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CALCULATION OF NONSTATIONARY MIXED CONVECTION OF BINARY GAS

MIXTURES IN THE PRESENCE OF LARGE DENSITY VARIATIONS

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Nonstationary mixed-convective flows of gas and gas mixtures are extremely widespread in nature and technology. Their study is necessary, for example, for developing safe methods for handling toxic and explosive mixtures, solving a number of ecological problems, and industrial hygiene. In spite of the considerably subsonic nature of such flows, the spatialtemporal variation of the density in the flow, due to the nonisothermality or difference in the molecular weights of the components of the mixture, can in many cases be very significant. Nevertheless, until recently, the theoretical analysis of mixed-convective flows, just as the solution of the problems of natural convection, was based primarily on the use of the socalled Boussinesq approximation [1], which is based on the assumption that the density variations in the flow are small. In [2, 3] a system of equations is formulated, which, in contrast to the Boussinesq approximation, can be used to describe the convection of binary gas mixtures in the presence of arbitrary finite variations of the density, which greatly expanded the possibilities of numerical modeling of such flows.

In this paper, the approach adopted in [2, 3] is generalized to the case of mixed-convective flows.

The basic difference between the derivation, proposed below, of the approximate system of equations of mixed convection and the analogous derivation of the system of equations of natural convection, described in [2, 3], lies in the choice of scales used to put the complete system of Navier-Stokes equations, on which the analysis is based, into dimensionless form. This difference is due to the appearance of an additional dimensional parameter - the characteristic velocity of forced convection - in problems of mixed convection. To illustrate the choice of scales, we shall examine the following problem. Let a region, with the shape of a rectangular parallelepiped, be filled with gas with molecular weight m2 at a temperature  $T_2$ . Initially, another gas, whose molecular weight is  $m_1$  and whose temperature is  $T_1$ (for definiteness  $T_2 > T_1$ ,  $m_2 > m_1$ ), begins to enter the volume with velocity  $v_1$  through the opening ef (Fig. 1). Simultaneously, the same gas that filled the volume initially is introduced into the region with velocity  $v_2$  through the opening *ab*. The mixture formed flows out of the volume through the opening cd. The problem is to calculate the development of the velocity, concentration, and temperature fields of the mixture in the volume as a function of time.

The problem described above is, on the one hand, quite typical for the class of flows under examination and, on the other, it is of certain practical interest, because it models the situation arising with activation of emergency forced exhaust ventilation when a foreign gas begins to enter an enclosure.

To put the system of Navier-Stokes equations, which describes the flow under study, into dimensionless form, we shall select as scales the following characteristic parameters of the problem: the average geometric value of the characteristic velocities of forced and natural convection  $v_0 = \sqrt{v_2(gL_2\epsilon_1)^{1/2}}$  as the velocity scale [here  $\epsilon_1 = (m_2/m_1 - 1)(T_2/T_1 - 1)$  in the case of nonisothermal flow of the gas mixture,  $\varepsilon_1 = \varepsilon_T = T_2/T_1 - 1$  in the case of nonisothermal

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flow of a homogeneous gas, and  $\varepsilon_1 = \varepsilon_M = m_2/m_1 - 1$  in the case of an isothermal flow of the mixture],  $t_0 = L_2/v_0$  for the time scale,  $T_0 = T_2$  for the temperature scale,  $m_0 = m_2$  for the molecular weight scale,  $\rho_0 = p_0 m_0/RT_0$  for the density scale ( $p_0$  is the pressure at the bottom of the region at t = 0),  $\mu_0 = \mu_2(T_0)$  for the scale of the coefficient of dynamic viscosity,  $D_0 = D_{1,2}(T_0, p_0)$  for the scale of the diffusion coefficient,  $\lambda_0 = \lambda_2(T_0)$  for the scale of the coefficient of thermal conductivity, and  $c_{p_0} = c_{p_2}(T_0)$  for the scale of the specific heat capacity at constant pressure.

Further, as done in [2, 3], we shall introduce together with the pressure p' the excess pressure p', defined by the relation  $p'_{+} = p' - p_0 \exp\left(-\frac{gm_0}{RT_0}x'_2\right)$  and we shall choose as the scale for this pressure the magnitude of the dynamic head  $\rho_0 v_0^2$ .

Transforming the system of Navier-Stokes equations, which includes the Navier-Stokes equation of motion, the equation of continuity for the mixture, the equation of balance of the mass of one of the components of the mixture neglecting thermo- and barodiffusion, the equation of energy balance neglecting diffusion thermoeffect and the equation of state for the mixture of perfect gases, into a dimensionless form using the scales introduced above, we obtain

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p_{+} - \frac{\rho - \exp\left(-\varepsilon x_{2}\right)}{\varepsilon_{1} \sqrt{Fr}} \mathbf{j} + \frac{1}{\sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}} \Phi; \qquad (1)$$

$$\frac{\partial \rho}{\partial t} + \nabla \left( \rho \mathbf{v} \right) = 0; \tag{2}$$

$$\rho \frac{dc}{dt} = \frac{1}{\operatorname{Sc} \sqrt[4]{\operatorname{Ar}^{1/2} \operatorname{Re}}} \nabla (\rho D \nabla C);$$
(3)

$$\rho c_p \frac{dT}{dt} = \frac{(k-1) \operatorname{M} \sqrt{\overline{e_1 e}} N_{\operatorname{dis}}}{\sqrt{\overline{k}} (e_{\mathrm{T}} + 1) \sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}} + \frac{(k-1)}{\sqrt{\overline{k}} (\varepsilon_{\mathrm{T}} + 1)} \frac{dp}{dt} + \frac{\nabla (\lambda \nabla T)}{\operatorname{Pr} \sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}} + \frac{(c_{p1} - c_{p2})}{\operatorname{Sc} \sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}} \rho D \nabla C \nabla T;$$

$$(4)$$

 $p_{+} \operatorname{M} \sqrt{k\varepsilon\varepsilon_{1}} + \exp\left(-\varepsilon x_{2}\right) = \rho T\left(\varepsilon_{r} + 1\right)\left(\varepsilon_{M}C + 1\right) = p.$ <sup>(5)</sup>

Here

$$\mathbf{\Phi} = 2\operatorname{div}\left(\mu\dot{S}\right) - \frac{2}{3}\nabla\left(\mu\mathbf{v}\right), \quad N_{\text{dis}} = 2\mu\dot{S}^2 - \frac{2}{3}\mu\left(\nabla\mathbf{v}\right)^2,$$

$$Re = \frac{\rho_0 v_2 L_2}{\mu_0}, \quad Fr = \frac{v_2^2}{g \varepsilon_1 L^2}, \quad Sc = \frac{\mu_0}{\rho_0 D_0}, \quad Ar = \frac{\rho_0^2 L_2^3 g \varepsilon_1}{\mu_0^2}, \quad Pr = \frac{c_{p_0} \mu_0}{\lambda_0}, \quad M = \frac{v_2}{\sqrt{k \rho_0 / \rho_0}}, \quad \varepsilon = \frac{m_0 g L_2}{R T_0}.$$

We shall examine a flow in which the Mach number M is much less than 1. Taking into account the fact that in most problems of practical significance the parameter of hydrostatic compressibility also assumes small values, it may be presumed that in order to describe such flows it is expedient to use the limiting form of the system of equations (1)-(5) with M and  $\varepsilon$  approaching zero. Passing to the limit indicated and transforming the equation of continuity (2) using (3)-(5), as done in [2], we obtain

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p_{+} - \frac{(\rho - 1)}{\varepsilon_{1}} \mathbf{j} \frac{1}{\sqrt{\mathbf{Fr}}} + \frac{1}{\sqrt{\mathbf{Ar}^{1/2} \mathbf{Re}}} \Phi;$$
(6)

$$\nabla \mathbf{v} = \frac{\nabla \left(\lambda \nabla T\right)}{\rho T c_p \Pr \left(\sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}\right)} + \frac{\left(c_{p1} - c_{p2}\right) D}{T c_p \operatorname{Sc} \left(\sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}\right)} \nabla C \nabla T + \frac{\varepsilon_{M}}{\left(\varepsilon_{M} C + 1\right) \operatorname{Sc} \left(\sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}\right)} \nabla \left(\rho D \nabla C\right); \tag{7}$$

$$\rho \frac{dC}{dt} = \frac{1}{\operatorname{Sc} \sqrt{\operatorname{Ar}^{1/2} \operatorname{Re}}} \nabla (\rho D \nabla C);$$
(8)

$$\rho c_p \frac{dT}{dt} = \frac{1}{\Pr{\sqrt{\operatorname{Ar}^{1/2}\operatorname{Re}}}} \nabla (\lambda \nabla T) + \frac{(c_{p1} - c_{p2})}{\operatorname{Sc}{\sqrt{\operatorname{Ar}^{1/2}\operatorname{Re}}}} \rho D \nabla C \nabla T;$$
(9)

$$(\varepsilon_{\rm M}C+1)(\varepsilon_{\rm T}+1)\rho T=1.$$
 (10)

From the mathematical point of view the system of equations (6)-(10) is analogous to the system of equations in the Boussinesq approximation. Indeed, just as the equation of in incompressibility  $\nabla \mathbf{v} = 0$ , which enters into the system of equations in the Boussinesq approximation, Eq. (7) is a nonevolutionary equation (it does not include time derivatives of the function sought). This is extremely important, because, as a result, efficient numerical methods, developed for integrating the system of equations in the Boussinesq approximation written in natural variables, can now be used to solve the system of equations (6)-(10) and it is thereby possible to avoid the difficulties arising when integrating the system of equations (1)-(5) in the case of considerably subsonic flows [4]. As an illustration of this, we shall examine the results of the solution of the problem described above based on the system of equations (6)-(10). We shall restrict our attention to the particular case of an isothermal flow of a mixture  $(T_1 = T_2)$ . In this case, the system of equations (6)-(10) greatly simplifies and assumes the form

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p_{+} + \frac{(\rho - 1)}{\epsilon_{\rm M}} \mathbf{j} + \frac{1}{\sqrt{\mathrm{Ar}^{1/2} \mathrm{Re}}} \Phi; \tag{11}$$

$$\nabla \mathbf{v} = \frac{\varepsilon_{\rm M}}{\rm Sc} \sqrt{Ar^{1/2} Re} \nabla (\rho \nabla C); \qquad (12)$$

$$\rho \frac{dC}{dt} = \frac{1}{\text{Sc } \sqrt[4]{\text{Ar}^{1/2} \text{Re}}} \nabla (\rho \nabla C);$$
(13)

$$\rho(\varepsilon_{\mathbf{M}}C+1) = 1. \tag{14}$$

The initial conditions for this system of equations for the problem under study are written as follows:

$$\mathbf{v} = 0, \ C = 0 \quad \text{at} \quad t = 0.$$
 (15)

As boundary conditions at the solid walls, we use the conditions of attachment for velocity and the conditions that the projection of the diffusion flux vector along the normal to the wall vanishes:

$$v_w = 0, \ (\partial C/\partial n)_w = 0. \tag{16}$$

Uniform profiles of the normal and zero values of the tangential components of the velocity vector are given on the segments  $\alpha$ b and ef, and the concentration of the light gas is assumed to equal zero and one, respectively.

"Soft" boundary conditions are used on the segment cd:

$$\partial \mathbf{v} / \partial x_1 = \partial c / \partial x_1 = 0. \tag{17}$$

The numerical integration of the system of equations (11)-(14) with the initial and boundary conditions (15), (17) was performed based on the use of one of the modifications of Harlow's SMAC method [5] on a uniform finite-difference grid with dimensions  $22 \times 22$ . Calculations on smaller grids  $(32 \times 32, 22 \times 42)$  showed that in this case the flows arising in the entire examined range of variation of the determining criteria of the problem are described with quite high accuracy. As far as the step in the integration over time is concerned, it is determined by the Courant condition  $u\Delta t/\Delta x < 1$  for an incompressible liquid. Thus, using the system of equations (11)-(14), there is no need in the unjustified, from the point of view of the accuracy of the calculation, decrease of the time step in accordance with Courant's condition for an incompressible gas  $(u + a)\Delta t/\Delta x < 1$  (a is the velocity of sound), which essentially eliminates the possibility of calculating the flow under examination based on the complete system of Navier-Stokes equations with the help of explicit schemes and requires the development of special very cumbersome implicit algorithms (see, for example, [6, 7]).

Let us examine the basic results of the calculations. First of all, the numerical parametric investigation performed (the values of the determining parameters, for which the calculations were performed, are presented in Table 1) showed that depending on the values of the determining parameters of the problem, two fundamentally different types of flows arise in the region. The first type is characterized by an asymptotic approach of all characteristics of the flow to some constant values in the limit  $t \to \infty$ . The second type, which is realized in a comparatively narrow range of variation of the determining criteria, is characterized by a nonmonotonic change in the parameters of the flow as a function of time and establishment of a quasistationary self-oscillatory flow regime in the limit  $t \to \infty$ . A graphic illustration of this is given in Fig. 2, which shows the dependence of the relative mass content of the light gas in the volume  $G = \iint \rho C dx_1 dx_2 / (\iint \rho dx_1 dx_2)$  on time for different values of determining parameters of the problem (the numbers on the curves correspond to the variants



in Table 1). The possibility of the appearance of self-oscillatory flow regimes in the problem under examination was first mentioned in [8]. We shall examine in greater detail the mechanism of this phenomenon. With a definite ratio of the intensities of the diffusion transport of mass and momentum, as well as natural and forced convection, characterized by the values of the parameters  $\sqrt{Ar^{1/2}}Re$ , Sc, Fr,  $v_{1,2} = v_1/v_2$ ,  $\varepsilon_1$ , at the initial stage of the process, the light gas accumulates in the lower part of the volume ABCD (ascending sections on curves 11, 12, in Fig. 2) as a result of the screening action of the stream of heavy gas entering through the opening ab. After this mass reaches some "critical" value, the buoyancy force displaces the "bubble" of light gas into the upper part of the region. In so doing, the bubble is intensively carried out of the volume through the outlet opening cd (descending sections on the curves in Fig. 2). The screening horizontal stream of heavy gas is then again reformed and the entire process described is repeated from the beginning. In this case, a quasi-stationary self-oscillatory flow regime is established with time. Its characteristic phases are shown in Fig. 3, where the fields of the velocity vector and isolines of the concentration of light gas at times t = 62 and 67 are illustrated for conditions corresponding to the regime N = 11 in Table 1.

Together with the values of the criteria  $\sqrt{\operatorname{Ar}^{1/2}\operatorname{Re}}$ , Fr,  $v_{1,2}$ ,  $\varepsilon_1$ , which, as is evident from Fig. 2, determine the flow regime arising in the volume ABCD, it also depends on the initial conditions. Thus, if at t = 0 the light, and not the heavy, gas fills the region, the self-oscillatory flow regime is not observed at all, which agrees completely with the mechanism of its development described above.

The results of investigations of the flows of the first type, characterized as already mentioned, by the establishment of a stationary regime in the limit  $t \rightarrow \infty$ , are presented in Figs. 2, 4-6. The nature of the dependence of the asymptotic value of G(t) in the limit  $t \rightarrow \infty$  on the values of the parameter  $v_{1,2}$  is somewhat unexpected. As is evident from a compari-

N	$\overline{V_{\rm Ar}^{1/2}{}_{\rm Re}}$	<sup>v</sup> 1,2	e1	Fr	Sc	N	$\sqrt{\mathrm{Ar}^{1/2}\mathrm{Re}}$	v <sub>1,2</sub>	81	Fr	Sc
1 2 3 4 5 6 7 8	$300 \\ 100 \\ 20 \\ 300 \\ 300 \\ 300 \\ 300 \\ 300 \\ 300 \\ 300 \\ 300 $	1 1 1 1 1, 0,75 1,5	1 1 0,2 0,01 1 1	0,25 0,25 0,25 0,25 0,25 1 1 1	1 1 1 1 1 1 1	9 10 11* 12* 13 14 15 16	300 300 300 300 300 300 300 100 20	$     \begin{bmatrix}       0,7 \\       0,04 \\       0,3 \\       0,$	$ \begin{array}{c} 1 \\ 1 \\ 0,1 \\ 1 \\ 10 \\ 1 \\ 1 \end{array} $	$\begin{array}{c} 0,25\\ 0,25\\ 0,25\\ 0,25\\ 0,25\\ 0,0625\\ 0,75\\ 0,25\\ 0,25\\ 0,25\end{array}$	1 1 1 1 1 1

TABLE 1

\* - Self-oscillatory regime.



Fig. 3





son of the dashed curves in Fig. 2, the indicated dependence is nonmonotonic. This means that under certain conditions the efficiency of ventilation of the volume ABCD, characterized by the quantity G(t), drops with increasing velocity of inflow of the ventilating gas. This can be explained based on the analysis of local characteristics of the flow, which exist under conditions corresponding to the variants N = 7 and 8 of the calculation. It is evident from Fig. 4a that in the first case the light gas cannot overcome the screening action of the stream of heavy gas, as a result of which it becomes concentrated primarily in the bottom of the region. In the second case, the heavy gas stream breaks up and a hydrodynamic situation is established such that the light mixture penetrates freely toward the "outlet" opening cd and leaves the volume (Fig. 4b). This explains the increase in the



ventilation efficiency. However, this situation occurs only in a comparatively narrow range of variation of the parameter  $v_{1,2}$ . For values of this parameter exceeding these limits, the dependence of G(t) on  $v_{1,2}$  has the opposite character (see Fig. 2); as  $v_{1,2}$  increases,  $G|_{t\to\infty}$ increases. This is explained by the fact that the change in the hydrodynamic environment, described above, leading first to an increase in ventilation efficiency with increasing  $v_{1,2}$ , later can no longer compensate the existing increase in volume of the light gas, entering into ABCD per unit time.

The effect of the parameter  $\sqrt{Ar^{1/2}Re}$  on the structure of the flow under study is illustrated in Fig. 5. A decrease of the value of this parameter increases the role of diffusion transport, which creates conditions for rapid mixing of the mixture. Thus, for  $\sqrt{Ar^{1/2}Re}=$  20 (regime N = 3), the mixture in ABCD has a more uniform composition (Fig. 5a), and there is more light gas in it than for values  $\sqrt{Ar^{1/2}Re}=$  100 or 300 (curves 1-3 in Fig. 2 and Fig. 5b, which shows the results of the calculation of variant N = 1).

It is of great interest to compare the results obtained based on the system of equations (11)-(14) with the corresponding results obtained by solving the same problem within the framework of the Boussinesq approximation. The results of this comparison, presented in Fig. 6 [the continuous curves show the solution of the system of equations (11)-(14) and the dashed curves show the Boussinesq approximation], indicate that as  $\varepsilon_1$  increases, the error introduced into the calculation as a result of the use of the Boussinesq approximation increases and already at  $\varepsilon_1 = 1$  (curve 1) reaches 25%. This conclusion is entirely natural, since as  $\varepsilon_1$  increases, the ratio of the densities of light and heavy gases increases, and the degree of density inhomogeneities in the flow therefore also increases.

The calculations showed that the error introduced into the calculation of G(t) with the use of the Boussinesq approximation does not exceed 5% only for  $\varepsilon_1 \leq 0.1$ .

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NUMERICAL INVESTIGATION OF A GAS JET WITH HEAVY PARTICLES ON THE BASIS

OF A TWO-PARAMETER MODEL OF TURBULENCE

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Theoretical [1-4] and experimental [5, 6] investigations recently executed show that disperse particles exert substantial influence on the gasdynamic parameters and turbulent structure of two-phase jets. Two fundamental problems occur in the theoretical investigation of flows of this kind: formulation of the initial system of equations and representation of the unknows correlation moments. The solution of the former is obtained in [7] by spatial averaging of the micro-equations describing the processes within the component phases; up to now the latter has been solved within the framework of the mixing-path theory [1-3]. The equation of turbulent viscosity transport for a "pure" gas has hence been applied in [2] in place of the Prandtl formula.

Utilized extensively at this time to investigate turbulent flows are two-parameter models containing the energy transport equations of turbulent pulsations and its dissipation velocity [8, 9]. Such models permit not only the computation of the average parameters and characteristics of the turbulence with the stream prehistory taken into account, but also taking account of the influence of the external effects to be given a better foundation. The transport equation of the fluctuating energy was utilized first in [4] to analyze a jet with a low drop concentration under the assumption of no average phase slip. The influence of the drops on the fluctuation energy is here taken into account approximately by the introduction of empirical corrections to the traditional terms describing the turbulent energy generation and dissipation; the scale of turbulence is considered proportional to the jet width.

An  $e - \varepsilon$  model is proposed in this paper for the numerical investigation of a turbulent gas jet with solid particles under conditions of a substantial nonequilibrium in the velocities of the component phases; expressions are obtained for the unknown correlation moments due to the presence of a disperse phase.

## 1. FORMULATION OF THE PROBLEM

The system of equations for the average quantities describing the outflow of a two-phase turbulent jet has the form

$$\frac{\partial u_g}{\partial y} + \frac{1}{y} \frac{\partial}{\partial y} (y v_g) = 0; \qquad (1.1)$$

$$\frac{\partial}{\partial x} \left( \rho_p u_p \right) + \frac{1}{y} \frac{\partial}{\partial y} \left( y \left( \rho_p v_p + \langle \rho'_p v'_p \rangle \right) \right) = 0; \tag{1.2}$$

$$\rho_g \left( u_g \frac{\partial u_g}{\partial x} + v_g \frac{\partial u_g}{\partial y} \right) + \frac{1}{y} \frac{\partial}{\partial y} \left( y \rho_g \left\langle u'_g v'_g \right\rangle \right) = -F_x; \tag{1.3}$$

$$\rho_{p}u_{p}\frac{\partial u_{p}}{\partial x} + \left(\rho_{p}v_{p} + \langle \rho_{p}^{'}v_{p}^{'}\rangle\right)\frac{\partial u_{p}}{\partial y} + \frac{1}{y}\frac{\partial}{\partial y}\left(y\rho_{p}\left\langle u_{p}^{'}v_{p}^{'}\right\rangle\right) = F_{x}; \qquad (1.4)$$

$$u_{g}\frac{\partial e}{\partial x} + v_{g}\frac{\partial e}{\partial y} = \frac{1}{y}\frac{\partial}{\partial y}\left(y\frac{\nu_{t}}{k_{2}}\frac{\partial e}{\partial y}\right) + \nu_{t}\left(\frac{\partial u_{g}}{\partial y}\right)^{2} - \varepsilon - \varepsilon_{p};$$
(1.5)

$$u_g \frac{\partial \varepsilon}{\partial x} + v_g \frac{\partial \varepsilon}{\partial y} = \frac{1}{y} \frac{\partial}{\partial y} \left( y \frac{v_t}{k_3} \frac{\partial \varepsilon}{\partial y} \right) + k_4 \frac{\varepsilon}{e} v_t \left( \frac{\partial u_g}{\partial y} \right)^2 - k_5 \frac{\varepsilon^2}{e} - \Phi_p, \tag{1.6}$$

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