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KINETIC THEORY OF TRANSFER PROCESSES

CONDENSATION COEFFICIENT: DEFINITIONS, ESTIMATIONS, MODERN EXPERIMENTAL AND CALCULATION DATA

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A brief analysis of different approaches to the calculation and measurement of the condensation coefficient of a vapor is presented. It is shown that, on frequent occasions, calculations give values of this coefficient that are at variance with the corresponding experimental data and that the condensation coefficient is determined most exactly on the basis of the molecular-kinetic theory. It was established that the spread in the literature data on the measured values of this coefficient is explained mainly by the fact that these values were obtained not in the immediate vicinity from the boundary between the gas and liquid phases but at a large distance (as compared to the mean free path of molecules) from it. Results of calculations of the condensation coefficient of argon by the method of molecular-dynamic simulation are presented.

Keywords: *condensation coefficient, velocity-distribution function of molecules, molecular-kinetic theory, molecular-dynamic simulation.*

Introduction. In the case where the processes of evaporation of a liquid and condensation of a gas (vapor) on its surface are investigated by the method of continuous-medium mechanics, corresponding boundary conditions are formulated depending on the features of the gas flow in a thin (Knudsen) layer [1]. The parameters of this flow are determined by the Boltzmann kinetic equation, for solution of which it is necessary to know the velocity-distribution function f_+ of the gas molecules flying from the phase boundary. It was shown in [2] that, of all the gas molecules falling on the surface of a liquid, only their part determined by the coefficient β is condensed on this surface, and the other part of the molecules $(1 - \beta)$ is reflected from it. Thus, in the general case, the function f_+ determining the velocity distribution of the molecules flying from the surface of the condensed phase is divided into two parts, the first of which f_e defines the evaporated molecules and the second one f_r defines the molecules reflected from the interface:

$$f_+ = f_e + (1 - \beta) f_r \ .$$

Here, the condensation coefficient β is determined as the ratio between the number of the molecules condensed on the liquid surface and the number of the molecules falling on it.

The authors of [3] investigated the evaporation of a liquid in a vacuum and established that the distribution function f_+ is fairly close to the Maxwell function. It was shown in [4] that, in the case where molecules are not reflected from the surface of a liquid in the process of its evaporation–condensation, "it would be reasonable to suggest that the molecules flying from the interface have a Maxwell velocity distribution." In [5], it was shown on the basis of the comparison of the results of the molecular-kinetic and molecular-dynamic calculations of the evaporation of a liquid in a vacuum that the velocity-distribution function of the molecules-flying from the interface corresponds to the semi-Maxwell semifunction in the case where the mass-flow velocity and the evaporation-surface temperature are equal to zero. Thus, to determine the velocity-distribution function of the molecules flying from the surface of a condensate, it is necessary to know the coefficient of condensation of molecules on this surface.

Methods of Determining the Condensation Coefficient. The notions of the coefficients of evaporation and condensation were introduced by M. Knudsen [6], who determined the evaporation coefficient as the ratio between the

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number of the molecules escaped from a liquid and the number of the molecules moving from the boundary between the liquid and the gas with zero Maxwell velocity and saturation density corresponding to the temperature of the interface. At a later time, this scheme of evaporation was called the diffusion. It is frequently supposed that the evaporation coefficient is equal in value to the condensation coefficient; however, it was shown in [7] that this supposition is correct only for the equilibrium state. It was established in [8] that the coefficients of evaporation β_e and condensation β_c of helium II are close to unity in the case of its low-intensity evaporation; in this case, $\beta_e \approx \beta_c$.

Different definitions of the condensation coefficient exist. For example, in [9], this coefficient was determined on the basis of the transient-state theory. In the series of works of Japanese authors [9–13], the condensation coefficient was determined by the method of molecular-dynamic simulation (MDS). In [10], the process of evaporation–condensation on the surface of argon at a temperature of 80 K was considered and its was shown that, for the equilibrium state of a liquid, the popular notion that the condensation represents a monomolecular reaction and the condensation coefficient is determined by the number of the vapor molecules reflected from the surface of a liquid is not always true. The point is that a gas molecule can be found on the surface of a liquid for a definite time with no transfer of its energy to the liquid, and then it can re-evaporate. In this case, it is impossible to differentiate the reflection from the re-evaporation and, in addition, molecular exchange is possible, with the result that the gas molecule falling on the surface of the liquid "dislodges" a liquid molecule from its surface. Therefore, to investigate the condensation process in detail (to follow the behavior of every molecule), it is necessary, in the view of the authors of [10], to estimate the energy transferred by a gas molecule falling on the surface of a liquid to the liquid molecules. Using this approach, the authors of [10] obtained, for the equilibrium state, the value 0.8 for the condensation coefficient. Analogous ideas were proposed in [11], where it was noted that an atom can be considered as condensed if it acquires a kinetic or a potential energy typical for the liquid atoms. In [12], with the use of correlation functions allowing one to determine the ratio β_r between the number of the gas molecules reflected from the surface of a liquid and the number of the gas molecules colliding with this surface, as well as the ratio β_{exch} between the number of the molecules participating in the molecular exchange and the total number of collisions, the following expression was obtained for the condensation coefficient: $\beta = 1 - (\beta_r + \beta_{exch})$. The authors of this work note that the molecular exchange is of crucial importance for any liquid (water, organic compounds). Dependences of the coefficients of condensation β, reflection β_r, and molecular exchange β_{exch} on the temperature of the surface of a liquid in the equilibrium state, obtained in [12], are presented in Fig. 1. It is interesting that, when the molecular exchange is disregarded, i.e., when it is assumed that $\beta = 1 - \beta_r$, the condensation coefficient is equal to ~0.9 throughout the temperature range being considered.

In [13], the following processes were investigated by the MDS method: 1) the evaporation–condensation of a pure liquid in the case where the liquid–vapor system is in the equilibrium state; 2) the evaporation–condensation of this liquid under the nonequilibrium conditions, and 3) the evaporation–condensation of a liquid mixture. The authors of this work separated four types of behavior of a gas (vapor) molecule near the boundary between a gas and a liquid: evaporation, reflection, condensation, and molecular exchange. They determined the condensation coefficient as the ratio between the number of the condensed molecules and the total number of the molecules falling on the surface of the liquid. Their calculations have shown that the condensation coefficient depends on the temperature of the liquid (Fig. 1). The authors of [13] speculated that this dependence is due to the molecular exchange. They note that, in the case where a condensate has a low temperature, the number of the liquid-phase molecules found near the interface is much larger than at a high temperature. In this case, the energy of a falling molecule is effectively scattered and, as a result, the molecule is condensed practically completely. However, when the number of the molecular bonds in a liquid is small, the energy of a falling gas molecule is transferred to a small number of liquid molecules, with the result that re-evaporation can take place, i.e., the falling gas molecule and a liquid molecule can exchange places. Moreover, it is shown in [13] that the coefficients of evaporation and condensation are more difficult to determine under nonequilibrium conditions. In this work, the situation where a hot vapor of argon contacts with a cold liquid argon film was considered. The initial temperature of the vapor was equal to 150 K, the temperature of the liquid was equal to 80 K, and the density of the vapor was critical (1/3). An examination of the liquid–vapor system with the indicated initial parameters during 100 ps gives the value of the condensation coefficient $\beta = 0.9$, which differs from the value 0.8 of this coefficient obtained under the equilibrium conditions.

The condensation of gas molecules on the surface of a liquid with transfer of their energy to the liquid molecules was investigated by Langmuir [2, 14], who supposed that the time necessary for the scattering of the energy obtained as a result of the collision of a gas molecule with one or several molecules on the surface of the liquid corresponds, in order of magnitude, to the period of vibrations of the liquid molecules in the condensed state. Taking into account the fact that energy is transferred rapidly from molecule to molecule, Langmuir speculated that the condensation coefficient is equal to unity. The authors of [15], where the condensation of a water vapor on the surface of a water with a temperature ranging from 268 to

300 K was investigated by the MDS method, also inferred that the condensation coefficient is close to unity for the indicated temperature range. It was shown in some works that the condensation coefficient depends on the vapor pressure [7, 16] and the temperature of the condensed phase [13].

A large number of works were devoted to the experimental determination of the evaporation and condensation coefficients of substances. It should be noted that the values of the condensation coefficient obtained in these works fall within the fairly large range. For example, the experimentally determined values of the condensation coefficient of water vary from $\sim 10^{-2}$ to 1. The experimental values of this coefficient presented in review [7] range from 0.006 to 1.00. The values of the condensation coefficient of water determined in [17, 18] fall within the range from 0.4 to 1.0. It is noted in [15] that the value of this coefficient determined in different experiments range from 0.01 to 1. It seems likely that the large spread in the experimental data on the condensation coefficient of water, obtained in the indicated works, is explained by the fact that this coefficient was measured by the nondirect method, i.e., at a large distance (as compared to the mean free path of the vapor molecules) from the interface. Moreover, even small differences between the experimental conditions (the presence of an impurity on the condensation surface, the difference between the temperatures of the surfaces of the liquids being investigated, and so on) can have a crucial influence on the measurement results [12, 19, 20].

The aforesaid allows the conclusion that the condensation coefficient is determined most exactly from the standpoint of the molecular-kinetic theory, because it is precisely this theory in which a clear geometric boundary between the gas and liquid phases, called the interface, at which the condensation coefficient should be determined, is used. However, in actual practice, the boundary between the gas and liquid phases is not clearly defined, i.e., it represents a thin transient layer (in the molecular-dynamic scale) with a density changing from the density of the liquid to the vapor density. The thickness of this layer comprises several distances between the molecules (atoms) in the condensed phase [5, 12]. From the standpoint of molecular dynamics, a clear boundary between the phases is also absent. The position of this boundary can be determined only with certain assumptions.

It seems likely that the problem on the boundary between the phases is more simply solved from the standpoint of the continuous-medium mechanics. Actually, since the spreading of the vapor–liquid interface is substantially smaller than the characteristic scales used in the continuous-medium mechanics, it may be suggested that the boundary between the gas and liquid phases is close to the nonspread geometric boundary between them. However, in this case the above-presented definition of the condensation coefficient becomes not entirely correct. If the condensation coefficient is determined as the ratio between the number of molecules falling on the surface of a liquid and remaining on it and the total number of molecules flying to this surface, the following contradictions arise. The molecules flying to the surface of the liquid can interact repeatedly (as a result of the collisions) with the vapor molecules found near the interface and, as a result, can reflect back to the gas phase. It is significant that, in this case, the molecules do not reflect from the interface, which, apparently explains literature data suggesting that the condensation coefficient decreases with increase in pressure. Actually, an increase in the pressure leads to an increase in the frequency of intermolecular collisions; because of this the probability that a molecule will reflect before it reaches the condensation surface increases. It may be that a flow of molecules moving from the boundary between a gas and a liquid as a result of the evaporation of the liquid will reflect completely the flow of molecules flying to the surface of the condensed phase. In this case, the condensation coefficient should be close to zero, because neither of the molecules will reach the surface of the condensed phase.

Kinetic Analysis of the Condensation Process. It should be noted that when the evaporation of a liquid and the condensation of a vapor on its surface are investigated from the standpoint of the molecular-kinetic theory, it is assumed that the temperature of the interface is known and remains constant throughout the evaporation–condensation process. Consequently, it is important to determine the condensation coefficient at a constant temperature of the condensation surface. Because of this, in the present work, the coefficient of evaporation of a liquid and the coefficient of condensation of a vapor on its surface were determined for the case where the temperature of the interface remains unchanged and the molecules flying to it have definite parameters. The obtained values of the evaporation and condensation coefficients should characterize the ability of the phase boundary to absorb or reflect the molecules falling on it.

If all the molecules flying to the boundary between the gas and liquid phases remain on it, i.e., if they are condensed during the kinetic-relaxation time (in the molecular-kinetic time scale), the condensation coefficient, by definition, is equal to unity. Consequently, it makes sense not to try to make a comprehensive molecular-dynamic description of the condensation process but only to determine (simulate) the conditions at which all the molecules falling on the condensation surface adhere to it, including due to their penetration into this surface.

In [21], the approximate expressions for the boundary "conditions of slipping" in the process of evaporation of a liquid and condensation of a vapor on its surface are presented. These expressions were obtained for a two-component mixture without considering the Knudsen layer on the assumption that the flow of molecules escaped from the surface of the liquid ($y = 0$) consists partially of the evaporated molecules determined by the coefficient β and the molecules reflected diffusely from the heated liquid surface on condition that the evaporation coefficient is equal to the condensation coefficient.

The following relations are true for a one-component gas:

$$\left|j\right| = \frac{2\beta}{2-\beta}\left(\frac{P_{\mathrm{s}}\left(T_{\mathrm{p.b}}\right)}{\sqrt{2\pi R T_{\mathrm{s}}}} - \frac{P_{\infty}}{\sqrt{2\pi R T_{\infty}}}\right),$$

$$V_x = l\,\frac{\partial V_x}{\partial y} + \frac{3}{4}\,l\left(\frac{2R}{\pi T}\right)^{1/2}\frac{\partial T}{\partial x},$$

$$T - T_{\mathrm{p.b}} = \frac{15}{8}\,l\,\frac{\partial T}{\partial y} - \frac{V_y}{8}\left(\frac{2\pi T}{R}\right)^{1/2}.$$

The first of these relations can be also used for a two-component mixture on condition that the pressures involved in it are the partial pressures of the evaporating and condensing components. In this case, the equality $(T_{\mathrm{p.b}} - T_{\infty})/T_{\mathrm{p.b}} << 1$ should be fulfilled.

In the late 1970s, the following approximate formula was proposed for calculating the density of a stationary one-dimensional mass flow of a condensing vapor propagating with a subsonic velocity [22]:

$$\left|j\right| = 1.67\,\frac{P_{\infty} - P_{\mathrm{s}}}{\sqrt{2\pi R T_{\infty}}}\left\{1 + 0.51\,\ln\left(\frac{P_{\infty}}{P_{\mathrm{s}}}\sqrt{\frac{T_{\mathrm{p.b}}}{T_{\infty}}}\right)\right\}. \tag{1}$$

This relation was obtained for the case where the molecules falling on the surface of a liquid are completely condensed, i.e., the condensation coefficient is equal to unity. In [23], an equation for calculating the evaporation–condensation process by the diffusion scheme of reflection of molecules from the interface at arbitrary evaporation and condensation coefficients has been derived.

In the case where the condensation coefficient differs from unity, formula (1) takes the form

$$\left|j\,\right|_{\beta\neq1}\Big| = 1.67\,\frac{P_{\infty} - P_0}{\sqrt{2\pi R T_{\infty}}}\left\{1 + 0.51\,\ln\left(\frac{P_{\infty}}{P_0}\sqrt{\frac{T_{\mathrm{p.b}}}{T_{\infty}}}\right)\right\}. \tag{1a}$$

The following relation is true for an ideal gas:

$$P_0 = \rho_0 R T_{\mathrm{p.b}}\,. \tag{2}$$

In accordance with [23],

$$\rho_0 = \rho_{\mathrm{s}}\left(1 - \frac{1-\beta}{\beta}\,\frac{j}{\rho_{\mathrm{s}}\sqrt{\dfrac{RT_{\mathrm{p.b}}}{2\pi}}}\right) = \rho_{\mathrm{s}}\left(1 + \frac{1-\beta}{\beta}\,\frac{\left|j\right|}{\rho_{\mathrm{s}}\sqrt{\dfrac{RT_{\mathrm{p.b}}}{2\pi}}}\right). \tag{3}$$

The system of three equations (1a), (2), and (3) includes, at definite values of $T_{\mathrm{p.b}}$, P_{s}, T_{∞}, and P_{∞}, the three unknowns $\left|j\right| = \left|j\,\right|_{\beta\neq1}\Big|$, ρ_0, and P_0, which can be determined from the solution of the indicated equations.

In 1988, an author of the present work [24] obtained an equation for determining the minimum (limiting) value of the condensation coefficient β_{lim}, at which condensation with a stationary one-dimensional vapor flow propagating with a definite velocity u_{∞} is possible. This equation was obtained in the following way. Since $\left|j\right| = \rho_{\infty}\big|_{\beta\neq1}\,|u_{\infty}|$, Eq. (3) can be written in the form

$$\rho_0 = \rho_s \left[1 + \frac{1-\beta}{\beta} \frac{\rho_\infty\big|_{\beta\neq1} |u_\infty|}{\rho_s \sqrt{\dfrac{RT_{\text{p.b}}}{2\pi}}} \right]. \tag{4}$$

In the case where the condensation coefficient is not equal to unity, ρ_s can be replaced by ρ_0, and the following relation can be used:

$$\frac{\rho_\infty\big|_{\beta\neq1}}{\rho_0} = \frac{\rho_\infty\big|_{\beta=1}}{\rho_s}. \tag{5}$$

Let us substitute ρ_0 from (5) into (4) and determine, from the expression obtained, the quantity $\rho_\infty\big|_{\beta\neq1}$:

$$\rho_\infty\big|_{\beta\neq1} = \frac{\rho_\infty\big|_{\beta=1}}{1 - \dfrac{1-\beta}{\beta} \dfrac{\rho_\infty\big|_{\beta=1}}{\rho_s} \dfrac{|u_\infty|}{\sqrt{RT_s/2\pi}}}. \tag{6}$$

From this expression, one can determine the minimum condensation coefficient at which the condensation with a definite rate u_∞ is possible. In this case, the denominator of (6) is zero, i.e., the quantity $\rho_\infty\big|_{\beta\neq1}$ tends to infinity. In the final analysis, from (6) we obtain

$$\beta_{\text{lim}} = \frac{1}{1 + \dfrac{1}{j'}}, \qquad j' = \frac{\left| j\big|_{\beta=1} \right|}{\rho_s \sqrt{\dfrac{RT_{\text{p.b}}}{2\pi}}}. \tag{7}$$

Sometimes it is useful to express formula (7) in terms of the Mach number. For example, in the case of monoatomic gas, where the velocity of sound is calculated by the formula $\alpha_\infty = \sqrt{\frac{5}{3} RT_\infty}$, we obtain

$$\beta_{\text{lim}} = \frac{1}{1 + \sqrt{\dfrac{3}{10\pi}} \dfrac{1}{\dfrac{\rho_\infty\big|_{\beta=1}}{\rho_s} \text{M}_\infty \sqrt{\dfrac{T_\infty}{T_s}}}}. \tag{8}$$

The use of formula (1), where $j = u_\infty \rho_\infty\big|_{\beta=1}$, in combination with formula (8) in the case where the mach number is determined as $\text{M}_\infty = u_\infty/a_\infty$ gives the following expression for β_{lim}:

$$\beta_{\text{lim}} = \frac{1}{1 + \dfrac{3}{5} \dfrac{\sqrt{\dfrac{T_\infty}{T_{\text{p.b}}}}}{\left\{ 1 + 0.51 \ln \left(\dfrac{P_\infty}{P_s} \sqrt{\dfrac{T_{\text{p.b}}}{T_\infty}} \right) \right\} \left(\dfrac{P_\infty}{P_s} - 1 \right)}}. \tag{9}$$

For example, at $\frac{P_\infty\big|_{\beta=1}}{P_s} = 4$ and $\frac{T_\infty}{T_{\text{p.b}}} = 2$, $\beta_{\text{lim}} = 0.84$. Consequently, at $\beta_{\text{lim}} < 0.844$, condensation is impossible.

Formulation of the MDS Problem. The coefficient of condensation of a vapor on the surface of a liquid film simulated by a system of N molecules in the form of a parallelepiped with sizes $L_x \times L_y \times L_z$ (Fig. 2) is determined.

The interaction between the ith and jth molecules is determined by the Lennard-Jones potential:

$$U(r_{ij}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right], \tag{10}$$

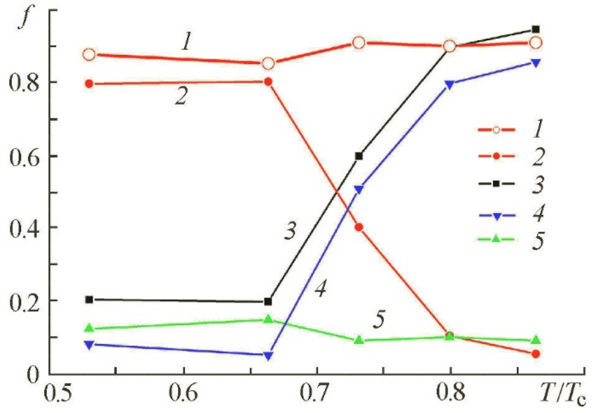

Fig. 1. Dependences of the condensation, reflection, and molecular-exchange coefficients on the surface temperature of a liquid: 1) $\beta = 1 - \beta_r$; 2) $\beta = 1 - (\beta_r + \beta_{exch})$; 3) $\beta_r + \beta_{exch}$; 4) β_{exch}; 5) β_r.

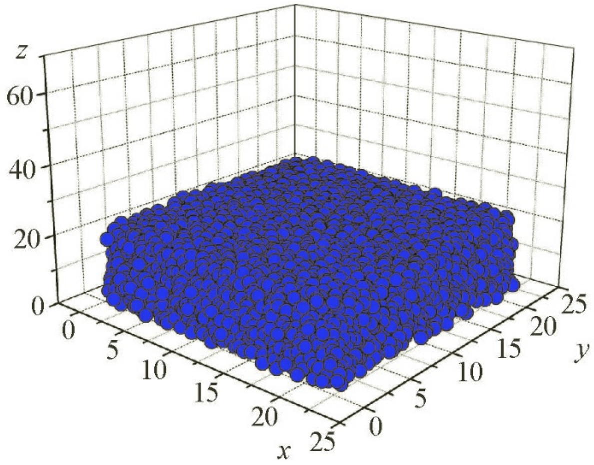

Fig. 2. Liquid film before the condensation process.

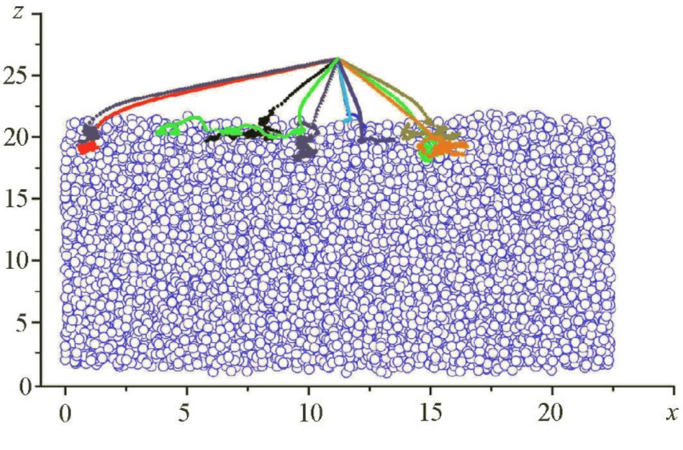

Fig. 3. Trajectories of the particles interacting with the liquid surface at $T_g = 1.07$ and $T_{liq} = 0.25$.

and the movement of molecules is defined using the molecular-dynamics method and the second Newton law

$$\mathbf{F}_i = m_i \frac{d^2\mathbf{r}_i}{dt^2}, \qquad i = 1, \dots, N, \tag{11}$$

where F_i is the interaction force determined by differentiation of potential (10) and m_i is the molecular mass.

The following dimensionless quantities were used in the calculations: the diameter of a molecule σ was used as the length unit, the potential well depth ε was used as the energy unit, the quantity $\sigma\sqrt{m/48\varepsilon}$ was used as the time unit, and the quantity ε/k was used as the temperature unit. The dimensionless temperature was determined by the formula

$$T = \frac{16}{N}\sum_{i=1}^{N} V_i^2, \tag{12}$$

where $V_i = v_i - u$.

For integration of Eq. (11), the initial coordinates and initial velocities of the molecules are prescribed. It is assumed that initially molecules are positioned at the sites of a simple cubic lattice inside the parallelepiped being considered and their velocities are distributed randomly in value and direction. In this case, the velocities of the molecules are normalized such that the temperature of the system formed by them, determined by their mean kinetic energy, has a definite value. The total number of molecules in the system $N = 8000$.

At the initial stage of simulation of the condensation of a vapor on the surface of a liquid having a definite temperature, the system is brought into the equilibrium state. At first, the temperature of the liquid is calculated in intervals of 10 time steps, and the values obtained are compared with the prescribed ones, after which the velocities of the molecules are changed such that they are equal. This procedure is carried out during 10,000 time steps, whereupon the process of scaling of the velocities of the molecules is terminated; however, the calculation is continued during additional 10,000 steps. At the first and second stages of the transformation of the system of particles into the equilibrium state, the periodic boundary conditions are used. After the first stage is completed, a liquid film with a definite surface temperature is obtained. Then, by an analogous method, the velocity distribution of the gas-phase molecules is determined; in this case, the temperature of the gas differs from the temperature of the liquid.

After the indicated stages of simulation are complited, we obtain a liquid film with a definite initial temperature, on which gas molecules moving with a definite velocity corresponding to the gas temperature are deposited. As noted above, the coefficient of condensation of a gas on a liquid should be determined in the case where the surface temperature of the liquid is constant, because this coefficient characterizes the ability of the liquid surface to entrain or reflect the gas molecules falling on it. To provide this condition, we assumed that the gas is condensed from the region positioned above the liquid surface (the region of $z > 22.0$ in Fig. 2). Of the set of all the gas molecules, the molecules moving to the liquid surface, i.e., the molecules for which the condition $V_z < 0$ is fulfilled, are selected. In this case, a molecule selected in this way begins to move from the point positioned at a cutoff-radius distance from the liquid surface. The choice of such a distance is explained by the fact that, at it, a gas molecule begins to "feel" the presence of the liquid phase and the liquid begins to "feel" the presence of the gas molecule. Therefore, the parameters of the movement of molecule (their velocity and coordinates in each time step) in the condensed and gas phases should be determined with account for the indicated effect. The observation of a gas molecule in the model system being considered continues until this molecule "submerges" into the liquid or rebounds from its surface. The method used for observation of each molecule allows one to differentiate the reflection from the molecular exchange. After this procedure is completed, another molecule selected from the set of gas molecules is observed. It should be noted that before the observation of the every next gas molecule, the liquid surface is brought into the initial state. Thus, each gas molecule falls on one and the same liquid surface and interacts only with the liquid-phase molecules.

Discussion of the Results Obtained. Results of determination of the coefficient of condensation of argon on the surface of its liquid film at $T_{\text{g}} = 1.07$ and $T_{\text{liq}} = 0.25$ are presented in Fig. 3. It is seen from this figure that all the molecules falling on the liquid surface are absorbed by it. An analysis of the trajectories of all the molecules falling on the liquid surface has shown that the condensation coefficient determined for the indicated gas and liquid temperatures comprises 0.999.

The results of calculations of the coefficient of condensation of the gas on the liquid surface at different gas and liquid temperatures are presented in Table 1. It is seen from this table that, in the case being considered, the condensation coefficient is close to unity, and it decreases insignificantly (approximately by 8%) when the temperature of the liquid increases by 3.2 times.

TABLE 1. Results of Calculation of the Coefficient of Condensation of Argon on Its Liquid Film at Different Temperatures of the Gas and Liquid Phases

T_g	T_{liq}	β
1.07	0.25	0.999
1.07	0.5	0.992
1.07	0.7	0.935
1.07	0.8	0.912

CONCLUSIONS

1. Several definitions of the coefficient of condensation of a gas on the surface of a liquid exist. In the case where this coefficient is determined at the molecular-kinetic level, the representation of it as the fraction of the gas molecules (of the total number of the gas molecules falling on the surface of the liquid) that remain on the liquid surface after the collisions with other gas molecules seems worthwhile.

2. The large spread in the experimental data on the evaporation and condensation coefficients, obtained over several decades, is explained mainly by the fact that the mass flows of molecules falling on the surface of a liquid were measured not in the immediate vicinity of the interface but at a large distance from it. The known Hertz–Knudsen formula is strictly true only for the free-molecular limit.

3. A calculation of the coefficient of condensation of argon on the surface of its liquid film with the use of the molecular-dynamic simulation method has given values of this coefficient as 0.9–1.0 for a ratio between the temperatures of the vapor and the liquid equal to 1.34–4.28.

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NOTATION

a_∞, sound velocity; j, mass flow density; k, Boltzman constant; l, mean free path of molecules; L_x, L_y, and L_z, sizes of the model liquid film in the directions x, y, and z; M_∞, Mach number; N, number of molecules in the model liquid film; P_s, equilibrium pressure of the vapor in the saturation state corresponding to the temperature $T_{p.b}$; R, individual gas constant; r_{ij}, distance between the ith and jth molecules; T, temperature; T_c, critical temperature; $T_{p.b}$, temperature of the phase boundary; T_∞ and P_∞, temperature and pressure of the vapor at a large distance (in the mean-free-path scale) from the phase boundary; t, time; $U(r_{ij})$, potential of interaction between the ith and jth molecules; u, mean-mass velocity of molecules; V_x, V_y, and V_z, projections of the relative velocity of gas molecules on the axis x, y, and z; v_i, velocity of the ith gas molecule; x, y, and z, Cartesian coordinates; β, β_e, β_r, and β_{exch}, coefficients of condensation, evaporation, reflection, and molecular exchange; β_{lim}, minimum value of the condensation coefficient; ε and σ, parameters of the molecular-interaction potential; ρ, vapor density. Subscripts: c, critical; e, evaporation; exch, exchange; g, gas; int, interface; liq, liquid; lim, limiting; r, reflection; s, saturation; p.b, phase boundary.

REFERENCES

1. M. N. Kogan, *Rarefied Gas Dynamics* [in Russian], Nauka, Moscow (1967).
2. I. Langmuir, Die Dissoziation des Wasserstoffs in Atome. III. Der Reaktionsmechanismus, *Zeits. Elektrochem.*, No. 26, 197 (1920).
3. V. V. Zhakhovskii and S. I. Anisimov, Numerical simulation of liquid evaporation by the method of molecular dynamics, *Zh. Élektrotekh. Fiz.*, **111**, Issue 4, 1328–1346 (1997).

4. J. W. Rose, Interphase matter transfer, the condensation coefficient and dropwise condensation, in: *Proc. 11th Int. Sci.-Techn. Conf.* (1998).
5. A. P. Kryukov and V. Yu. Levashov, Molecular-dynamic simulation of the processes of evaporation and condensation. Comparison with kinetic calculations, in: *Proc. 14th Minsk Int. Forum on Heat and Mass Transfer*, September 10–13, 2012, ITMO NANB, Minsk (2012), Vol. 1, Pt. 2, pp. 521–529.
6. M. Knudsen, Die maximale Verdampfungsgeschwindigkeit des Quecksilbers, *Ann. Phys., IY. B*, No. 47, 697 (1915).
7. R. Marek and J. Straub, Analysis of the evaporation coefficient and the condensation coefficient of water, *Int. J. Heat Mass Transf.*, No. 44, 39–53 (2001).
8. A. P. Kryukov and V. Yu. Levashov, About evaporation–condensation coefficients on the vapor–liquid interface of high thermal conductivity matters, *Int. J. Heat Mass Transf.*, No. 54, 3042–3048 (2011).
9. G. Nagayama and T. Tsuruta, A general expression for the condensation coefficient based on the transition state theory and molecular dynamics simulation, *J. Chem. Phys.*, **118**, No. 3, 1392–1399 (2003).
10. M. Matsumoto, K. Yasuoka, and Y. Kataoka, Molecular simulation of evaporation and condensation, *Fluid Phase Equilibria*, **104**, 431–439 (1995).
11. T. Tsuruta, H. Tanaka, and T. Masuoka, Condensation/evaporation coefficient and velocity distributions at liquid–vapor interface, *Int. J. Heat Mass Transf.*, No. 42, 4107 (1999).
12. M. Matsumoto, Molecular dynamics simulation of interphase transport at liquid surfaces, *Fluid Phase Equilibria*, No. 125, 195–203 (1996).
13. M. Matsumoto, Molecular dynamics of fluid phase change, *Fluid Phase Equilibria*, No. 144, 307–314 (1998).
14. I. Langmuir, The evaporation, condensation and reflection of molecules and the mechanism of adsorption, *Phys. Rev.*, No. 8, 149–176 (1916).
15. J. Julin, M. Shiraiwa, R. E. H. Miles, et al., Mass accommodation of water: Bridging the gap between molecular dynamics simulations and kinetic condensation models, *J. Phys. Chem.* A, No. 117, 410–420 (2013).
16. V. P. Isachenko, *Condensation Heat Transfer* [in Russian], Énergiya, Moscow (1997).
17. A. I. Neizvestnyi and L. I. Onishchenko, Experimental determination of the coefficient of condensation of a distilled water, *Izv. Akad. Nauk SSSR*, *Fiz. Atmos. Okeana*, **15**, No. 10, 1052–1059 (1979).
18. A. I. Neizvestnyi, G. B. Kotov, and L. I. Onishchenko, Determination of the coefficient of condensation of water during growth of micron-size droplets on hydroscopic condensation nuclei, *Izv. Akad. Nauk SSSR*, *Fiz. Atmos. Okeana*, **15**, No. 1, 74–81 (1979).
19. J. Niknejad and J. W. Rose, Interphase matter transfer: an experimental study of condensation of mercury, in: *Proc. R. Soc. Lond. A*, No. 378, 305 (1981).
20. A. K. Kosasie and J. W. Rose, New measurements for condensation of mercury — implications for interphase mass transfer, in: *Proc. 7th ASME National Heat Transf. Conf.*, San Diego, USA (1992).
21. N. V. Pavlyukevich, G. E. Gorelik, V. V. Levdanskii, et al., *Physical Kinetics and Transfer Processes with Phase Transformations* [in Russian], Nauka i Tekhnika, Minsk (1980).
22. D. A. Labuntsov and A. P. Kryukov, Analysis of intensive evaporation and condensation, *Int. J. Heat Mass Transf.*, **22**, 989–1002 (1979).
23. M. N. Kogan and N. K. Makashev, On the role of the Knudsen layer in the theory of heterogeneous reactions and in flows with surface reactions, *Izv. Akad. Nauk SSSR*, *Mekh. Zhidk. Gaza*, No. 6, 3–12 (1971).
24. A. P. Kryukov, Influence of the condensation coefficient on the flow of vapor with sub- and supersonic velocities in the process of condensation, *Izv. Akad. Nauk SSSR*, *Mekh. Zhidk. Gaza*, No. 2, 189–192 (1988).