INVESTIGATION OF FLOWS OF A GAS-DUST MIXTURE BY THE METHODS OF MOLECULAR-KINETIC THEORY

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Using a direct numerical solution of the Boltzmann kinetic equation the problem of the flow of a gas-dust mixture is investigated with allowance for the motion of the dust. The qualitative analysis made has shown that in describing the flow of gas-dust mixtures it becomes possible to simplify the system of kinetic equations. The dependences of the density, the temperature, and the velocity of the gas on the coordinate have been obtained for different concentrations and velocities of the dust particles.

The present work is a continuation of [1–3], where consideration has been given to the issues of modeling, based on the methods of molecular-kinetic theory of description, gas-mixture flows in the presence of dust particles distributed in the flow region in question. The main feature of such flows is that the masses and collision cross sections of the components differ by several orders of magnitude. In [1, 2], the influence of dust on the character of flow has been studied; it has been assumed that the dust is uniformly distributed in the flow region and is at rest. In these works, we proposed an algorithm of transformation of the distribution function of gas molecules by velocities as a result of the interaction with dust particles, considered different geometries of the dust particles [2], and took into account the possibility for the gas to condense on the dust particles [3]. Unlike the works cited above, the present paper is devoted to the issues of modeling of the flow of a gas–dust mixture with allowance for the motion of the dust.

To describe the flow of a gas-dust mixture we must solve the system of Boltzmann kinetic equations that is written in general form as follows:

a)
$$\frac{\partial f_g}{\partial t} + \xi_x \frac{\partial f_g}{\partial x} = J_{gg} + J_{gp}$$
, b) $\frac{\partial f_p}{\partial t} + \xi_x \frac{\partial f_p}{\partial x} = J_{pp} + J_{pg}$. (1)

The system of equations (1) consists of two integro-differential equations whose solution is a rather difficult problem. Each of the equations involves cross collision integrals, i.e., J_{gp} and J_{pg} . The collision integral is a complex five-dimensional integral whose computation with a sufficient degree of accuracy turns out to be possible only when random cubature formulas are used [4]. Solution of the Boltzmann equations (1) containing four integrals for a two-component mixture is an even more difficult problem. In the present work, we consider the issue of the possibility of a simpler description of the flow of a gas-dust mixture with significantly differing masses of the components. This description is carried out based on (1a) using the method of direct numerical solution of the Boltzmann equation [4]. It is well known that as the ratio of the sizes and masses of the interacting particles of the mixture components increases it becomes more difficult to evaluate the collision integrals and to solve the Boltzmann equations. The procedure of [1-3] developed by the authors and employed in this work makes it possible, in solving Eq. (1a), to obviate a calculation of the multidimensional integral J_{gp} and replace it by the procedure of step-by-step computation of the distribution function of gas molecules by velocities which takes into account the interaction of these molecules with a solid particle.

The qualitative analysis presented below has shown that when mixtures with significantly differing masses of the components are considered it becomes possible to eliminate the second equation of system (1). Expression

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(1a) does not contain the equation for the dust-distribution function but takes into account changes in gas parameters due to the collisions with dust particles.

Qualitative Analysis of the Flow of a Gas-Dust Mixture. It has been assumed in the investigation that the flow region is uniformly covered with a moving dust. For a mass of the dust particles of $M_p \approx 10^4 - 10^{10} m_g$ the standard deviation of the velocity of motion of individual dust particles from the average velocity of motion of the dust is two orders of magnitude or more lower than for the gas. In describing the influence of the moving dust on the gas, this circumstance enables us to disregard the spread in the velocities of solid particles and to assume that the flow region is uniformly covered with dust particles moving with approximately the same velocities (see Appendix). The velocities of the dust particles are directed along the OX axis or are in opposition to it; the magnitude of the velocity varies. The dust particles are considered to be spherical.

By carrying out qualitative evaluations of the characteristic relaxation times, we can show that the distribution function of the dust particles changes little upon collision with the gas molecules. In [5], it has been shown that one can obtain the following expressions for the hard-sphere model:

$$\dot{\tau}_{gg} = 1, \quad \dot{\tau}_{gp} = \frac{4n_g}{n_p} \left(\frac{d_g}{D_p}\right)^2, \quad \dot{\tau}_{pg} = \frac{4D_p}{d_g}, \quad \dot{\tau}_{pp} = \frac{n_g}{n_p} \left(\frac{d_g}{D_p}\right)^{1/2}.$$
(2)

Here $\tau'_{ij} = \tau_{ij}/\tau_{gg}$ is the dimensionless characteristic mean free time of particles of the *i* type relative to particles of the *j* type (in what follows we will drop the primes on dimensionless quantities). To obtain the estimates (2) we employed expression (Π) (see Appendix).

As has been noted above, the dust particles are distributed uniformly in the flow region, i.e., the density is $n_p = \text{const.}$ Then, from the given relations, it follows that in the case in question the relaxation times are functions of the following quantities: n_g , d_p , and D_p .

Assuming that the collision cross sections are prescribed (see next section) and varying n_g from a certain value to zero, we obtain the plots of the characteristic relaxation times (Fig. 1). Figure 1a shows the relaxation times on condition that the dust particles are distributed in the flow region with a density of $n_p = 2.43 \cdot 10^{23} \text{ m}^{-3}$. The analogous plots for a value of $n_p = 1.22 \cdot 10^{24} \text{ m}^{-3}$ are presented in Fig. 1b. In constructing them, we assumed that $D_p = 93.8 \text{ Å}$ and $d_g = 3.7 \text{ Å}$, while the quantity n_g varied within the limits from 0 to $4.83 \cdot 10^{24} \text{ m}^{-3}$ (the OX axis). The value of the logarithm corresponding to the relaxation time was plotted on the *OY* axis.

From Fig. 1 it is clear that $\tau_{gp} \ll \tau_{gg}$. Thus, for the case of the highest concentration of the gas (Fig. 1b) $(n_g = 4.83 \cdot 10^{24} \text{ m}^{-3}) \tau_{gp}$ is nearly 40 times shorter than τ_{gg} while with decrease in n_g this difference increases. Consequently, the number of gas molecules colliding with dust particles over a finite period of time Δt is larger than the number of molecules colliding with each other. As a result, the gas distribution with parameters determined by two processes of collision, i.e., gas-dust and gas-gas, will be established after the time Δt .



Fig. 2. Scheme of solution of the problem.

It has been noted earlier that to describe the flow of a gas-dust mixture one must solve the system of Boltzmann equations (1). As follows from (1), the distribution function of dust particles can change as a result of two kinds of collisions: dust-gas and dust-dust.

The relaxation time τ_{pg} when the relaxation of the dust on the gas occurs is the longest (it is nearly 10^2 times longer than all the remaining times). This leads to the fact that dust parameters do not change due to the collisions with gas molecules, and evaluation of the collision integral J_{pg} can be obviated in the calculations. Consequently, the distribution function of dust particles by velocities changes on the scales of the relaxation times of the gas only as a result of the collisions of the particles with each other. However, it is necessary to note that if the dust-distribution function changes (as a result of the collisions of the dust with the dust), the gas responds to the "new" parameter of the dust rather quickly (since τ_{gp} is short). This fact enables us to independently calculate the dust-distribution function for the flows of gas–dust mixtures at each time step and then to take these new dust parameters into account in calculating the gas-distribution function. Thus, in certain cases we can solve two independent equations — one for the gas (with allowance for the transformation of the distribution function function function in question), the dust parameters remain constant and, as a consequence, evaluation of the collision integral J_{pp} can be obviated.

Thus, on the scale of the time τ_{gg} , the distribution function of dust molecules is a "slow" variable since it virtually does not change as a result of collisions with gas molecules.

From what has been said above it follows that in the case of flow of a gas-dust mixture with significantly differing masses of components one can employ just Eq. (1a).

Formulation of the Problem. Method of Solution. In the work, we consider the problem of determination of the flows of a gas-dust mixture with allowance for the motion of dust particles. The scheme of the problem is presented in Fig. 2.

From the left-hand surface (x = 0), evaporation of a gas (nitrogen) occurs. The gas is totally absorbed on the right-hand surface (x = 5). The region x = 0-5 is covered with dust particles. The temperature of the gas at the inlet to the flow region is $T_0 = 300$ K and the pressure is $P_0 = 20$ kPa. All the values for the densities and the temperatures are given in relation to the basis parameters for which we took the temperature T_0 and the density of nitrogen $n_g = 4.83 \cdot 10^{24} \text{ m}^{-3}$ corresponding to the value of the pressure P_0 . The coordinate x is given in the mean free paths of gas molecules for these parameters. It has been assumed that the flow region is uniformly covered with a moving dust. Consideration was given to two cases where the concentration of the dust was $n_p =$ $2.43 \cdot 10^{23} \text{ m}^3$ and $n_p = 1.22 \cdot 10^{24} \text{ m}^{-3}$. The left-hand and right-hand surfaces are absolutely transparent to dust. All the dust particles move with the same velocities which are directed along the *OX* axis or are in opposition to it. As an example the velocity of motion of the dust was assumed to be equal to two and three thermal velocities of motion of the gas molecules. It was considered that the dust particles represent spherical particles of diameter $D_p = 93.8 \text{ Å}$; their surface temperature was taken to be constant and equal to 300 K.

As has been noted above, to solve the kinetic equation (1a) we employ the method of [4] which involves the finite-difference approximation of the differential side of the equation and Korobov's special formulas to evaluate the integral of gas–gas collisions with a high degree of accuracy. Within the framework of the discrete model it is assumed that the molecules can have values of the velocities determined by a fixed velocity grid. The fun-



Fig. 3. Concentration distribution of the gas along the *OX* axis for the case of motion of the dust from the surface x = 0 (a) and toward the surface x = 0 (b).

damental equation is replaced by a system of a large number (of about several hundred or thousand) of finite-difference equations with a nonlinear right-hand side. This system is solved using the iteration procedure.

In evaluating the integral of gas-dust collisions, we employ the procedure of transformation of the distribution function presented in [1–3] in detail. Its essence is as follows. Only part of the gas molecules will collide with a solid particle over the finite period of time Δt . The velocity-distribution function will be a combination of two parts, i.e., of the first, constant part corresponding to the gas molecules that did not interact with the solid particle and the second part of the distribution function transformed as a result of collisions with dust particles. When the mass and size of the solid particles are large, the interaction between the dust particles and the gas molecules can be represented as the reflection of the latter from the surfaces of macroscopic bodies according to the model adopted, for example, the diffuse one.

In solving (1a), the initial and boundary conditions are specified as follows. It is assumed that gas molecules leave the surface x=0 with a Maxwellian distribution ($n_g=1$ and T=1) and a zero transport velocity (diffuse scheme). All the molecules arriving at the surface x=5 are totally condensed, i.e., there are no molecules escaping from this surface: $f_g \rightarrow 0$ for $\xi_x < 0$. As the initial condition (at t=0) it is assumed that $f_g \rightarrow 0$ in the entire calculational region.

Finally, we find, from Eq. (1a), the distribution function of the gas molecules by velocities for each point of the flow. The macroparameters (density, temperature, mass-mean velocity) are computed as moments of the distribution function [6].

Results of the Solution and Their Analysis. Results of the solution of the problem on gas flow through a region covered with a moving dust are presented in Figs. 3–5. Each figure shows two cases: (1) the velocity of motion of the dust flow is 2 and 3 magnitudes of the thermal velocity of the gas molecules; the concentration of the dust is $n_p = 2.43 \cdot 10^{23} \text{ m}^3$ and (2) the velocity of motion of the dust flow is the same, while the concentration of the dust is $n_p = 1.22 \cdot 10^{24} \text{ m}^{-3}$. As has been noted above, n_g is a basis parameter; therefore, $n_g = 4.83 \cdot 10^{24} \text{ m}^{-3}$ everywhere.

Figures 3a, 4a, and 5a show the density, temperature, and velocity distributions of the gas for the situation where the direction of the velocity of motion of the dust coincides with the OX axis. The results obtained for the dust moving in the opposite direction, i.e., to the plane x = 0, are presented in Figs. 3b, 4b, and 5b. It is clear from the plots that the presence of the moving dust in the flow region can substantially change the character of flow. The increase in the concentration of the dust causes the number density of the gas to decrease more slowly (see Fig. 3). Furthermore, the influence of the magnitude and direction of the dust velocity is pronounced.

It is well known that the kinetic temperature is a moment of the distribution function and represents the variance of molecular velocities. In passage of the gas through the layer of dust, the magnitude of the variance depends on two basic factors: (1) reflection from the surface of dust particles moving in space with velocities of the order of the thermal velocities of gas molecules and (2) increase in the number of collisions of gas molecules with dust particles. From the dependences presented in Fig. 4a it is evident that the increase in the concentration of the dust leads to a decrease in the gas temperature. Such behavior is attributable to the fact that the gas ve-



Fig. 4. Gas temperature vs. coordinate in the case of motion of the dust from the surface x = 0 (a) and toward the surface x = 0 (b).



Fig. 5. Change in the transport velocity of flow of the gas along the OX axis in the case of motion of the dust in the positive (a) and negative (b) directions.

locity adapts itself to the dust velocity as a result of collisions with dust particles (the number of such collisions is the larger n_p), which leads to a decrease in the variance of the distribution function characterizing the gas temperature). As is evident from Fig. 4b, for the case where the density of the solid particles is $n_p = 2.43 \cdot 10^{23} \text{ m}^{-3}$ the concentration of gas molecules is higher at the beginning of the calculational region (Fig. 3b) and the gas–dust collisions are rather frequent. We also note that the average velocity of the dust particles is directed to the surface x = 0 from which the gas molecules move as a result of evaporation. The interaction of these flows opposite in direction leads to an increase in the variance and as a consequence to an increase in the gas temperature. A fast decrease in the concentration of the gas in the direction of the *OX* axis leads to the fact that the collisions of the gas molecules with the dust particles and with each other become less frequent and the gas motion acquires increasing freedom. Finally, the variance (and consequently the temperature) decreases. In this case the dependence of the temperature curves for a concentration of the dust of $n_p = 1.22 \cdot 10^{24} \text{ m}^{-3}$ only in the region from x = 0 to x = 1.5. The reason is that for such a value of n_p the gas density decreases very rapidly and becomes comparable to the computational error when x > 1.5.

Figure 5 illustrates the process of acceleration or deceleration of the gas as a result of the interaction with the dust particles. From Fig. 5a it is evident that the average velocity of the gas increases but does not become equal to the velocity of the dust. Thus, for the case where $n_p = 2.43 \cdot 10^{23} \text{ m}^{-3}$ and $U_p = 3.0$ the maximum velocity of the gas is nearly 1.4. This is due to the fact that the character of flow is determined not only by the gas–dust collisions but by the gas–gas collisions as well. Figure 5b analogously demonstrates that the average velocity of the gas molecules and the more rapidly, the more frequent are the collisions between the gas molecules and the dust particles. Thus, for the case where $n_p = 2.43 \cdot 10^{23} \text{ m}^{-3}$ and $U_p = -3$ the gas velocity for the coordinate x = 0 is lower than the velocity for x = 5. This is attributed to the fact that the concentration of the gas is higher



Fig. App. Velocity-distribution functions for nitrogen molecules and dust particles.

for x = 0 (Fig. 3b) and as a consequence collisions of the gas-dust type are much more frequent. Accordingly, as a result of these rather frequent collisions of the gas molecules with the dust particles, the values of the positively directed velocities of the molecules which are caused by the diffuse character of evaporation from the left-hand (x = 0) surface decrease so that the average velocity of the gas becomes close to zero.

Thus, the qualitative analysis carried out and the results of the solution of the problem have shown that in considering the flows of gas-dust mixtures with allowance for the motion of the dust, one can obviate, under certain conditions, evaluation of the integral of dust-gas collisions (J_{pg}) and consider the system of kinetic equations for the dust and the gas separately at each time step.

APPENDIX

In the work, we consider a mixture of nitrogen (diameter of the collision cross section $d_g = 3.7 \text{ Å}$) and dust particles (diameter $D_p = 93.8 \text{ Å}$). As is shown in [5], for the case of a dense packing of molecules in a dust particle (the dust particle is not a snowflake of a sort) one can obtain the following relation between the diameters (collision cross sections) and masses of the colliding components:

$$\frac{D_{\rm p}}{d_{\rm g}} = \left(\frac{M_{\rm p}}{m_{\rm g}}\right)^{1/3}.$$
 (App)

Let us consider the relations between thermal velocities for nitrogen molecules and dust particles. By employing expression (App) we can write

$$u_{\rm g} = \sqrt{\frac{2kT_0}{m_{\rm g}}} , \ u_{\rm p} = \sqrt{\frac{2kT_0}{M_{\rm p}}} = \left(\frac{d_{\rm g}}{D_{\rm p}}\right)^{3/2} \sqrt{\frac{2kT_0}{m_{\rm g}}}$$

Thus, with increase in the diameter (or mass) of a dust particle the ratio u_p/u_g decreases and tends to zero when $D_p/d_g \rightarrow \infty$.

Let us assume that the distribution function of the gas (nitrogen) molecules by velocities has a Maxwellian form:

$$f_{\rm g} = n_{\rm g} \left(\frac{m_{\rm g}}{2\pi kT_0}\right)^{3/2} \exp\left(-\frac{m_{\rm g}\xi_{\rm g}^2}{2kT_0}\right).$$

The corresponding distribution function for the dust particles is

$$f_{\rm p} = n_{\rm p} \left(\frac{M_{\rm p}}{2\pi kT_0}\right)^{3/2} \exp\left(-\frac{M_{\rm p}\xi_{\rm p}^2}{2kT_0}\right).$$

From the given relations and expressions for the thermal velocities of the components it is evident that for the case where $M_p/m_g \gg 1$ the modulus of the exponent of the distribution function of the dust particles is much larger than the corresponding quantity for the gas function. This leads to the fact that the distribution function of the dust particles decreases much more rapidly than the distribution function of the gas molecules.

Let us consider, as an example, the plots of the distribution function for the nitrogen molecules and the dust particles. In constructing them, we have assumed that $n_g = 4.83 \cdot 10^{24} \text{ m}^{-3}$, $n_p = 2.43 \cdot 10^{23} \text{ m}^{-3}$, and $T_0 = 300 \text{ K}$ (these parameters were employed in solving the problem considered in the main part of the paper), the mass of a dust particle is computed from expression (App), and the velocities ξ_p and ξ_g varied from $-3u_g$ to $+3u_g$ (see Fig. App).

In describing the flow of a mixture consisting of light (gas) and heavy (dust) components, it may be considered that the velocity-distribution function of the dust particles on the velocity scale of the gas molecules is a delta function, in practice.

This work was carried out with financial support from the Russian Foundation for Basic Research (project Nos. 00-02-16273, 0.1-02-06215, and partially 00-15-96543).

NOTATION

 f_g , velocity-distribution function of the gas molecules; f_p , velocity-distribution function for the dust particles; ξ_x , component of the vector of the velocity ξ along the x axis; ξ , velocity of a molecule (dust particle) in a laboratory coordinate system; x, coordinate in the physical space; t, time; J_{gg} , collision integral describing the interaction of the gas molecules with each other; J_{gp} , collision integral describing the interaction of the gas molecules; J_{pp} integral of collisions of the dust particles with each other; J_{pp} , integral of collisions of the dust particles with the gas molecules; M_p , mass of the dust particle; m_g , mass of the gas molecule; D_p , diameter of the dust particle; d_g , diameter of the collision cross section of the gas molecules; n_g , concentration of gas molecules; n_p , concentration of solid particles; τ_{ij} , characteristic mean free time of particles of the *i* type relative to particles of the *j* type; *k*, Boltzmann constant; u_g , transport velocity of flow of the gas; u_p , average velocity of flow of the dust; *T*, gas temperature, T_0 , temperature of the gas at the inlet to the flow region; P_0 , pressure of the gas at the inlet to the flow region. Subscripts: x, coordinate in the physical space; g, gas component of the mixture.

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