

RECONDENSATION IN THE PRESENCE OF A NONCONDENSABLE COMPONENT

A. P. Kryukov, V. Yu. Levashov,
and I. N. Shishkova

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Flows of two-component mixtures with vapor condensation on cooled surfaces are analyzed by the methods of molecular-kinetic theory. The mixture contains a noncondensable component whose average density remains constant in the region under study. The influence of the gas on the process of recondensation of the vapor and the interaction of the components of the mixture in the cases of equal and different molecular weights are studied. The problems posed are investigated using the method of direct numerical solution of the kinetic Boltzmann equation modified for the mixture of gases. Special emphasis is placed on computation of direct and cross collision integrals.

Problems in solving which one must take into account the nonequilibrium of transfer processes are topical for many situations of practical importance.

In a number of practical applications, one frequently has such regimes of flow in which the regularities of flows of a continuous medium, on the one hand, and those of a free-molecular medium, on the other, cease to hold.

Under such conditions, intermolecular collisions turn out to be insufficient for the superposition of a large number of random interactions to completely counterbalance their probabilistic character and to make it possible to use the regularities of a continuous medium. At the same time, collisions between gas or vapor particles are rather frequent and they cannot be disregarded, as in the case of a free-molecular regime of flow. Therefore, it is expedient to describe rarefied-gas flows at the level of the velocity-distribution function of molecules.

The problem of calculation of the parameters of gas or vapor flows is also complicated by the presence of at least two components of the gas which interact with each other and by the phase transitions on cooled surfaces.

Correct investigation of such flows is possible by the methods of molecular-kinetic theory. The motion and interaction of gas or vapor molecules are described based on the kinetic equation. In the present work, we use, as such an equation, the traditional Boltzmann equation, which, for a two-component mixture, becomes the system of equations

$$\frac{\partial f_a}{\partial t} + \xi_a \frac{\partial f_a}{\partial \mathbf{r}} = J_{aa} + J_{ab}, \quad \frac{\partial f_b}{\partial t} + \xi_b \frac{\partial f_b}{\partial \mathbf{r}} = J_{bb} + J_{ba}. \quad (1)$$

In this work, we use collision integrals written in the following form:

$$J_{ij} = \frac{\sigma}{2} \int_{-\infty}^{+\infty} d\xi_{j1x} \int_{-\infty}^{+\infty} d\xi_{j1y} \int_{-\infty}^{+\infty} d\xi_{j1z} \int_0^\pi \int_0^{2\pi} \left(f_i' f_{j1}' - f_i f_{j1} \right) |\xi_i - \xi_{j1}| \sin \theta d\theta, \quad (2)$$

where i and j may be assumed as a and a , a and b , b and b , and b and a , depending on the sort of colliding molecules; $f_i \equiv f(\mathbf{r}, t, \xi_i)$; $f_{j1} \equiv f(\mathbf{r}, t, \xi_{j1})$, $f_i' \equiv f(\mathbf{r}, t, \xi_i')$, $f_{j1}' \equiv f(\mathbf{r}, t, \xi_{j1}')$; ξ_i and ξ_{j1} are the molecular velocities of the mixture components before the collision and ξ_i' and ξ_{j1}' are the velocities after the collision; $\sigma = \frac{1}{4} \pi \left(\frac{d_i + d_j}{2} \right)^2$ is the middle collision cross section for the i and j particles.

Moscow Power Institute (Technical University), 14 Krasnokazarmennaya Str., Moscow, 112250, Russia; email: KryukovA.P.@mpei.ru. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 78, No. 4, pp. 15–21, July–August, 2005. Original article submitted July 21, 2004.

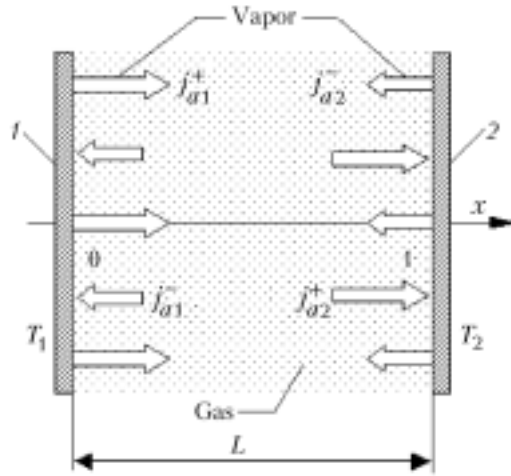


Fig. 1. Scheme of the problem.

System (1) consists of two integro-differential equations to solve which we use the method of direct numerical solution of the kinetic Boltzmann equation (the method is presented in [1] in detail). The sets of velocity-distribution functions of molecules for both components of the mixture are a result of the solution of system (1). The macroparameters — density, temperature, pressure, mass and energy fluxes — and other moments of the distribution function are determined by integration over the three-dimensional velocity space. In particular, for each of the components we have

$$n = \int f d\xi, \quad u_x = \frac{1}{n} \int \xi_x f d\xi, \quad j_x = \int \xi_x f d\xi, \quad \frac{3}{2} nkT = \frac{1}{2} m \int (\xi - \mathbf{u})^2 f d\xi, \quad (3)$$

where u_x and j_x is the velocity and the mass flux in the x direction respectively.

Formulation of the Problem. A scheme of the problem is shown in Fig. 1. The vapor (component a) arrives from bounding surfaces at the region under study. The space between the surfaces is filled with noncondensable gas (component b), whose amount remains constant throughout the process.

The distribution functions for molecules leaving the interfaces were prescribed in the form of half-Maxwellians with parameters n and T and a zero transport velocity. For the vapor we have $n_a = n_{a1}$, $T = T_1$ and $n_1 = n_{a2}$, $T = T_2$ on surfaces 1 and 2 respectively. The quantities n_{a1} , n_{a2} , T_1 , and T_2 are known. It was assumed that $n_{a1} = 2n_{a2}$ in the calculations. Surfaces 1 and 2 are impermeable to gases; therefore, we determined n_{b1} and n_{b2} for $x = 0$ and $x = L$ from the nonflow conditions. It was assumed that $T_1(x = 0) \approx T_2(x = L)$.

At the initial instant of time, the concentration of gas particles was taken to be the same throughout the region under study and to be $n_{b0} = n_{a2}$ or $n_{b0} = 0.1n_{a2}$ and $0.5n_{a2}$ in different variants of calculation.

A number of computations were carried for mechanically identical molecules: $m_a = m_b$ and $d_a = d_b$. Thereafter, the algorithm was modified for arbitrary masses and diameters. We give in the work results of calculations for $m_a = 10m_b$ and $d_a = 1.68d_b$ (argon-helium mixture) and $m_a = 0.001m_b$ and $d_a = 0.1d_b$ (mixture of vapor molecules and large particles as the noncondensable component) as an example. To describe the interaction of the mixture components a and b we used the model of rigid elastic spheres.

The vapor concentration n_{a2} and the surface temperature T_2 were taken as the basic ones in the work.

The problem on recondensation of a vapor in the presence of a noncondensable component was solved for the Knudsen numbers $\text{Kn} = 0.5, 0.1, \text{ and } 0.01$. The Kn number is equal to λ_{a2}/L , where λ_{a2} is the mean free path of the vapor with parameters n_{a2} and T_2 .

Method of Solution. In solving Eqs. (1), we used a numerical procedure involving a conservative finite-difference approximation of the differential parts of the equations. We prescribed a fixed grid with steps Δx , Δt , and $\Delta \xi$ in the five-dimensional phase space $(x, t, \xi_x, \xi_y, \xi_z)$ and replaced the system of equations (1) by a system consisting of a large number (of the order of several hundred or thousand) of finite-difference equations with a nonlinear right-hand side. In a one-dimensional formulation for the problem on recondensation of a mixture, they have the form

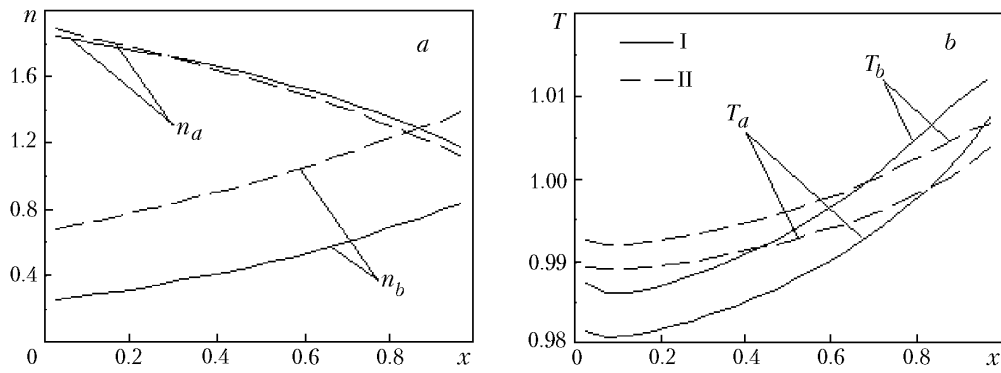


Fig. 2. Concentrations (a) and temperatures (b) of the vapor and the gas vs. x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.5$ (I) and 1.0 (II).

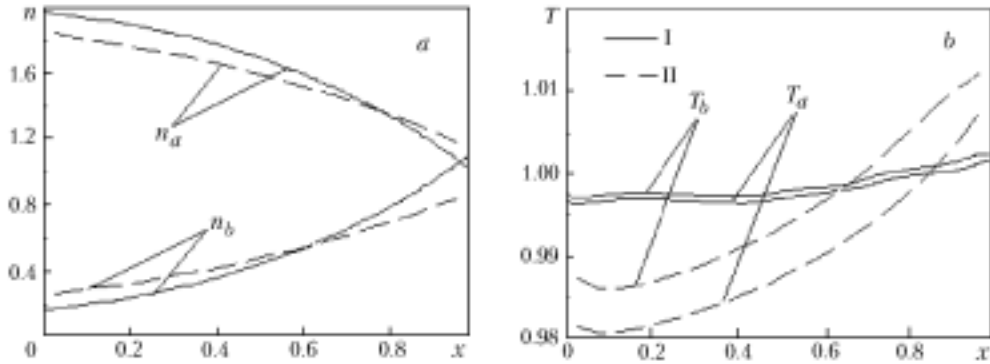


Fig. 3. Concentrations (a) and temperatures (b) of the vapor and the gas vs. x for $\text{Kn} = 0.01$ (I) and 0.1 (II) when $n_{b0}/n_{a2} = 0.5$.

$$\frac{\Delta f_a^k}{\Delta t} + \xi_{ax}^k \frac{\Delta f_a^k}{\Delta x} = J_{aa}^k + J_{ab}^k, \quad \frac{\Delta f_b^k}{\Delta t} + \xi_{bx}^k \frac{\Delta f_b^k}{\Delta x} = J_{bb}^k + J_{ba}^k, \quad (4)$$

where k is the cell number in the velocity space.

In solving the system of equations (4), we used the algorithm of splitting by physical processes: molecular motion without collisions and spatially homogeneous relaxation

$$\frac{\Delta f_a^k}{\Delta t} + \xi_{ax}^k \frac{\Delta f_a^k}{\Delta x} = 0, \quad \frac{\Delta f_b^k}{\Delta t} + \xi_{bx}^k \frac{\Delta f_b^k}{\Delta x} = 0;$$

$$\frac{\Delta f_a^k}{\Delta t} = J_{aa}^k + J_{ab}^k, \quad \frac{\Delta f_b^k}{\Delta t} = J_{bb}^k + J_{ba}^k.$$

In solving the problem, special emphasis was placed on computation of direct and cross collision integrals. Fivefold multiple integrals were computed using random cubature formulas with special Korobov distributions [2], which ensured the accuracy necessary for solution of the problem. For a number of random nodes of the order of 10^3 , the error of computation of the multiple integral amounts to about 3%.

Calculation Results. The results of calculations are given in Figs. 2–7. In all the figures, the concentrations and the temperatures are given in relation to n_{a2} and T_2 respectively. The dimension of the domain under study L is taken to be unity.

Figure 2 shows the stationary dependences of the concentrations and temperatures of the vapor and the gas on x for $\text{Kn} = 0.1$ with $n_{b0}/n_{a2} = 0.5$ and 1.0 for mechanically identical molecules. It is seen that the dimensionless con-

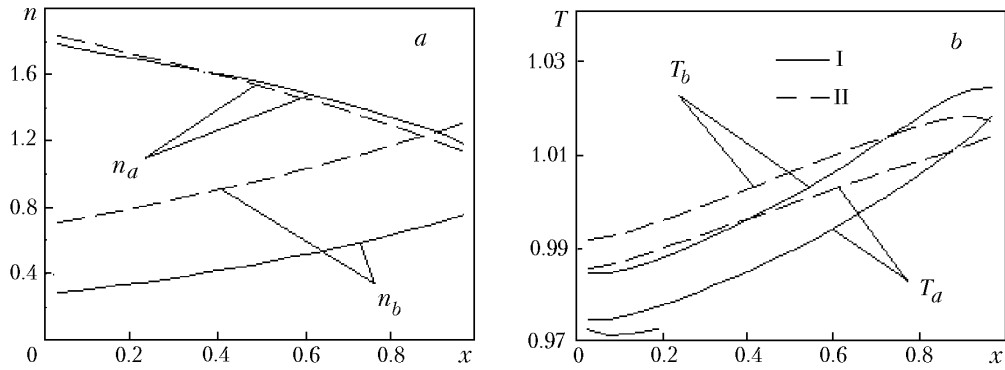


Fig. 4. Concentrations (a) and temperatures (b) of the vapor and the gas vs. x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.5$ (I) and 1.0 (II), $m_a = 10m_b$, and $d_a = 1.68d_b$.

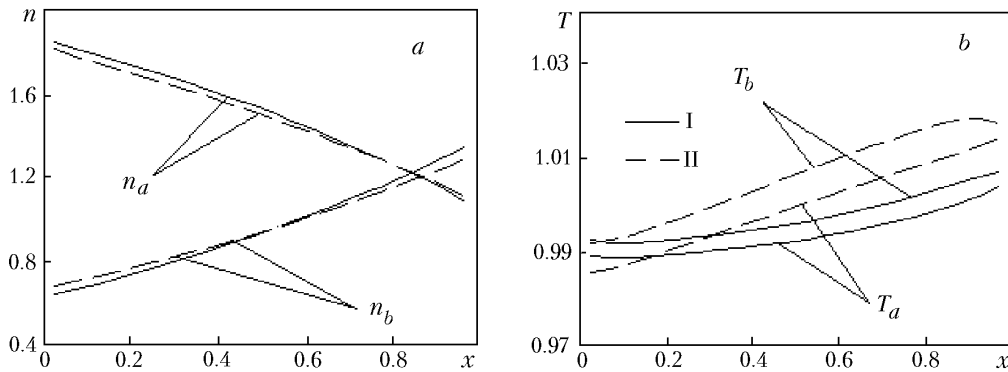


Fig. 5. Concentrations (a) and temperatures (b) of the vapor and the gas vs. x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 1.0$, $m_a = m_b$ and $d_a = d_b$ (I) and $m_a = 10m_b$ and $d_a = 1.68d_b$ (II).

centration of the vapor changes from a value of ~ 1.83 near interface 1 to a value of ~ 1.18 near phase boundary 2. A twofold increase in the initial concentration of the gas exerts no substantial influence on n_a as a function of the coordinate. In the process of interpenetration of the components, the mass of the gas is redistributed in the space under study so that its concentration near phase boundary 2 is more than twice as high as the concentration near interface 1.

Figure 3 illustrates the influence of the Knudsen number on the concentration and temperature distributions of the components of the mixture in the domain under study. The results of calculations are given for $\text{Kn} = 0.01$ and 0.1 when $n_{b0}/n_{a2} = 0.5$. The molecules are mechanically identical. It follows from the figure that the curvature of the $n_a(x)$ and $n_b(x)$ lines increases as the state of the mixture approaches the limit of a continuous medium ($\text{Kn} = 0.01$), and the concentration near the interfaces is closer to n_{a1} and n_{a2} respectively.

In the following step of investigation, we solved a number of problems on recondensation of the vapor in the presence of a noncondensable gas in the case where the masses of the mixture components and the molecular diameters were different (Figs. 4–6).

Figure 4 gives the dependences of the concentrations and temperatures of the vapor and the gas on x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.5$ and 1.0. In these calculations, the masses and molecular diameters of the components correspond to the argon (vapor)–helium (gas) mixture: $m_a = 10m_b$ and $d_a = 1.68d_b$. Figure 5 shows the dependence of the concentration of the mixture components and of the temperature on x for $\text{Kn} = 0.1$ and $n_{b0}/n_{a2} = 1.0$ for the case of mechanically identical molecules $m_a = m_b$, and $d_a = d_b$, and the argon–helium mixture: $m_a = 10m_b$ and $d_a = 1.68d_b$. The observed behavior of the concentrations and the temperatures is similar, in principle, to the case $m_a = m_b$ and $d_a = d_b$ (Fig. 2).

A change in the vapor velocity along x is presented in Fig. 6 for mechanically identical molecules (Fig. 6a) and the argon–helium mixture (Fig. 6b) when $n_{b0}/n_{a2} = 0.5$ and $n_{b0}/n_{a2} = 1.0$. In this figure, the velocity is given in

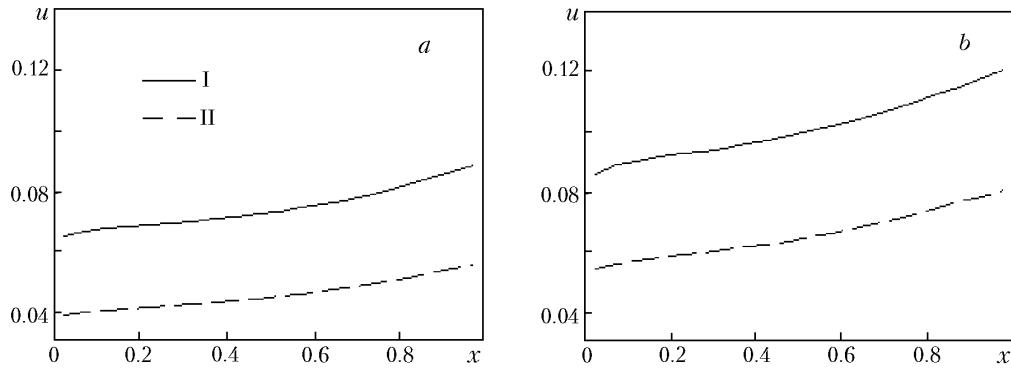


Fig. 6. Vapor velocity vs. x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.5$ (I) and 1.0 (II), $m_a = m_b$ and $d_a = d_b$ (a) and $m_a = 10m_b$ and $d_a = 1.68d_b$ (b).

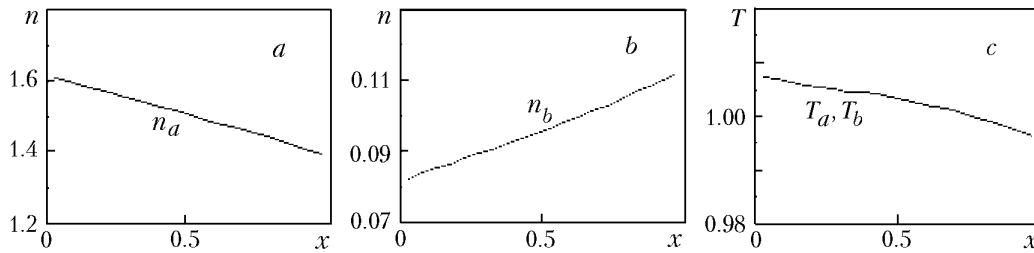


Fig. 7. Concentrations of the mixture components (a and b) and temperature (c) vs. x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.1$, $m_a = 0.001m_b$, and $d_a = 0.1d_b$.

dimensionless form $u/\sqrt{R_a T_2}$, where R_a is the individual gas constant for the vapor and T_2 is the temperature of surface 2. Unlike the concentration and the temperature, the velocity u substantially depends on both the quantity n_{b0} and the relation of the masses and diameters of the mixture components. A twofold increase in the concentration of the noncondensable gas leads to a reduction of approximately 1.4 times in the velocity of flow of the vapor in both cases. Also, it is noteworthy that when $m_a = 10m_b$ and $d_a = 1.68d_b$ the average velocity of the vapor flow turns out to be approximately 1.5 times higher than that for mechanically identical molecules. Since the concentrations for these types of mixtures are similar (Fig. 5), the significant growth in the velocity means a substantial increase in the mass of the vapor flow through the domain under study.

Subsequently, the algorithm used in the work was applied to solution of the problem on flow of a mixture with strongly differing masses and diameters for the components: $m_a = 0.001m_b$ and $d_a = 0.1d_b$. Figure 7 shows the dependences of the concentration of the mixture components and the temperature on x for $\text{Kn} = 0.1$ when $n_{b0}/n_{a2} = 0.1$. Here the heavy component acts as noncondensable gas b and the light component acts as vapor a . As is seen in Fig. 7, the vapor arriving at the domain activates particles exceeding one thousand times its molecules in mass, which finally becomes responsible for their redistribution in space. The concentration of heavy component b near interface 1 is approximately 1.4 times lower than that near interface 2.

Comparison of the Data of Other Authors. In the work presented, we compared the results obtained to the data of [3] (Fig. 8).

To solve the problem on recondensation of the vapor in the presence of a noncondensable gas Aoki et al. [3] adapted the Bird method of Monte Carlo direct statistical simulation presented, for example, in [4].

The main idea of the method is as follows. The gas is simulated by a set of a rather large (but finite) number of particles that behave in accordance with the hypotheses of kinetic theory. Tracking the evolution of the entire ensemble of particles in the volume, one may compute the average macroscopic quantities and the distribution function if necessary.

In each time step, the process of evolution is split into two steps: (1) free separation with the corresponding boundary conditions and (2) collision relaxation.

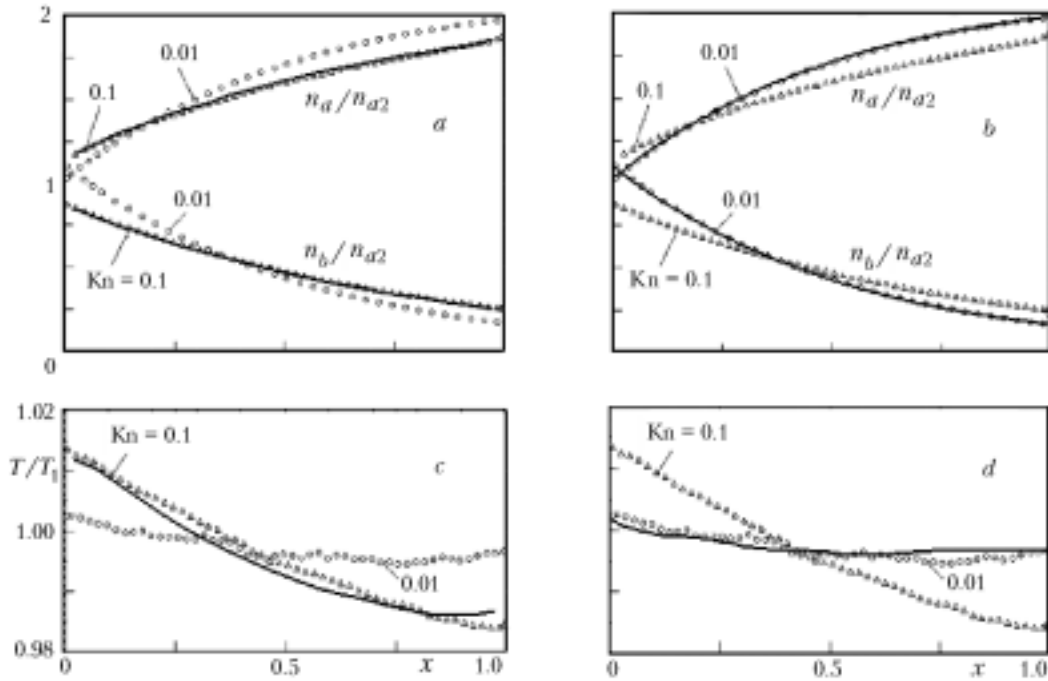


Fig. 8. Comparison of the results obtained by the authors for $Kn = 0.1$ (a and c) and 0.01 (b and d) (curves) to the data of [3] (points) when $n_{b0}/n_{a2} = 0.5$ for the concentrations (a and b) and temperatures (c and d) of the vapor and the gas.

Realization of the first step presents no fundamental difficulties: all the molecules are shifted in accordance with their velocities and interact with the boundaries of the domain if necessary.

Fundamental is the second step, on whose successful realization the success of the method depends.

Superficially the principle of splitting is the same as that in the corresponding scheme of solution of the Boltzmann equation. The step of free movements simply coincides if we have in mind that the velocities are random and not fixed in statistical simulation. The relaxation step in [3] is implemented differently than in the method used by the authors of the present work. Nonetheless, Fig. 8 shows good agreement of the results obtained by these different methods for the present class of problems.

The authors have been unable to find works where the problem on recondensation of the vapor in the presence of a noncondensable gas would be solved for molecules of different masses and diameters.

CONCLUSIONS

1. The results of solution of the problems for mechanically identical molecules, which have been obtained by two different methods in a wide range of Knudsen numbers, are in good agreement.

2. The algorithm developed enables one to calculate the processes of recondensation in the presence of a gas whose molecules significantly differ from the vapor molecules in mass and diameter, with no limitations being imposed on the concentration of the components.

3. The calculation results presented for the mixture with a large ratio of masses and diameters for different components (1000 and 10 respectively) enable one to evaluate their mutual influence and to determine the density and temperature distributions in recondensation.

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NOTATION

d_a , diameter of a molecule of component a ; d_b , diameter of a molecule of component b ; $f_a(\mathbf{r}, t, \xi_a)$, velocity-distribution function of molecules for the vapor; $f_b(\mathbf{r}, t, \xi_b)$, velocity-distribution function of molecules for the gas; J_{aa} , collision integral describing the interaction of vapor molecules with each other; J_{ab} , collision integral describing the interaction of vapor molecules and gas molecules; J_{bb} , collision integral describing the interaction of gas molecules with each other; J_{ba} , collision integral describing the interaction of gas molecules and vapor molecules; j , mass-flux density; Kn, Knudsen number; L , dimension of the domain under study; m_a , mass of a molecule of component a ; m_b , mass of a molecule of component b ; n , concentration; $\mathbf{r}(x, y, z)$, Cartesian coordinates; t , time; T , temperature; u , mass-flux velocity; θ and ε , angular parameters of collision; λ_0 , mean free path of component a ; ξ_a , molecular velocity for component a ; ξ_b , molecular velocity for component b .

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