Special Regimes under Diffusion in Gaseous Mixtures

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Abstract: The features of the occurrence of convective flows during diffusion in multicomponent gas mixtures are considered. Experimental data and results of a numerical analysis of the emergence of convective motions during diffusion in three-component gas mixtures are presented. It is shown that the analysis of the stability of three-component gas mixtures can be carried out both in the framework of the linear stability theory and modern methods of numerical simulation.

1. Introduction

Molecular diffusion can lead to instability of the mechanical equilibrium of the mixture with the subsequent occurrence of natural convection, which noticeably intensifies the total mass transfer. In experiments on the study of mixing in multicomponent systems at different pressures and compositions [1], and diffusion of a mixture of solution vapors into an inert gas [2], convective flows were observed leading to a synergistic effect associated with a significant increase in the rate of mixing of the system components.

The solution of issues related to the determination of the mechanism of change of the regimes "diffusion – convection" in multicomponent gas mixtures and the parameters determining the occurrence of the convective mode are important for fundamental and applied problems of convective mass transfer.

2. Experimental data

In the ternary gas mixtures (for example 0.5538 H_2 + 0.4462 N_2 – CH_4 and 0.8846 H_2 + 0.1154 CH_4 – He [3], 0.5504 CH_4 (1) + 0.4496 Ar (2) – N_2 (3), 0.5143 He (1) + 0.4857 Ar (2) – 0.5148 CH_4 (3) + 0.4852 Ar (2) and 0.8366 CH_4 (1) + 0.1634 R12 (2) – n-C_4H_{10} (3) [4]) a regime change can occur, due to the difference in diffusion coefficients. The parameters defining such a transition are the pressure and the initial composition of the mixture [3, 4]. In this case, it is possible to realize the conditions when the transfer of the component with the highest molecular weight will be prior to the others. This situation that is not typical for the diffusion can be explained by the occurrence of convective structured formations.

3. Numerical analysis

Diffusion mixing near the boundary of the change of kinetic regimes can be described by the general system of hydrodynamic equations, which includes the Navier-Stokes equations written in the Boussinesq approximation, preserving the number of particles of a mixture and components [1, 3, 4]. This system of equations can be solved analytically using the linear stability theory [3] or by means of the splitting scheme for physical parameters [4].

First approach allows in terms of diffusion Rayleigh numbers to obtain the maps of stability for the ternary gas mixtures determining regime change "diffusion – concentration gravitational convection" for the vertical channels. Thus, in order to evaluate the theoretical effect of pressure (or other influencing parameter) on the occurrence of convection under the isothermal mixing of ternary gas mixture is necessary to consider the location of the partial Rayleigh numbers (as points) relative to the boundary line on the plane (Ra_1, Ra_2). If the partial Rayleigh numbers lie below the boundary line, then the diffusion process is observed in the system. If the partial Rayleigh numbers are in the area between the boundary line and zero density gradient line, then the stability paradox occurs in the system, i.e. there is an unstable diffusion mixing. If the partial Rayleigh numbers are situated above the boundary line, then the convective mixing is observed in the mixture.

The numerical model for the study of isothermal transfer in three-component gas mixtures permits to determine and analyse the behaviour of isoconcentration lines of the components. The main feature of the transition from the diffusion mode to the convective mode is the appearance of nonlinear isoconcentration lines due to a significant difference in the coefficients of mutual diffusion of the components. With increasing pressure or content in the mixture of the component with the highest molecular weight, the curvature of the isoconcentration lines increases which is the cause of the occurrence of convective instability. With unstable mixing, a pulsating transfer mode is possible, which is associated with the occurrence of structural convective formations.

4. Summary

Thus, the proposed mathematical models for the study of isothermal transfer in three-component gas mixtures allows for determining the conditions under which the change of regimes "diffusion – concentration gravitational convection" occurs.

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