

ABSTRACT

Doctoral thesis for the degree of PhD on the specialty 8D05302 - "Physics" by Zhussanbayeva Aiyim

Research topic: Emergence and evolution of structured flows at boundary of the «diffusion – concentration convection» regime change in isothermal multicomponent mixing in gas mixtures.

Purpose of research: experimental and numerical investigation of mechanical equilibrium of isothermal ternary gas mixtures, determination of dynamic characteristics of arising concentration gravity currents under different conditions (pressure, mixture composition, ratio between diffusion coefficients), obtaining computational data on the effect of differences in diffusion coefficients of components on the determination of the boundaries of the transition "diffusion - convection".

Objectives of the research:

- to analyze for stability of mechanical equilibrium and determination of baric and concentration conditions of kinetic regimes of mixing in multicomponent mixtures, in which there is a transition from diffusive modes to convective ones;
- to determine of thermophysical and geometrical parameters causing the appearance of supercritical flows caused by instability of mechanical equilibrium of isothermal ternary gas mixtures;
- to investigate of influence of diffusion mechanisms on hydrodynamics of the initial phase of supercritical flow at different pressures and initial compositions of multicomponent mixtures.

Research methods:

Scientific methods of research are based on the fundamental laws of physical kinetics and multicomponent mass transfer. To achieve the set objectives, it is planned to use experimental and computational-theoretical methods of research:

Experimental methods of research.

- Two - column method (areas of investigated parameters: pressure from 0.1 MPa to 3.0 MPa; temperature from 278 K to 353 K).

Theoretical and numerical methods of investigation.

- The method of analysis for stability of mechanical equilibrium in the Boussinesq approximation adapted to the case of isothermal ternary gas mixtures.
- The method of small perturbations and perturbations of finite amplitude.
- Methods of similarity theory.
- Numerical method of splitting by physical parameters.

The main provisions submitted for defense (proven scientific hypothesis and also conclusions that are new knowledge):

- 1) The change of mixing regimes "diffusion - convection" in ternary gas mixture systems $H_2 + CO_2 - N_2$, $N_2 + R_{12} - n-C_4H_{10}$ depends on the pressure and concentration of the gas with the highest molecular weight in the system.

2) The intensity of convective mixing, arising due to the instability of the mechanical equilibrium of the mixture at the initial stage, depends on the pressure and initial composition of the mixture.

3) Diffusion-convection stability cartograms for mixtures $H_2 + CO_2 - N_2$, $N_2 + R_{12} - n-C_4H_{10}$ as a function of initial mixture composition and pressure.

4) Numerically detected pulsation mode of pressure in flat vertical channels at separate stages of convective structures formation.

Description of the main results of the study:

1. to determined, that at diffusion in gas mixtures under certain conditions, it is possible to occur effects not typical for the Fickian description. Their experimental realization is possible on devices, which for binary systems allow to measure successfully the coefficients of mutual diffusion of gases. Correct translation of the described methods to the case of multicomponent mixing allows us to recommend them for experimental studies at the diffusion-convection transition boundary.

2. to studied the change of regimes «diffusion - concentration gravitational convection» in three-component gas mixtures containing carbon dioxide and freon-12 at different pressures and compositions experimentally. The distribution of component concentration and mixture density in vertical cylindrical channel in the area of parameters determining transition «diffusion-convection» is analyzed. Cartograms fixing the boundaries of increasing (convection) and damped (diffusion) convective disturbances are presented and compared with experimental data.

3. to described an algorithm for calculating isoconcentration distributions in vertical channels, which allow characterizing the change of regimes «diffusion – convection» and detailing the evolution of convective currents in the initial stage of emergence. The basic sign of the «diffusion-convection» transition is appearance of nonlinear isoconcentration lines. Curvature of isoconcentration lines is possible at certain content of the component with the largest molecular weight in mixture, as well as pressure.

Novelty and importance of the results obtained:

The 1st experimentally investigated the transition «diffusion – convection» at different compositions and pressures in system $H_2 + CO_2 - N_2$;

The 2nd numerically investigated convective stability of the mixture in vertical diffusion channel for the system $H_2 + CO_2 - N_2$;

The 3rd studied the influence of the difference in the diffusion coefficients of components on the mixing intensity in gas mixtures near the area of transition to convective regime of mass transfer;

The 4th calculated the distributions of component concentrations, pressure and average velocity at occurrence of supercritical-convective flows in ternary gas mixtures at different initial compositions.

Compliance with the directions of development of science or state programs:

The dissertation work was implemented in accordance with the plans of fundamental research work of Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan «Grant financing of scientific research» on the topics: «Occurrence of concentration gravitational convection at

multicomponent diffusion in steadily - stratified media» (2021 - 2023, code AP09259248, state registration number 0121RK00258); «Development of an innovative method of purification of isothermal gas mixtures from carbon dioxide in conditions of instability of mechanical equilibrium» (2022 - 2024, code AP14870237, state registration number 0122RK00463).

The contribution of the doctoral student to the preparation of each publication (the contribution of the author of the dissertation work is shown as a percentage of the total volume of the publication):

The content of the dissertation work is represented in the 8 articles and international conferences:

1. Diffusion mechanisms for the occurrence of the instability of mechanical equilibrium of a ternary gas mixture containing carbon dioxide (Switzerland) // *Fluids*, 2021 y. 6(5), P. 1-7, 177 (Scopus). (Co-authored by: Kosov V. N., Fedorenko O.V., Kalimov A.B. 60%);

2. Features of isothermal multicomponent mixing of gas mixtures containing methanes at convective instability // «BULLETIN KazNPU». Series of the «Physics and mathematical sciences», 2020 y. № 3 (71), – P. 102- 105. (Co-authored by: Kosov V. N., Mukamedenkyzy V. 60%);

3. Numerical research of characteristic mixing times of isothermal three-component steam-gas systems // «BULLETIN KarSU ». Series of the «Physics», 2022 y. №2, – P. 133-140. (Co-authored by: Mukamedenkyzy V., Kosov V. N., Akzholova A.A. 60%);

4. Instability of mechanical equilibrium and some features of concentration convection in isothermal ternary gaseous systems. // «BULLETIN KazNU ». Series of the «Physical Sciences and Technology», 2022 y. №1-2. – P. 55 – 61. (Co-authored by: Kosov V. N., Fedorenko O.V., Zhaneli M. 60%);

5. Численное исследование влияния давления на неустойчивость механического равновесия в трехкомпонентных газовых смесях при изотермических условиях // «Проблемы науки». Series of the «Physics and mathematical sciences», Moscow, 2017 y., №5(18), – P. 5-7. (100%);

6. Features of multicomponent mixing of isothermal gas mixtures at convective instability // Proceedings of IX International Scientific and Methodical Conference «Mathematical Modeling and Information Technologies in Education and Science (MMITES)» dedicated to the 75th anniversary of Doctor of Pedagogical Sciences, Professor E.Y. Bidaibekov and 35th anniversary of school informatics Almaty, Kazakhstan, October 1-3, 2020. – P. 75 – 79. (Co-authored by: Kosov V. N., Mukamedenkyzy V., 60%);

7. Численное исследование возникновения конвективных возмущений в изотермических трехкомпонентных парогазовых системах // Proceedings of VII International Scientific and Technical Conference of students, graduate students and young scientists of the Kazakhstan, «Creativity of the young – innovative development of the Kazakhstan» – Ust-Kamenogorsk, Kazakhstan, April 8 - 9, 2021. – Part IV. P. 116 – 120. (Co-authored by: Mukamedenkyzy V., Kosov V.N., 60%);

8. Специфика возникновения структурированных течений при смене режимов «диффузия – концентрационная конвекция» для изотермического тройного смешения // Proceedings of XVI Minsk International Forum on Heat and Mass Transfer «Convective-Radiation Heat Transfer». – Minsk, Belarus, May 16-19, 2022. – P. 41-45. (Co-authored by: Kosov V.N., Fedorenko O.V., Bitibaeva J.M., Меурамбекuly E. 60%).