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Numerical Study of the Diffusion of Two Gases Equally Diluted by Third Component

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A special case that is often considered when solving practical problems in multicomponent mass transfer is the diffusion of two or more gases through a layer of diluent gas (ballast gas). A very interesting problem is the case when different diluent gases with different properties are used in the diffusion process, which, apparently, makes it possible to control the nature of the flow of mass-exchange processes, for example, in chemical reactions. If ballast gas is used as an indicator, then it is possible to estimate the actual molecular transfer of components and describe the features of multicomponent diffusion (Duncan et al. 1962, Dil'man et al. 2010, Toor 1957).

Diffusion studies in multicomponent gas mixtures with ballast gas have shown that the role of hydrodynamic transport is great (Kosov et al. 1981). Therefore, to evaluate its effect on the diffusion of two main components is undoubtedly important.

If two main gases are diluted equally by different ballast gases, then the diffusion coefficients of the main gases will depend on which diluent gas (light or heavy) is in the mixture. By appropriately selecting the diluent gas, one can either accelerate or slow down the diffusion mass transfer of the main components.

A numerical study of the instability of mechanical equilibrium in systems with ballast gas can be carried out on basis of the approach described in (Kossov et al. 2017). However, the possibilities of this method are limited. In the study of nonstationary processes, the proposed approach does not allow to determine accurately the critical conditions for the "diffusion-convection" transition. It is also difficult to describe the dynamics of convective currents on basis of the stability theory and to estimate the kinetics of multicomponent mass transfer under conditions of developed instability. Such questions can be solved with the help of numerical methods of mathematical modeling.

The macroscopic motion of an isothermal three-component gas mixture is described by the general system of equations involving the Navier-Stokes equations, conservation equations of the particle number of mixture and components in the Boussinesq approximation. For the numerical solution of this equations system is used the splitting scheme on physical parameters. The spatial derivatives are approximated on the uniform spatial grid. The time derivatives are approximated by differences ahead with the first order. On the first stage, the transference of the number of motion is done due to the convection and diffusion. The intermediate velocity field is solved by the five-point sweep method specified by Navon (1987) with the fourth order of accuracy in space and the third order of accuracy with respect to time using the explicit scheme of Adams-Bachfort for convective terms and implicit scheme of Crank-Nicolson for the diffusion members defined by Kim and Moin (1985). On the second stage, based on the found intermediate velocity field, there is the pressure field. Intermediate velocity field is at the use of fractional step method. By analogy with Abdibekova et al. (2014) we have used the sweep method at each stage of sweep fractional step method to find the stage significance of intermediate field speed. On the third stage, it is assumed that transference is done only due to pressure gradient, where the final velocity field is recalculated. On the fourth stage the concentration of components mixture are calculated on basis of five-point sweep method using the Adam-Bachfort scheme taking into account the found velocity fields. The calculations were carried out on a uniform rectangular staggered grid. The calculations are done for actual physical parameters of geometrical characteristics of the channel. The main assumption in modeling is the two-dimensional flows limitation.

The results of numerical experiment have shown that by appropriately selecting the diluent gas, one can either intensify or slow down, or leave without change the process of transfer of those gases that diffuse in its medium.

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