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# VAPOR FLOW WITH EVAPORATION–CONDENSATION ON SOLID PARTICLES

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*Strongly nonequilibrium vapor (gas) flows in a region filled by solid particles are considered with allowance for particle-size variation due to evaporation–condensation on the particle surface. The study is performed by directly solving the kinetic Boltzmann equation with allowance for the transformation of the distribution function of gas molecules due to their interaction with dust particles.*

**Key words:** *dusty flow, vapor flow, condensation, evaporation, numerical calculation.*

**Introduction.** In various industries, a necessity has recently arisen in developing new procedures for predicting dusty gas flows with particle sizes ranging from some hundreds of angstroms to some tens or hundreds of micrometers. The development of a kinetic approach based on the Boltzmann equation for predicting homogeneous or heterogeneous condensation of vapor or vapor–gas mixtures in the presence of dust particles, drops, or clusters is a new research line in this field. The kinetic Boltzmann equation is theoretically rigorous, and the description of the motion and interaction of gas or vapor molecules, based on this equation, is well substantiated and quite adequate to the physical process.

The main specific feature in predicting strongly nonequilibrium flows of gas–dust mixtures, as compared to similar molecular-kinetic problems, is the presence of dust particles and condensation centers in the vapor or vapor–gas mixture; the size and mass of these particles can be several orders of magnitude greater than the size and mass of molecules. That is why the interaction between the molecules and condensation centers cannot be described by the Boltzmann collision integral for coupled interaction of gas molecules.

An approach that treat solid particles, in contrast to molecules, as macroscopic bodies and require the problem of gas flow around such a body to be solved is known. The area of application of this method is limited since it treats only a single solid particle, leaving aside the collective influence of dust particles on the gas flow. If the concentration of solid particles is high enough, statistical effects acquire fundamental significance and need to be taken into account.

In recent years, a new procedure for predicting the characteristics of gas–particle mixtures has been proposed [1]; in this procedure, the potential for a dust particle is calculated as the sum of potentials of individual molecules composing this particle, to be subsequently substituted into the collision integral. This approach makes it possible to solve many important problems and predict diffusion of dust particles several hundred angstroms in diameter. The use of the collision integral in its traditional form implies that the medium is sufficiently rarefied and the gas–particle collisions always involve no more than two participants, which somewhat narrows the applicability area of this method.

There exist methods for predicting dusty gas flows that are well substantiated from the theoretical standpoint but do not allow one to solve particular problems because they are too complex and cumbersome. For instance, Bogdanov et al. [2] developed a kinetic approach intended for predicting gas–particle flows. Yet, no solution of particular problems was obtained because the numerical implementation of this approach turned out to be too difficult. Broverman et al. [3] proposed another approach. A Monte Carlo simulation of mass transfer during substance filtration through a high-porosity bed with allowance for possible absorption of gas molecules impinging

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onto the surface was performed; yet, no change in geometric parameters of the porous medium due to evaporation–condensation was considered. Volkov and Semenov [4] examined a gas flow induced by a supersonic gas flow around a cylinder with entrainment of foreign disperse particles penetrating into the shock layer. The effect of the admixture was taken into account by introducing additional terms into the Navier–Stokes equations.

In the present paper, we propose an approach based on direct numerical solution of the kinetic Boltzmann equation, which takes into account both the gas interaction with solid particles and intermolecular collisions [5]. Since the condensation centers are large enough, their collisions with molecules can be described as an interaction of gas molecules with a large-size body (in particular, with the body surface) using various reflection models for gas molecules. At the same time, the dust distributed in the flow field consists of microscopic particles $10^{-7}$–$10^{-5}$ m in diameter, and their concentration in many problems of practical importance is sufficiently high to describe the processes at the level of the distribution function. Hence, to study nonequilibrium processes with participation of such particles, one can and has to use methods of the molecular-kinetic theory. The interaction involved in the description makes it possible to take into account gas condensation on solid-particle surfaces, the increase in the thickness of the deposited layer, and the associated time variation of collision cross-sections of dust particles, drops, or clusters.

**Mathematical Description.** Generally, the system of the kinetic Boltzmann equations for two-species flows can be written as

$$\frac{\partial f_g}{\partial t} + \xi_x \frac{\partial f_g}{\partial x} = J_{gg} + J_{gp}, \qquad \frac{\partial f_p}{\partial t} + \xi_x \frac{\partial f_p}{\partial x} = J_{pp} + J_{pg}. \tag{1}$$

Here, $x$ is the coordinate, $t$ is the time, $f_g$ and $f_p$ are the velocity distribution functions of gas molecules and dust particles, $\xi_x$ is the $x$-component of the velocity vector $\boldsymbol{\xi}$, $J_{gg}$ and $J_{pp}$ are the collision integrals that describe the interaction among particles of one component, and $J_{gp}$ and $J_{pg}$ are the collision integrals that describe the interaction of dissimilar particles.

In writing the expression for the collision integral, we use the notation proposed by Kogan [6]:

$$J = \int \ldots \int_{\Omega} (f' f_1' - f f_1) |\boldsymbol{\xi} - \boldsymbol{\xi}_1| \, d\Omega, \qquad d\Omega = db \, d\varepsilon \, d\boldsymbol{\xi}_1. \tag{2}$$

Here, $\boldsymbol{\xi}$ and $\boldsymbol{\xi}_1$ are the velocities of two molecules prior to the collision, $f \equiv f(\boldsymbol{\xi})$ and $f_1 \equiv f(\boldsymbol{\xi}_1)$ are the velocity distribution functions of the molecules, $f' \equiv f(\boldsymbol{\xi}')$, $f_1' \equiv f(\boldsymbol{\xi}_1')$ ($\boldsymbol{\xi}'$ and $\boldsymbol{\xi}_1'$ are the velocities of the molecules after the collision), $b$ is the impact parameter, and $\varepsilon$ is the angular impact parameter. With increasing mass and size ratios of particles of the two components, the solution of (1) becomes more difficult.

The difficulties in the joint solution of Eqs. (1) are primarily related to the presence of four collision integrals in the system, two of them being cross integrals that describe the interaction between dissimilar components in the mixture.

If the mass of the solid particle is much greater than the molecular mass, the velocity of solid particles is low compared to the thermal velocity of molecules. For instance, if the mass ratio equals $10^4$–$10^{10}$, the difference between the mean velocities amounts to $10^2$–$10^5$; for this reason, the motion of dust particles is almost unnoticeable on the background of the gas motion. It should be noted, however, that, if the dust distribution function changes (owing to dust–dust collisions), the gas will very soon “adjust” itself to the “new” dust parameters. In calculation of dusty gas flows, this fact allows one to independently calculate the dust distribution function at each time step and then take into account these new dust parameters in calculating the gas distribution function. Thus, in certain cases, it is possible to solve, instead of system (1), two independent equations: one for the gas, with allowance for the change in its distribution function due to interaction with solid particles, and the other for the dust.

If, in solving the problem, of primary interest is the gas flow under fixed dust parameters (e.g., modeling of flows through porous media), one can use only one equation from system (1), which describes the gas flow, for gas–dust mixtures with disparate masses of the components. Here, the multiple integral $J_{gp}$ is to be replaced by the distribution-function transformation procedure developed by the present authors.

**Method of the Solution.** The present study of gas flows with condensation centers is based on the kinetic Boltzmann equation, which has the following form in the one-dimensional unsteady formulation:

$$\frac{\partial f_g}{\partial t} + \xi_x \frac{\partial f_g}{\partial x} = J_{gg} + J_{gp}. \tag{3}$$

Since the mixture consists of particles of different sizes, it is rather difficult to find $J_{gp}$. To avoid the difficulties, we treat the collisions of molecules with condensation centers as the interaction of molecules with large-size bodies (in particular, with the body surface), using various models of reflection of gas molecules. The solution of (3) yields the velocity distribution function of the molecules. The macroparameters (density, temperature, pressure, mass fluxes, energy, and other moments of the distribution function) can be found by integration over the three-dimensional velocity space:

$$n = \int f \, d\boldsymbol{\xi}, \qquad u = \frac{1}{n} \int \xi f \, d\boldsymbol{\xi}, \qquad j = m \int \xi f \, d\boldsymbol{\xi}, \qquad \frac{3}{2} nkT = \frac{1}{2} m \int (\xi - u)^2 f \, d\boldsymbol{\xi}.$$

Here $n$ is the concentration of gas molecules, $T$ is the temperature, $k$ is the Boltzmann constant, and $m$ is the molecular mass.

In solving the kinetic Boltzmann equation (3), the numerical procedure of [7] is used, which comprises a conservative finite-difference approximation of the differential part of the equation and special Korobov formulas for calculating the quintuple gas–gas collision integral with sufficient accuracy. Within the framework of the discrete model, it is assumed that the molecular velocity is determined by a fixed velocity grid. The basic equation is replaced by a set of many (several hundreds or thousands) finite-difference equations with nonlinear right sides.

The main stages in the algorithm used are as follows:

1. Motion without collisions:

$$\frac{\Delta f^k}{\Delta t} + \xi_x^k \frac{\Delta f^k}{\Delta x} = 0.$$

2. Spatially uniform gas–gas relaxation:

$$\frac{\Delta f^k}{\Delta t} = J_{gg}^k.$$

Stages 1 and 2 form the basis of the method of direct solution of the kinetic Boltzmann equation [7].

3. Transformation of the velocity distribution function of gas molecules due to their interaction with the surfaces of solid particles.

4. Calculation of macroparameters.

Calculation of the change in the gas distribution function due to gas interaction with the dust is the key point in the approach proposed.

Transformation of the velocity distribution function of gas molecules is illustrated by Fig. 1. The transformation procedure is as follows. Within the framework of the discrete model, it is assumed that the molecule velocities $\boldsymbol{\xi}_k$ are determined by a fixed velocity grid. During a finite time interval $\Delta t$, only some part ($n^r$) of all gas molecules with a concentration $n$ will impinge onto the solid particle. Thus, the velocity distribution function $f_k$ of gas molecules will include an unchanged component $f_k^n$ due to molecules not interacting with solid particles and a component $f_k^r$ undergoing collision-induced transformation (the subscript $k$ denotes the $k$th nodal point of the velocity grid):

$$f_k = f_k^n + f_k^r.$$

The total number of gas molecules per unit volume that collide with dust particles during the time $\Delta t$ is

$$n_k^r = N_p n_k \pi D_*^2 g \, \Delta t / 4. \tag{4}$$

Here, $D_* = D_p + d$ ($D_p$ is the solid-particle diameter), $d$ is the gas-molecule diameter, $g$ is the absolute velocity of gas molecules with respect to solid particles, $N_p$ is the concentration of solid particles, and $n_k = f_k \Delta\xi^3$ is the concentration of gas molecules whose velocity is $\boldsymbol{\xi}_k$.

One can use Eq. (4) to determine the distribution function $f_k^r$ for the total number of molecules impinging onto dust particles during the time $\Delta t$.

As gas molecules interact with the solid surface, these molecules suffer scattering according to the reflection model, e.g., diffuse scattering. The molecules with identical pre-collision velocities $\boldsymbol{\xi}_k$ acquire different post-collision velocities in line with the Maxwellian distribution. The density of reflected gas molecules $n_{\rm ref}^k$ can be found from the impermeability condition. If the condensation factor $\beta$ equals zero ($\beta = 0$), then we have

$$n_{\rm ref}^k = n_r^k |\boldsymbol{\xi}_k| \Big/ \sqrt{RT_p/(2\pi)}\,,$$

where $T_p$ is the dust-particle temperature. If $\beta \neq 0$, the density of reflected molecules can be found with allowance for condensation:

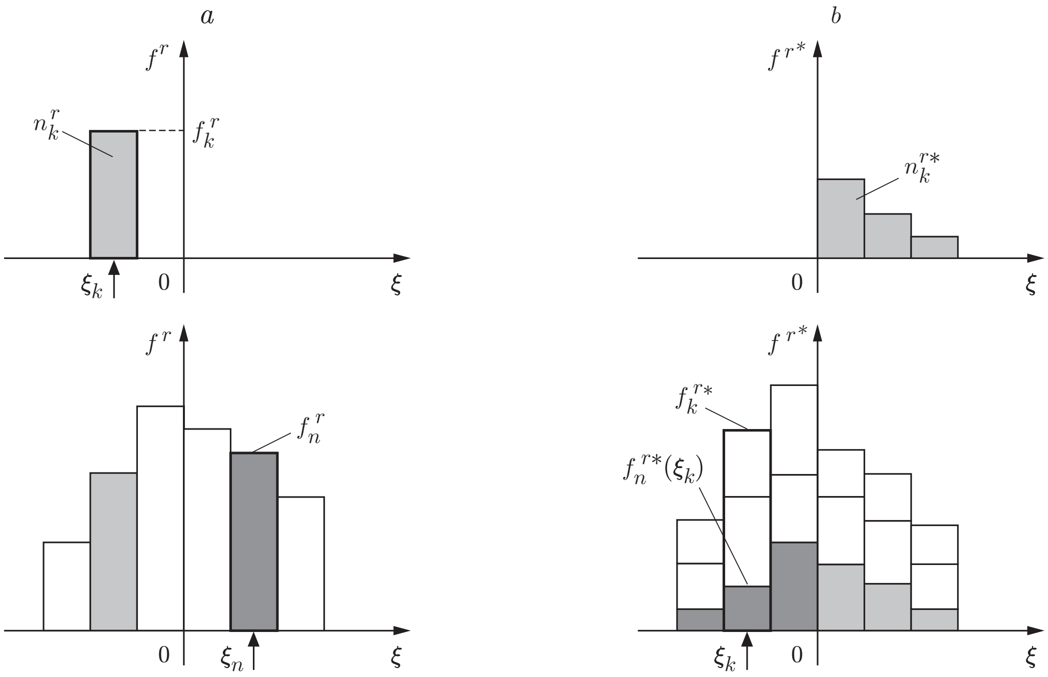

Fig. 1. Transformation of the distribution function due to gas–dust interaction: prior to the interaction (a) and after the interaction (b).

$$n_{\rm ref}^k = (1-\beta)n_r^k|\boldsymbol{\xi}_k|\Big/\sqrt{RT_p/(2\pi)}.$$

The condensation factor is

$$\beta = (j_{\rm inc} - j_{\rm ref})/j_{\rm inc},$$

where $j_{\rm inc}$ and $j_{\rm ref}$ are the incident and reflected specific mass fluxes, respectively.

A similar procedure is to be performed at each nodal point $\boldsymbol{\xi}_k$ of the velocity grid.

The velocity distribution function of gas molecules after their collision with solid particles, $f_k^{r*}$, can be found by summation over all values of the reflected functions $f^*(\xi_n)$ at all velocity points $\xi_n$:

$$f_k^{r*} = \sum_{n=1}^{M} f_n^{r*}(\xi_k), \tag{5}$$

where $M$ is the total number of nodal points in the velocity grid. Expression (5) shows that each group of molecules whose pre-collision velocity is $\xi_n$ contributes to the post-collision distribution function $f_k^{r*}$.

Determining $f_k^{r*}$ by the algorithm described above, one can find the velocity distribution function of gas molecules after their collision with solid particles:

$$f_k^* = f_k^n + f_k^{r*}.$$

Repeating this procedure at all velocity points, one can find the distribution function in the entire phase space.

Next, the approach suggested above can be extended to the case of variable particle sizes, this variation being dependent on the total number of gas molecules stuck to the dust particle, which is determined in the course of the solution.

If the condensation factor is $\beta \neq 0$, the increase in size of solid particles due to gas (vapor) condensation can be substantial; this circumstance should be taken into account in treating the gas–dust interaction. In this case, the time-dependent dust-particle diameter is

$$D_p(t) = 2\{3(V + \sigma V_m)/(4\pi)\}^{1/3}. \tag{6}$$

Here, $V_m$ is the volume of molecules deposited onto the surface of a solid particle during the time $\Delta t$, $V$ is the volume of the dust particle at the previous time step, i.e., in the time interval $t - \Delta t$, and $\sigma$ is a quantity that

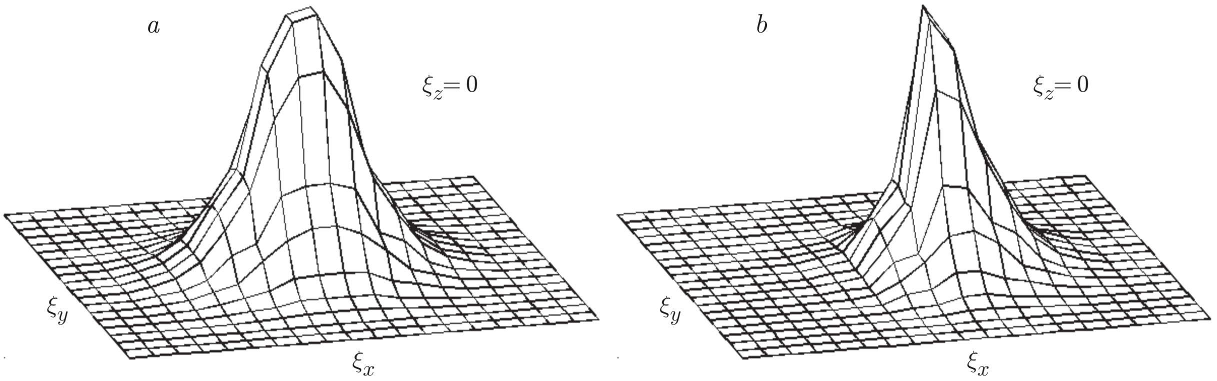

Fig. 2. Examples of the gas–molecule velocity distribution function near the interface between the phases: inside the porous body (a) and in the gas phase (b).

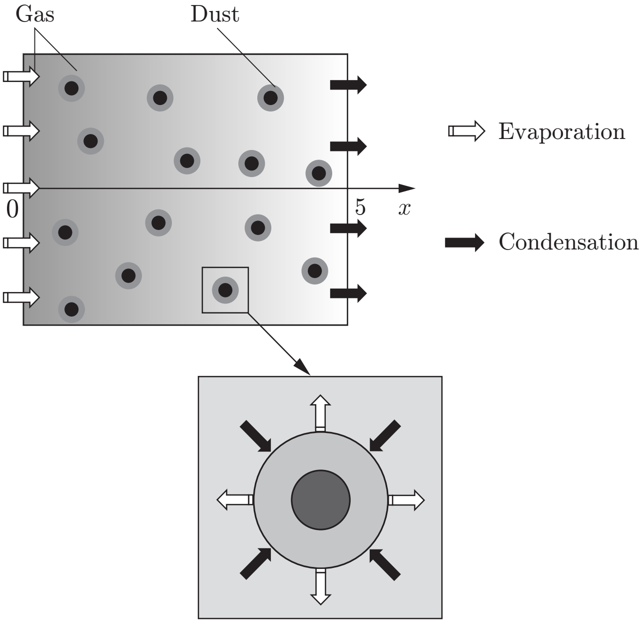

Fig. 3. Schematic of the problem.

characterizes condensate looseness. Thus, the diameter $D_* = D_p(t) + d$ should be inserted into Eq. (4) at each time step.

The approach proposed was verified on problem of gas flow through porous media [8, 9]. The porous body was modeled by the well-known "dusty gas" applied to particles shaped as spheres and cylinders. The resultant permeabilities were compared with available experimental data [10]. Figure 2 shows three-dimensional sections of the distribution function for the gas at various points in the calculation domain. The function is seen to be nonequilibrium even in the case of slow gas diffusion through the porous medium; for this reason, the molecular-kinetic approach can be applied to such problems and yields adequate results.

**Problem of Gas Flow Through a Dusty Region with Evaporation–Condensation on Solid Particles.** The schematic of the problem is shown in Fig. 3. Nitrogen (molecular weight 28 and molecular diameter $d = 3.7$ Å) enters the calculation domain through the surface $x = 0$. The velocity distribution function for the incoming gas is set as a half-Maxwellian with a base temperature $T_0 = 78$ K, concentration $n_0 = 1.0 \cdot 10^{26}$ m$^{-3}$, and zero transport velocity. At the initial time ($t = 0$), the number density of nitrogen molecules in the region under study is $1.0 \cdot 10^{21}$ m$^{-3}$. At the boundary $x = 5$, complete condensation of molecules occurs. The collisions between the nitrogen molecules are described within the framework of the hard-sphere model. The internal degrees of freedom are not excited.

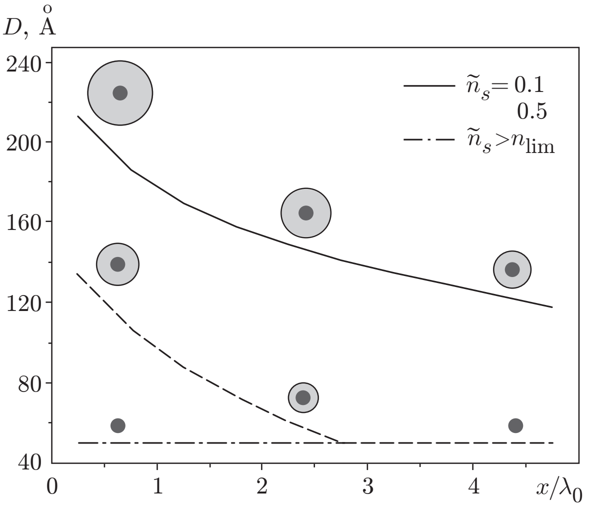

Fig. 4. Diameter of solid particles versus the coordinate.

Motionless solid particles (condensation centers) are uniformly distributed throughout the volume under study. Their concentration is $N_p = 0.0001n_0$, yielding the mean distance between the particles $r \approx 4.5 \cdot 10^{-8}$ m. The particle diameter at the initial time is $D_p = 93.8$ Å. Thus, the ratio is $\lambda_0/D_p \approx 1.7$. The time evolution of the gas density and solid-particle size is controlled by two opposite processes, evaporation and condensation, proceeding on solid surfaces. In the present calculations, the condensation factor is $\beta = 1$. Thus, we assume that nitrogen molecules impinging onto the particle surface get stuck to it; as a result, a deposited layer is formed, and the dust-particle diameter changes. Simultaneously, there exists a flux of molecules evaporating from the surface.

An increase (decrease) in the particle diameter prevails if the evaporation intensity is low (high). The evaporation process is characterized by the density of evaporating particles $\tilde{n}_s = n_s/n_0$ determined from the saturation curve depending on the temperature at the interface between the phases, i.e., at the dust-particle surface in our case. The distribution function of evaporating particles is set as a half-Maxwellian with a density $\tilde{n}_s$, surface temperature $\tilde{T}_s = T_s/T_0$, and zero transport velocity. In the present calculations, we had $\tilde{n}_s = 0.1$–$1.0$, which corresponds to particle surface temperatures $\tilde{T}_s \approx 0.8$–$1.0$.

The problem is unsteady. Both the solid-particle size and the distribution function of reflected gas molecules are time-dependent functions.

**Results.** As the calculation data show, the presence of solid particles in the region under study substantially affects the gas flow. The interaction of these particles with gas molecules becomes even more substantial in the case of evaporation–condensation proceeding at dust-particle surfaces. Because of two opposite processes, namely, the growth of the deposited layer of gas molecules and the evaporation of these molecules from the surface, the collision cross-sections are time-dependent quantities. An increase in the collision cross-sections increases the probability of gas-molecule deposition onto condensation centers. At the same time, the surface area of dust particles increases; as a consequence, the mass flux of evaporating particles into the ambient space also increases.

It should be noted that the present work was primarily aimed at studying specific properties of vapor flows interacting with dust particles in the case of appreciable variations of the condensation-center size. Solid particles up to several hundred angstrom in size were considered, and the deposited layer thickness was $D_p$.

Figure 4 shows the diameters of solid particles versus the coordinate for various densities of evaporating molecules $\tilde{n}_s$ ($\beta = 1$) in the case of a steady gas flow, i.e., for the steady solution ($\lambda_0 = 1.6 \cdot 10^{-8}$ m is the mean free path of gas molecules at $T = T_0$). The conventional representations of solid particles in this figure illustrate the relative thickness of the deposited layer on solid surfaces. The condensation-center diameter is seen to exhibit notable variations along the $x$-axis. For instance, in the vicinity of the left boundary, through which the gas enters the region under study, the particle size is greater than near the right boundary, where the gas is more rarefied. For instance, for a density of evaporating particles $\tilde{n}_s = 0.1$, the diameters of dust particles vary almost twofold (and the collision cross-sections, accordingly, by a factor of four). As the evaporation intensity increases ($\tilde{n}_s = 0.5$), the flux of condensing particles in the region $x > 2.8\lambda_0$ no longer compensates for the flux of evaporating particles

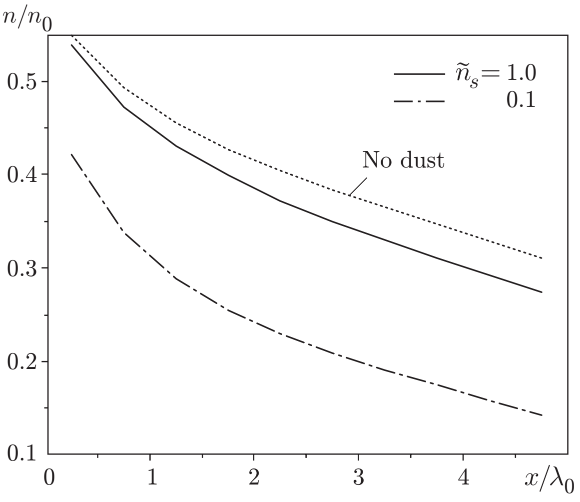

Fig. 5

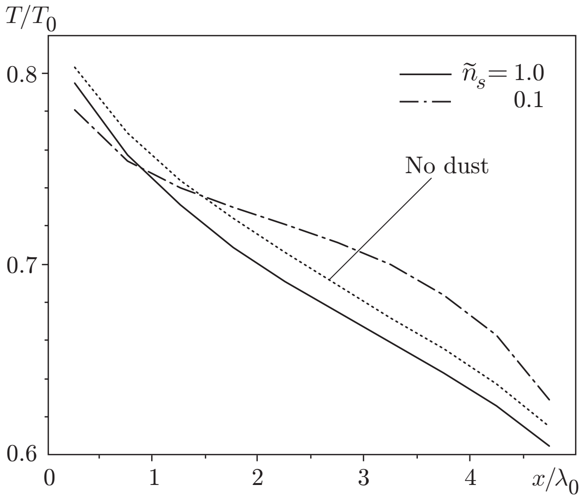

Fig. 6

Fig. 5. Vapor (gas) concentration versus the coordinate.

Fig. 6. Vapor (gas) temperature versus the coordinate.

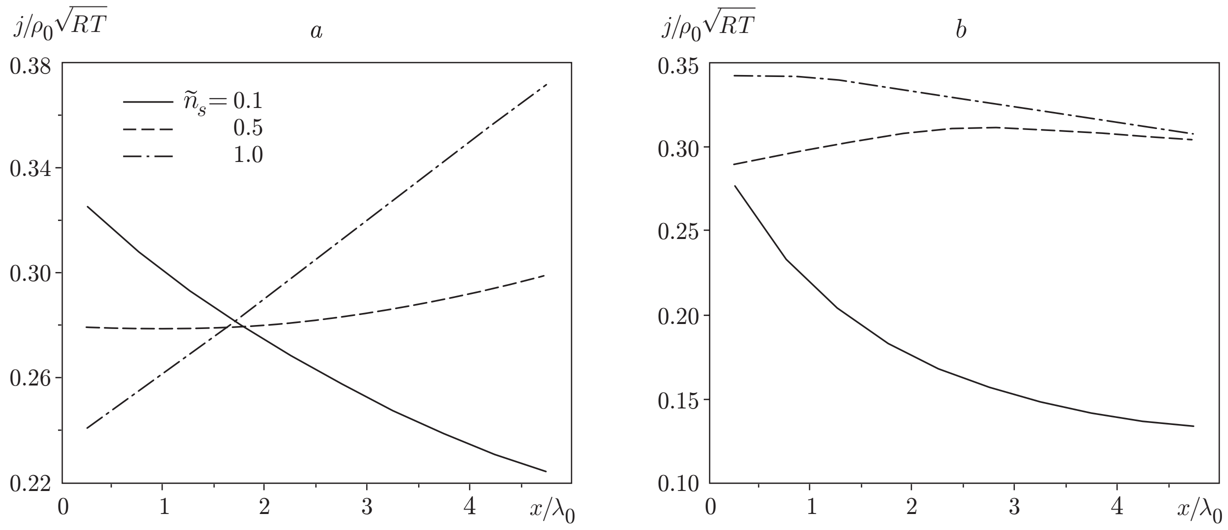

Fig. 7. Change in the vapor mass flux versus the coordinate: at the initial stage of the process (a) and steady solution (b).

because of insufficient gas density. The deposited layer is no longer formed on the dust particles. It should be noted that the minimum diameter of solid particles in the present study was 50 Å. The calculations show that there exists a certain limiting density of evaporating particles, $\tilde{n}_{\rm lim}$; for $\tilde{n}_s > \tilde{n}_{\rm lim}$, the increase in the dust-particle diameter becomes impossible throughout the whole region under study, because the mass entrainment due to evaporation prevails over the mass income due to condensation. For the parameters adopted in the present study, the limiting density of evaporating molecules is $\tilde{n}_{\rm lim} \approx 0.65$.

Figures 5 and 6 show the steady gas concentration and temperature as functions of the coordinate; for comparison, the data calculated for a vapor flow with ignored interaction with dust particles are also plotted. The curve $n(x)/n_0$ for $\tilde{n}_s = 1.0$ is profoundly shifted upward, as compared to the curve for $\tilde{n}_s = 0.1$. Such a behavior can be explained by the fact that the deposited layer thickness and the condensation-center size for $\tilde{n}_s = 1.0$ are smaller since evaporation is more intense. In the absence of dust, the vapor density in the calculation region is notably higher than the corresponding values for $\tilde{n}_s = 0.1$. In the latter case, a strong “pump-out” effect of condensation on dust particles is manifested.

In contrast to concentration, the temperature is less affected by intensity of evaporation on solid particles. The curves $T(x)/T_0$ for $\tilde{n}_s = 0.1$ and 1.0 differ quantitatively rather than qualitatively (see Fig. 6).

Figure 7 shows the densities of the mass flux versus the coordinate. The behavior of the curves $\tilde{j}(x) = j/(\rho_0\sqrt{RT})$ is governed by the joint action of three dominating factors: 1) evaporation of molecules from solid surfaces; 2) condensation on dust particles; 3) resistance of the system of particles to the directional gas flow. It is seen from Fig. 7a that the mass flux density for $\tilde{n}_s = 1.0$ at the early stage of the process increases along the $x$ axis approximately from 0.24 to 0.37. The reason is that, with such intense evaporation, molecules leaving the solid surfaces add to the gas flow that enters the region of interest. The opposite situation is observed for $\tilde{n}_s = 0.1$; here, the condensation prevails, and the mass flux density decreases. If the density of evaporating molecules is low, the main tendency is retained even after the steady state is reached. For $\tilde{n}_s = 1.0$, a steady flow is formed, in which the mass flux $\tilde{j}(x)$ varies from 0.3 to 0.35. The case $\tilde{n}_s = 0.5$ is remarkable for an almost perfect balance between evaporation and condensation during the whole time and throughout the entire flow region.

**Conclusions.** A new procedure for predicting gas flows through dusty regions with evaporation–condensation on dust particles is proposed.

The dust particles present in the calculation domain substantially affect the flow character.

In the problem considered, the size of dust particles varies owing to two opposite processes, evaporation and condensation. There exists a limiting evaporation intensity making the growth of particle size impossible because of immediate complete evaporation of the substance deposited onto the surface.

The results of the present paper were reported at the Russian Workshop “Kinetic Theory and Dynamics of Rarefied Gases” dedicated to the 130th anniversary of the publication of Boltzmann equation (Novosibirsk, December 2–7, 2002).

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