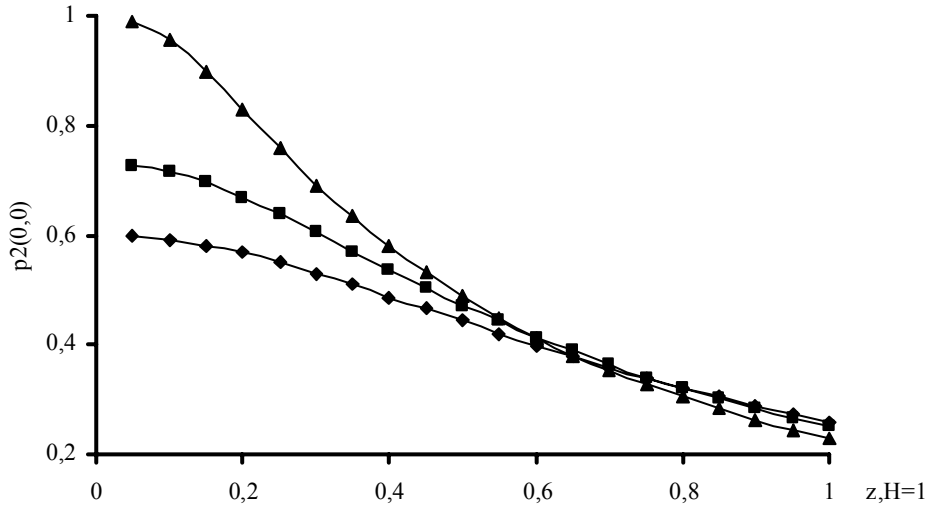


Figure 9 - Particles dissemination density heightwise the walls of slotted systems. H = 1. N = 0. r = 0. ▲- a = $2 \cdot 10^{-8}$m, ■–a = $0.25 \cdot 10^{-8}$m, ●– a = $0.125 \cdot 10^{-8}$m

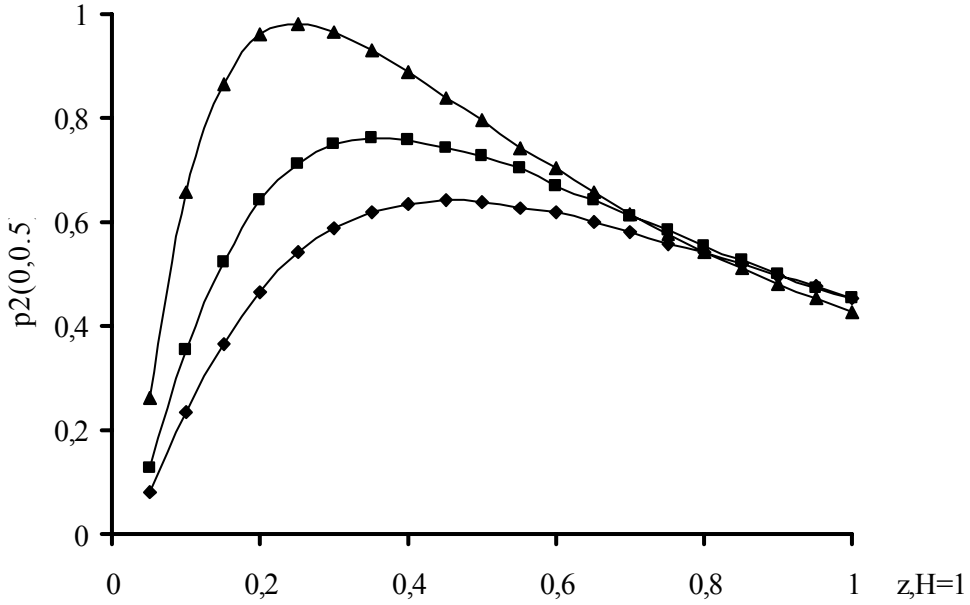


Figure 10 - Particles dissemination density heightwise the walls of slotted systems. H = 1. N=0. r=0.5, ▲- a = $2 \cdot 10^{-8}$m, ■ –a = $0.25 \cdot 10^{-8}$m, ●- a = $0.125 \cdot 10^{-8}$m

Figure 11 depicts the results of particles dissemination calculations p4, escaping from slotted systems after all collisions with walls, and accumulated on a flat surface which is fixed over the top edge of system at a distance equal to H. Due to the insufficiently big number of particles напыляемых on the surface there appears a significant deviation from the appreciated average values. The graphs show that the disseminations are symmetric by the middle of the system.

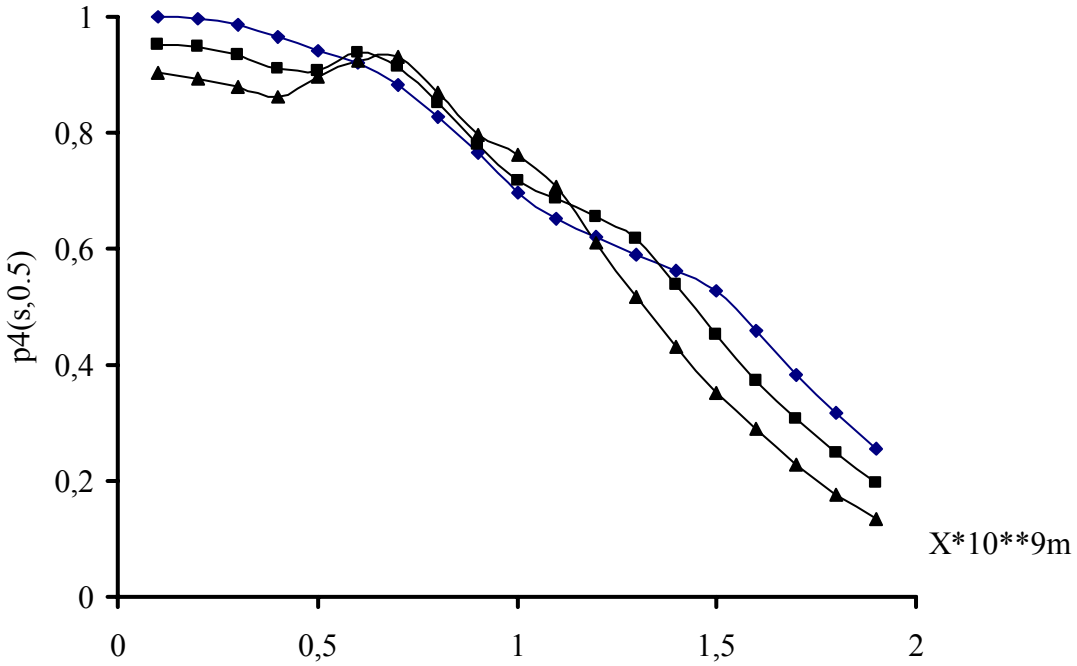


Fig. 11. Particles dissemination density on spraying surfaces. H = 1. N = s. r = 0.5. ▲ - a = $2 \cdot 10^{-8}$m, ■–a = $0.25 \cdot 10^{-8}$m, ● – a = $0.125 \cdot 10^{-8}$m

Figure 12 represents the results of an additional energy calculation, which is taken away by the particles which escape from the system. Data value has been defined as the ratio of a sum of the energies all escaping particles to this number of particles. Afterwards the average kinetic energy has been subtracted from that additional energy and the result divided on the kinetic energy. It is necessary to note, that the effect given is observed for values of parameter r $\neq$ 0. At a value of parameter to r = 0 the aforesaid effect is not observed (particles any to additional energy do not carry away). The additional energy is connected with the fact, that the particles when overcoming a potential barrier lose a part of kinetic energy, equal to U amount, but an average energy of the escaped particles appears to be more than an average energy of particles in the condensed phase.

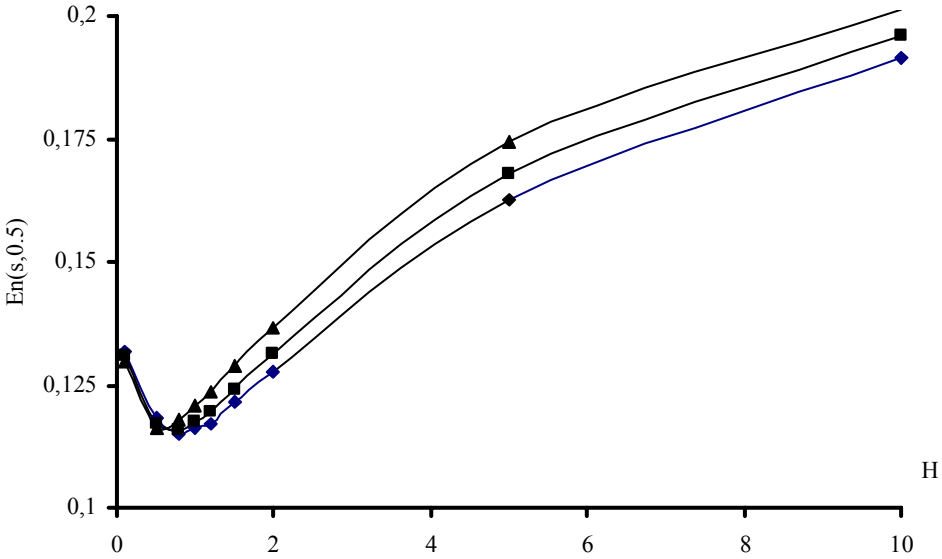


Figure 12 - Normalized additional energy, taken away by particles from slotted systems. N = s. r = 0.5. ▲- a = $2 \cdot 10^{-8}$m, ■–a = $0.25 \cdot 10^{-8}$m, ●– a = $0.125 \cdot 10^{-8}$m

The results of calculations of cylindrical systems escaped particles probabilities W1 (s) are given on Figure 12. The curves of distributions for cylindrical systems are similar to those of distributions for slotted systems; however the particles escapes probabilities from cylindrical systems decrease noticeably faster. The parameter *a* in case of cylindrical systems is equal to a diameter of the cylinder. All other distributions are found between minimal and maximal values.

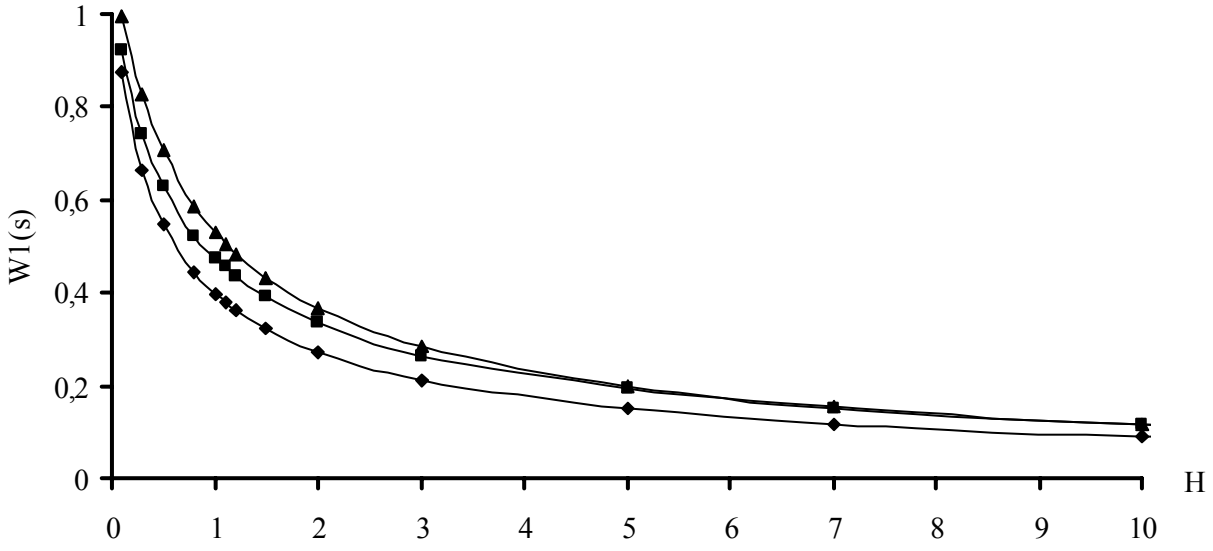


Figure 13 - Particles escapes probabilities from cylindrical systems. N = s. r = 0.
● - a = $0.125 \cdot 10^{-8}$m, ▲–a = $2 \cdot 10^{-8}$m, r = 0.5. ■ – a = $2 \cdot 10^{-8}$m.

Figure 13 shows the distributions of the additional normalized energies taken away by particles from cylindrical systems. A general view of distributions is similar to those in slotted systems but minimum sharper and gradual then.

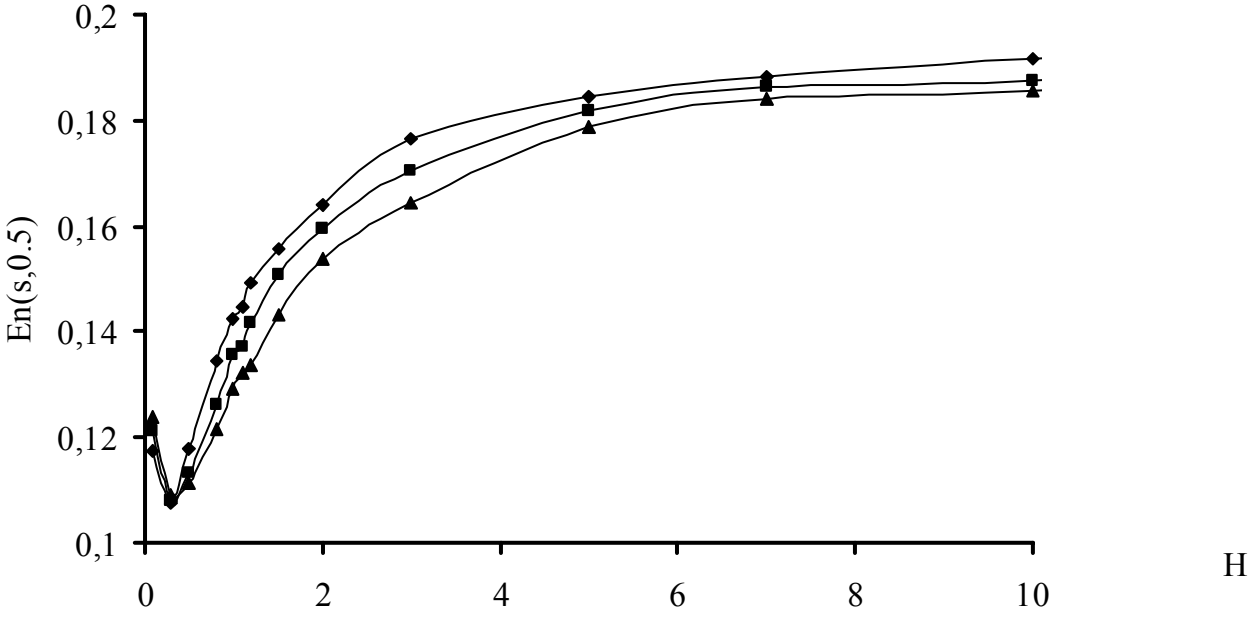


Figure 13 - Normalized additional energy, taken away by particles from cylindrical system. N = s. r=0.5. ▲- a = $2 \cdot 10^{-8}$m, ■– a = $0.25 \cdot 10^{-8}$m, ●– a = $0.125 \cdot 10^{-8}$m

The analysis of the experiments conducted shows that all probabilities and distributions of particles escapes have been insignificantly changing within the fluctuations of parameter r > 4. The simple geometry of the considered systems allows conducting real experimental researches on the process of heat and mass transfer in nanosystems. Such nanosystems might be used, for example, in cooling of electronic nanosystems. Taking into account the fact of small aerosol particles and viruses motion in dilute gas can be examined as a free molecular mode motion. It is possible to use these nanosystems as filters for catching these viruses.

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