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Peculiarities of the rise of structured formations at the boundary of the change of the regimes "diffusion–concentration convection" at an isothermal mixing of a binary mixture equally diluted by the third component*

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The peculiarities of the change of the regimes "diffusion–gravitational concentration convection" have been studied numerically. It is shown that at a certain mixture composition and pressure, substantially nonlinear distributions of the concentrations of components arise at the expense of the difference in the diffusion coefficients of components, which lead to the corresponding distribution of the gaseous mixture density. This is a reason for the formation of structured formations and the rise of convective instability in the mixtures under study. The time of the rise of convective flows and of the mean velocity of the components transfer has been estimated. Obtained results are compared with experimental data.

Key words: diffusion, convection, pressure, concentration, instability.

Introduction

The investigation of the multi-component transfer regimes related to a correct determination of the velocities, concentration and temperature fields of mixing gaseous and condensed mixtures is one of the topical problems in the advanced thermophysics [1], which are studied widely at the combustion of various fuel types, combustion of natural gases, evaporation and condensation of multiphase systems [2–4]. The existence of mixing regimes obviously has a threshold character that is it is determined by the critical Rayleigh numbers and the critical

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pressure values. In this connection, the determination of the boundary of the change of mixing regimes and the prediction of their state appear important for convective heat and mass transfer problems both in the fundamental and applied respects.

In the experiments on the investigation of a multi-component mixing in gaseous systems at elevated pressures [5], the diffusion of a mixture of vapors into an inert gas [6], convective flows were registered, which lead to a considerable growth of partial fluxes of components. The revealed synergetic effect [5, 6] was shown to be related to a considerable increase in the mixing rate and a preferable transfer of the mixture component, which is the heaviest one in terms of the density. Following the physical meaning, the rise and the development of the concentration component must occur within the framework of conventional concepts of the Rayleigh thermal tasks [7, 8]. However, for the situations studied in the works [5, 6] when the motions arise at a stable stratification in the isothermal mixture, it is necessary to account for the influence of several concentration gradients. The investigations [9, 10] have shown that in three-component systems with a significant difference in molecular weights M_i of the components and coefficients of mutual diffusion D_{ij} [11], there are the regions of decaying and increasing disturbances. Depending on the gradient of the mixture density, different mechanisms of the components mixing may take place: both the diffusion ones and the ones caused by convective instability. It was shown in the work [12] that at the diffusion of a binary system, which is equally diluted by the third component, the nonlinear partial concentration dependencies on the coordinate may take place, which lead to the formation of a nonmonotonous distribution of the mixture density, which may also serve a reason for the gravitational convective instability. Along with that, it is necessary to note that the possibilities of the approach [7, 8] extended for the case of the mixing of isothermal ternary gaseous mixtures are limited and do not enable the description of the dynamics of convective flows and the time of the unstable regime onset. In the works on the investigation of the unsteady evaporation of solutions with regard for convection in gaseous phase [13, 14], the numerical approaches were proposed for modeling a complex mass transfer, which have shown a good agreement between the results of numerical experiment and experimental data about the estimate of the evaporation rate of a binary solution to an inert gas. One should assume that for the case of the diffusion in ternary mixtures, the numerical modeling of mixing processes near the boundary of the change of kinetic regimes will enable a more detailed elucidation of typical peculiarities of the multi-component mass transfer.

In the present work, a computational model is proposed for studying the isothermal transfer of a binary gas mixture, which is equally diluted by the third component, by means of the two-dimensional modeling in a vertical cylindrical duct of finite sizes. The obtained results of numerical investigation are compared with experimental data.

Governing equations of convective disturbances at diffusion. Numerical algorithm

One can describe the change of the regimes "diffusion–concentration convection" in three-component gas mixtures by a system of fluid dynamics equations for perturbed quantities in the Oberbeck–Boussinesq approximation [7]. This system consists of the Navier–Stokes equation, the conservation law for the number of particles of the mixture and of the components, and with regard for the independent diffusion condition $\sum_{i=1}^{3} \mathbf{j}_i = 0$ and $\sum_{i-1}^{3} c_i = 1$, it has the form [9, 10]

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\nabla\mathbf{u})\right] = -\nabla p + \eta\nabla^2\mathbf{u} + \left(\frac{\eta}{3} + \xi\right)\nabla\operatorname{div}\mathbf{u} + \rho\mathbf{g},$$

$$\frac{\partial n}{\partial t} + \operatorname{div}(n\mathbf{v}) = 0, \quad \frac{\partial c_i}{\partial t} + \mathbf{v}\nabla c_i = -\operatorname{div}\mathbf{j}, \tag{1}$$