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INVESTIGATION OF MIXING IN BINARY GAS MIXTURES UNDER MECHANICAL EQUILIBRIUM INSTABILITY

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Abstract. *Mixing processes in binary and multicomponent gas systems are characterized by a significant variety of observed regimes. The main objective of the study is to determine the boundary between diffusion and convective regimes, as well as to identify the parameters that control the convective regime. The change in modes from "isothermal diffusion" to "gravitational concentration convection" was studied using the ANSYS Fluent software package, which allows investigating the evolution of convective flows at the initial stage of mixing and determining the limits of mechanical equilibrium stability of the system. The observed correspondence between computational and experimental results verifies the proposed method for determining the boundary between diffusion and convective transport in gas mixtures. The novelty lies in reconstructing the spatiotemporal evolution of the isoconcentration fields for binary mixtures at different pressures and relating the convective flow structures to the observed mode transitions. The approach provides a verified method for locating the diffusion–convection boundary and for refining diffusion and thermal-diffusion coefficient measurements.*

Keywords: diffusion, convection, mechanical equilibrium, binary gas mixture.

1. Introduction

The fundamental cause of natural convection in liquids and gases is a disturbance in mechanical equilibrium caused by inhomogeneities in the distribution of density, temperature, and concentration of components [1]. The phenomenon of natural convection underlies many natural processes, such as atmospheric circulation and the transport of water masses in the oceans [2, 3]. The occurrence and development of convection in viscous media is due to the combined action of a number of physical mechanisms. The loss of mechanical equilibrium stability can be explained by various amplifications of hydrodynamic disturbances caused by density fluctuations [1]. Diffusion is a critically important control parameter in a class of problems describing the change in kinetic regimes under the action of simultaneously applied temperature and concentration gradients. Analysis of the stability parameters of the system is necessary not only to determine the boundaries of the growth of hydrodynamic perturbations, but also to predict the areas of their attenuation, since it is in these areas that it is possible to accurately measure the diffusion and thermal diffusion coefficients, which are of great practical importance [4, 5]. This determines the relevance of research in this area, which is valuable both for a fundamental understanding of the physical nature of the effects under study and for solving applied problems. Modeling natural convection requires consideration of a wide range of parameters determined by boundary conditions and system geometry. Models are significantly complicated by the need

to integrate factors such as coupled heat and mass transfer, chemical transformations, internal heat sources, and the presence of phase boundaries [5].

The transition between kinetic mixing modes is determined by the disruption of the mechanical equilibrium of the system. A mode change can be caused by the emergence of density gradients [6], which are formed under the influence of heat flows, composition heterogeneity, or applied external fields. When considering binary mixtures in a system, conjugate temperature and concentration gradients arise [7]. Their interaction causes the development of complex, often unstable, convective modes. The loss of mechanical equilibrium stability in binary gas mixtures is determined by a complex of factors, including spatial temperature gradients, differential compression, and external force fields. When the threshold values of the control parameters are reached, modes are formed in the system that are associated with a change in the dominant transport mechanism from molecular diffusion to convective motion. Under conditions of gravitational stratification, convective flows [8], driven by the difference in the densities of the components, evolve into complex macroscopic structures. Experimental studies [9, 10] have confirmed the validity of approaches [7, 8] for describing regions of non-isothermal diffusion and thermal concentration convection.

It should be noted that studies [5-7,11] considered convection arising from non-isothermal mass transfer and thermal diffusion under the action of a temperature gradient. As shown in [12], during isothermal mixing of multicomponent systems, the difference in diffusion coefficients causes an inversion of the mixture density, which leads to effects that require additional study compared to those presented in works on non-isothermal mixing. In [13], a large number of studies were summarized that were conducted for isothermal cases of multicomponent mixing at the boundary between diffusion and gravitational convection modes under various thermophysical factors.

Numerical studies of the evolution of convective mixing in isothermal mixtures have revealed a variety of transition regimes from diffusion to convection and have determined the characteristic mixing times inherent in diffusion and combined mixing types [14-17]. At the same time, it should be noted that the convective mixing effects recorded in [13-15] are derived from the simultaneous action of several concentration gradients. Therefore, it seems important to study the change in kinetic regimes in the presence of a minimum number of concentration gradients that correspond to binary systems when the condition of increasing mixture density with height is realized. In [9,10,18], the features of convective mixing in isothermal binary mixtures with unstable mixture density stratification were investigated. Within the framework of stability theory [1,7], relations were obtained that register the transition from diffusion to the Rayleigh–Taylor convection analogue [19]. At the same time, studies related to the dynamics of isoconcentration fields at given compositions and pressures have not yet sufficiently established the relationship between the structures of convective flows and the evolution of their development.

Unlike the authors' previous, mainly experimental and stability-theory studies [9, 10, 18], this work uses 3D CFD modelling to reconstruct the spatiotemporal evolution of the isoconcentration fields and to link the structure of the convective flows directly to the mode transitions. The novelty lies in establishing, for isothermal binary mixtures at different pressures, the connection between the spatial organization of convective flows and the "diffusion–convection" and "convection–convection" transitions, including identification of the critical pressure of mechanical-equilibrium instability.

This work proposes to numerically investigate, using the ANSYS Fluent software package [20], the initial stage of the spatial-temporal evolution of concentration fields arising from the instability of the mechanical equilibrium of a gas system at different pressures for isothermal binary mixtures. It is planned to compare the numerical results with experimental data. It is expected that the presented comparison will provide a better understanding of the mechanisms of transition from a diffusion state to a convective state, which will allow recommendations to be developed for a more detailed description of mixing processes in binary systems.

2. Problem formulation and numerical methods

The experimental studies obtained in [9-10] in the pressure range of 0.338–2.5 MPa at a temperature of 298 K using an experimental setup implementing the two-flask method, the diagram of which is shown in Fig. 1, were taken as the objects of study. The diffusion apparatus consisted of two flasks of equal volume $V_u = V_l = 55.6$ cm^3, which were connected by a diffusion channel with a diameter of $d = 0.4$ cm and a length of $L = 6.4$ cm. The duration of the experiments was 17 min, except for the experiments at a pressure of 0.29 MPa, for which the duration was increased to 60 min. The ANSYS Fluent software package provides the ability to

perform three-dimensional modeling of diffusion channels of arbitrary geometry [19], as well as visual visualization of physical processes described by the selected system of equations.

A combined approach to mesh generation was used to discretize the computational domain when modeling a binary gas mixture. The cylindrical elements of the system were approximated by an unstructured mesh based on triangular finite elements, while the diffusion channel was described by a structured mesh of square elements. This mesh generation strategy allows the geometric features of different parts of the installation to be adequately taken into account. The choice of a characteristic mesh cell size of 2 mm ensures correct reproduction of the model geometry and stable convergence of the numerical solution [20]. A mesh sensitivity analysis carried out for a representative case (p = 1.49 MPa) on co-arser and finer grids showed that the predicted nitrogen concentration in the lower flask varied by less than about 1.5% upon refinement, confirming that the results are essentially grid-independent. The mesh of about 385 000 elements was therefore adopted as an optimal compromise between accuracy and computational cost.

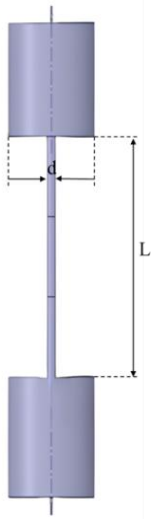


Fig. 1. Three-dimensional model of a diffusion cell and the calculated simulation area

The use of a hybrid mesh combining triangular and square elements provides an optimal balance between modeling accuracy and computational efficiency. The use of triangular cells in cylindrical regions allows for the correct approximation of curved surfaces, while the structured mesh in the diffusion channel significantly reduces computational costs. The proposed approach is consistent with modern practices for constructing computational meshes for numerical modeling of processes in binary gas mixtures, where the choice of element types and sizes is determined by the balance between the geometric complexity of the domain and the accuracy requirements of the calculations.

Mass transfer modeling in the N_2-*He* system was performed under initial conditions, when nitrogen is located in the upper flask and helium in the lower one [10]. This configuration, determined by the difference in molecular weights of the gases, creates a pronounced gravitational stratification of the mixture density, allowing the processes of mechanical equilibrium disruption to be investigated. Within the framework of mathematical modeling, the assumption was made that the physicochemical characteristics of the gas environment are constant. The numerical values of the corresponding parameters were obtained from the built-in database of substances in the ANSYS Fluent software package. Since the process is isothermal at 298 K, the temperature-dependent transport properties remain practically constant within a single run, while the pressure dependence is retained through the binary diffusion coefficient D_{12} (Eq. 6) and the mixture density is computed from the state model as a function of composition; the assumption loses accuracy only under strongly non-isothermal or near-critical conditions.

Since the apparatus is modeled as a closed system, impermeability conditions are set at all its boundaries. This type of boundary condition mathematically excludes the possibility of any mass transfer through the control surface, thereby ensuring the isolation of the system from the external environment in terms of material components. To ensure the isothermal nature of the mixing process, appropriate thermal boundary conditions were used, and the enclosure structure of the apparatus was modeled as a solid wall made of structural stainless

steel whose thermodynamic and strength characteristics were also taken from the standard ANSYS Fluent materials library [18].

Convective flows caused by mechanical equilibrium instability demonstrate complex evolutionary dynamics at the initial stage. The evolution of convective flows includes a sequence of stages: linear growth of small convective perturbations, nonlinear interaction of instability modes, transition to a turbulent regime with the formation of multiscale vortex structures, and other specific features determined by the parameters of the system [21]. To analyze partial flows in media with convective flows of variable intensity, it is advisable to use the k-ω turbulence model [22,23], which allows adequate description of mass transfer processes over a wide range. The initial and boundary conditions were set as follows: at the initial moment of time, the upper and lower chambers of the diffusion apparatus contained different binary gas mixtures. The molar fractions of the components were determined using the patch method for the corresponding grid zones.

In ANSYS Fluent, binary gas mixtures are modeled using component transport equations (mass fractions Y_1 and Y_2) and equations of motion. Mass transfer is described by convective-diffusive equations that take into account molecular and turbulent diffusion, and the density of the mixture is calculated according to the selected state model. The formulas include the transport equation for mass fraction [22-23]:

$$\frac{\partial(\rho Y_1)}{\partial t} + \nabla(\rho\vec{u}Y_1) = \nabla\left(\rho D_{eff}\nabla Y_1\right) + S_1$$
$$\frac{\partial(\rho Y_2)}{\partial t} + \nabla(\rho\vec{u}Y_2) = \nabla(\rho D_{eff}\ \nabla Y_2\ ) + S_2 \quad (1)$$

where D_{eff} is the effective diffusion coefficient, S_1 and S_2 are generalized source terms that account for possible mass sources or sinks of components. In the context of the problem under consideration, there are no additional mass sources.

The standard *k–ω* model is based on a system of semi-empirical transport equations, including equations for turbulent kinetic energy *k* and its specific dissipation rate *ω*, where *ω* is interpreted as the ratio of turbulent energy dissipation rate *ε* to *k* [23]. The standard k–ω model was chosen because, unlike the k–ε family, it integrates directly to the wall without wall functions and retains accuracy at low turbulent Reynolds numbers, so it correctly reproduces transitional and near-laminar regimes and naturally reduces to molecular transport in regions where turbulence production vanishes. This makes it suitable for the present problem, in which the flow evolves from a purely diffusive state through a transitional convective stage to locally developed convection.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho\vec{u}k) = \frac{\partial}{\partial x_j}\left(\Gamma_k\frac{\partial k}{\partial x_j}\right) + G_k - Y_k + S_k + G_k$$
$$\frac{\partial}{\partial t}(\rho\omega) + \frac{\partial}{\partial x_i}(\rho\vec{u}\omega) = \frac{\partial}{\partial x_j}\left(\Gamma_\omega\frac{\partial \omega}{\partial x_j}\right) + G_\omega - Y_\omega + S_\omega + G_\omega \quad (2)$$

G_k – describes the generation of kinetic energy of turbulence caused by average velocity gradients; ρ is the density of the medium; $\vec{u} = (u_x, u_y, u_z)$ – velocity vector; G_ω – characterizes the generation of the specific dissipation rate ω. In the presented system of equations, Γ_k and Γ_ω characterize the effective turbulent diffusion for *k* and *ω*, respectively; Y_k and $Y\omega$ are dissipation terms; S_k and S_ω are user source terms, which are assumed to be zero in this work [24]. The indices i, j imply summation over coordinates ($i, j = 1, 2, 3$).

The effective diffusion coefficients for the *k–ω* model are given by the formulas:

$$\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}$$
$$\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega} \quad (3)$$

Prandtl turbulence numbers σ_k and σ_ω determine the efficiency of diffusion transfer of turbulent kinetic energy and the rate of its dissipation. Within the framework of the model used, constant values $\sigma_k = \sigma_\omega = 2$ are assumed. Molecular viscosity μ is supplemented by turbulent viscosity μ_t, which is a function of *k* and *ω*:

$$\mu_t = \alpha^* \frac{\rho k}{\omega} \quad (4)$$

where α^* is a coefficient that dampens turbulent viscosity and has a constant value of $\alpha^*=1$ [23]. Diffusion flows $\overrightarrow{J_1}$ and $\overrightarrow{J_2}$ for substances 1 and 2, respectively, are calculated using the formulas:

$$\overrightarrow{J_1} = -\left(\rho D_{12} + \frac{\mu_t}{Sc_t}\right)\nabla Y_1$$
$$\overrightarrow{J_2} = -\left(\rho D_{12} + \frac{\mu_t}{Sc_t}\right)\nabla Y_2 \quad (5)$$

In the presented model: μ_t is the turbulent viscosity; Sc_t is the Schmidt number, defined as $Sc_t = \mu_t/(\rho D_t)$; the standard value of Sc_t is taken to be 0.7. D_{12} is the binary diffusion coefficient; T is the temperature. It should be noted that in developed turbulent flows, the contribution of turbulent diffusion usually exceeds molecular diffusion. However, in the problem under consideration, corresponding to the initial and transitional stages of mixing, molecular diffusion processes continue to play a significant role.

Binary diffusion coefficient D_{12} is determined within the framework of Chapman-Enskog kinetic theory [25] using the formula:

$$D_{12} = 0.00186 \frac{\left[T^3\left(\frac{1}{M_{w,1}} + \frac{1}{M_{w,2}}\right)\right]^{\frac{1}{2}}}{p_{abs}\sigma_{12}^2 \Omega_D} \quad (6)$$

where M_w - molar mass (g/mol), T - temperature (K), p_{abs} - absolute pressure (atm), Ω_D - dimensionless diffusion collision integral, quantitatively characterizing the intensity of molecular interactions in the system.

An approach based on the pressure method was used for all calculation models. For spatial discretization of computational fluid dynamics equations, the schemes listed in Table 1 were used, which were tested and validated in [23, 26].

The parameters listed characterize the configuration of the numerical solution in the ANSYS Fluent environment, detailing the methods used to discretize the basic equations, approximation schemes, and computational algorithms involved in the modeling process. The PRESTO! (PREssure STaggering Option) scheme computes pressure on staggered face control volumes, avoiding the interpolation errors of standard schemes, and is therefore recommended for flows with strong body forces and steep density gradients, such as the buoyancy-driven concentration convection considered here. The selected and tested combination of discretization schemes guarantees an optimal balance between the accuracy of the numerical solution and computational efficiency, which is particularly critical for problems with the combined influence of convective and diffusion processes, and makes it the preferred choice for this class of problems [24].

Table 1. Solution methods

Quantity	Discretization
Gradient	Least Square Cell Based
Pressure	PRESTO!
Momentum	Second Order Upwind
Turbulent Kinetic Energy	Second Order Upwind
Specific Dissipation Rate	Second Order Upwind
Pseudo Time Method	Off
Transient Formulation	Second Order Implicit

3. Results of numerical studies and comparison with experimental data

Numerical simulation of the dynamics of binary gas mixtures was performed in the ANSYS Fluent 2025 R2 software environment using a Lenovo LOQ 15IAX9 computing complex equipped with an Intel Core i5-12450HX processor, 16 GB of RAM, and an NVIDIA GeForce RTX 3050 graphics accelerator. Depending on the complexity of the calculation scenario and the characteristics of iterative convergence, the duration of

a single computational experiment ranged from 20 to 72 minutes. To assess the reproducibility of the results obtained, each series of calculations was performed three times.

In order to validate the numerical approach adopted to describe the kinetic transition "diffusion–convection" and "convection–convection" over a wide range of pressures, the simulation results were compared with the experimental data presented in [9, 10] and summarized in Table 2. The computational mesh and discretization schemes are described in Section 2.

The experimental data [9,10] presented in Figure 2 illustrate the effect of pressure on the behavior of the *N_2–He* binary gas mixture. At low pressures, there is good agreement between the concentrations calculated under the assumption of diffusion and the experimental concentrations, which indicates the predominance of the diffusion mechanism of mass transfer. In this pressure range, the binary diffusion coefficient has relatively high values, and density stratification remains stable, as a result of which any local disturbances are effectively suppressed by molecular diffusion. With an increase in pressure starting from a certain critical value (0.518 MPa), the concentration of components increases, which indicates a loss of mechanical equilibrium stability of the system and the emergence of convective currents, i.e., a boundary transition "diffusion-convection" is recorded. This transition is caused by a decrease in the mutual diffusion coefficient with a simultaneous increase in density gradients, as a result of which the characteristic diffusion equilibration time becomes comparable to the growth time of gravity-induced perturbations. At this point, the system reaches a limiting state in which small density and concentration perturbations cease to decay. Further pressure increase leads to an increase in the concentration of components, which corresponds to the convective type of mixing. In the specified pressure range, mass transfer is determined by the development of concentration-driven gravitational convection, leading to intensification of component transfer. However, starting at a pressure of 1.1 MPa, the intensity of convective mixing begins to decrease, and at a pressure of 1.8 MPa, the intensity of mixing decreases, which is typical for diffusion rather than gravitational convection. This behavior may be associated with the restructuring and enlargement of convective structures, as well as with an increase in viscous and stabilizing effects at high pressures, which leads to a decrease in the efficiency of convective mass transfer.

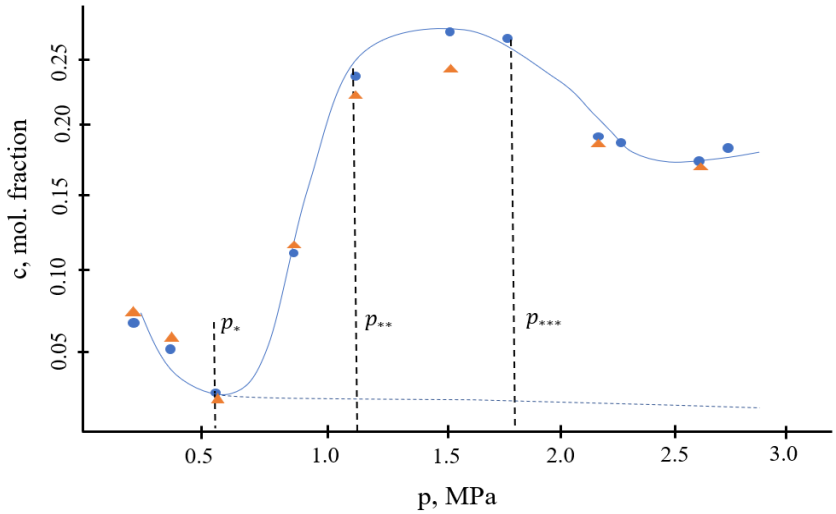


Fig. 2. Pressure dependence of nitogen transfer from upper flask to the lower flask in the *N_2-He* system: until $p_* \approx$ 0.518 MPa – diffusion mode; from p_* to $p_{**} \approx$ 1.1 MPa – the occurrence and development of convection; from p_{**} to $p_{***} \approx$ 1.8 MPa – transition from one type of convective mixing to another; from p_{***} – decrease in convection intensity. ● – experimental points [9,10], ▲ – Points calculated using Ansys Fluent, solid curve – polynomial approximation, dotted curve – calculation based on Stefan-Maxwell theory

The change of mixing regimes with pressure reflects the competition between the buoyancy forces that drive convection and the diffusive and viscous mechanisms that dissipate it. As the pressure increases, the binary diffusion coefficient decreases (Eq. 6), which weakens the diffusive smoothing of concentration gradients and sharpens the density stratification. Once the solutal Rayleigh number exceeds its critical value, the mechanical equilibrium loses stability and concentration-driven convection sets in. In the range from p=0.52 to 1.1 MPa the driving density gradients dominate over dissipation, and fine-scale plume-like structures analogous to Rayleigh–Taylor fingers develop, providing a large interfacial area and intense convective

transport. At higher pressures, the further reduction of D_{12} is accompanied by an increase in density and in momentum dissipation, so that the characteristic scale of the convective structures grows: the plumes merge into larger and slower circulation cells with a smaller specific interfacial area. As a result, although convection persists, its efficiency decreases and the integral mass-transfer rate approaches values typical of the diffusion regime — this restructuring, rather than a complete suppression of convection, is the physical mechanism behind the "convection–convection" transition.

The table 2 shows experimental and calculated values of concentrations both in the diffusion approximation (according to Stefan-Maxwell equations) and taking into account convective perturbations according to the k-ω turbulence model. Analysis of experimental and numerical data shows good convergence and demonstrates that when critical pressure values are reached in the system, a transition from diffusion mode to concentration convection is observed. The formation of convective flows at certain time intervals is a key indicator of a disturbance in the mechanical equilibrium of the system. The observed process is consistent with the theoretical provisions of convective stability theory. Based on the analysis of the time dependencies of the average molar fractions and isoconcentration isoline maps, two types of transitions were identified: the "diffusion → convection" transition is recorded at the moment of isoline curvature and the appearance of local circulation flows; the "convection → convection" transition corresponds to the restructuring of the flow structure, including due to the action of convective mechanisms. With a further increase in pressure, convection persists, but its nature changes, which manifests itself in the restructuring of the spatial structure of the flows and the stabilization of average concentrations.

Table 2. Concentrations of diffused nitrogen from the upper flask to the lower flask for the *N_2-He* system at various pressures and T=298 K, τ = 17 minutes

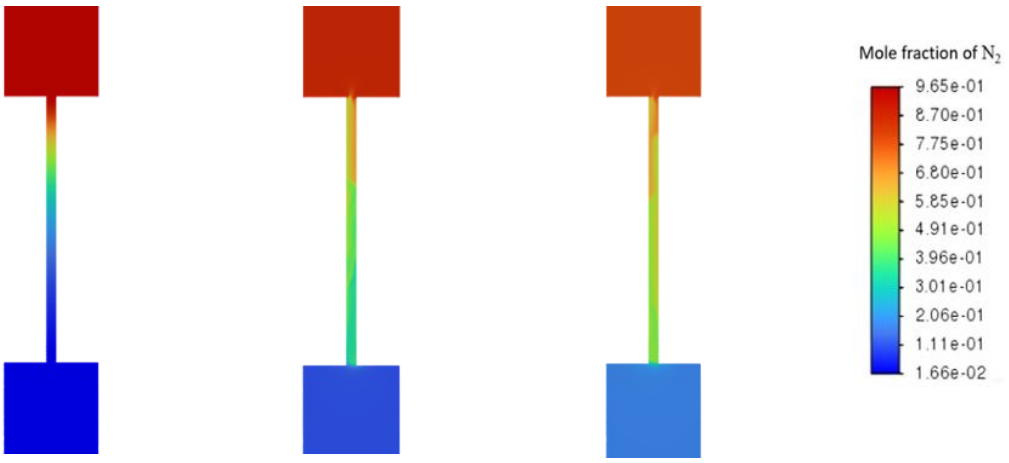
P, MPa	$C_{experiment}$	C_{theory}	C_{Ansys}
0,338	0,065	0,064	0,069
0,437	0,051	0,051	0,055
0,518	0,043	0,046	0,040
0,798	0,161	0,030	0,165
1,030	0,244	0,024	0,226
1,490	0,273	0,016	0,239
2,210	0,184	0,022	0,181
2,655	0,173	0,028	0,170

The agreement between the calculated and experimental concentrations was quantified by the relative deviation. The mean absolute relative error over the whole pressure range is about 5.8%, with a maximum of about 12.5% near p = 1.49 MPa, where convective mixing is most intense, this confirms quantitatively the satisfactory predictive accuracy of the model.

The comparison of experimental data with calculated concentration profiles confirms that the initial stage of the diffusion process occurs within a time range that is significant for the overall mixing process. The numerical results obtained demonstrate satisfactory agreement with experimental observations. Figure 3 shows the instantaneous distribution of the concentration field of a binary gas mixture *N_2–He* at a fixed time τ=510 s at different pressure values. This method of data presentation allows us to reveal the influence of pressure on the spatial organization of mass transfer without resorting to integral mixing characteristics.

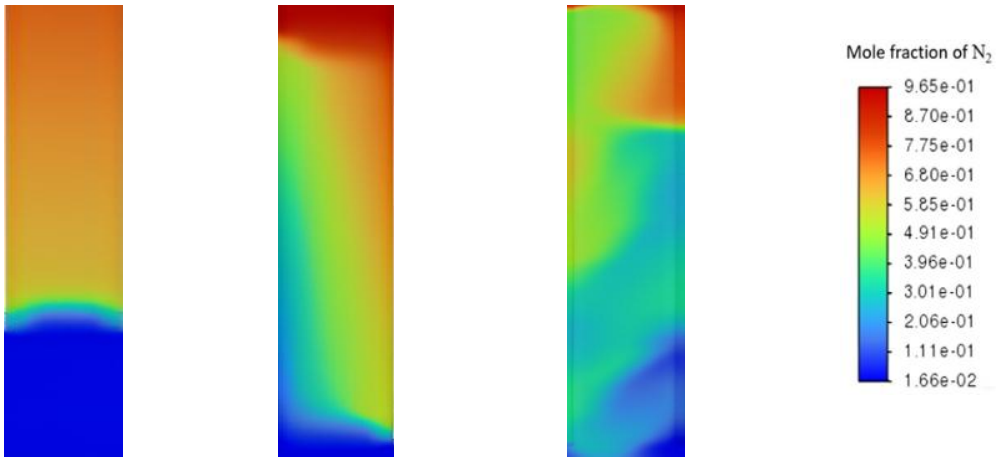
Analysis of the concentration distributions shown in Fig. 3 shows that when the pressure changes, the structure of the concentration field undergoes a sequential rearrangement—from a quasi-one-dimensional distribution to spatially inhomogeneous configurations. At low pressures, the concentration field is characterized by an ordered structure with a dominant direction of transport along the diffusion channel axis and the absence of pronounced transverse gradients, which corresponds to the distribution shown in Fig. 3a.

As the pressure in the system increases, spatial disturbances intensify, manifesting themselves in the curvature of isoconcentration lines and the formation of local inhomogeneities in the distribution of components (Fig. 3b). These changes indicate a complication of the spatial structure of mass transfer and an increase in the role of transverse concentration redistributions. With a further increase in pressure, the concentration field becomes significantly heterogeneous (Fig. 3c), reflecting the intense spatial redistribution of components within the system and the formation of stable concentration configurations. The further temporal evolution and spatial organization of these structures are shown in Figure 4.



a) b) c)

Fig. 3. Mixing dynamics for the *N_2-He* system at time τ = 510 s depending on mixing modes: a) p=0.437 MPa; b) p=0.798 MPa; c) p=1.49 MPa



a) b) c)

Fig. 4. Convective flows formed in the diffusion channel for the *N_2-He* system at p=1.49 MPa, T=298 K as a function of time: a) τ = 1 s; b) τ = 2 s; c) τ = 7 s

The sequence of instantaneous distributions allows us to trace the characteristic stages of the evolution of concentration-driven convection after the system loses its mechanical equilibrium stability.

At the initial stage of mixing, the concentration field remains generally ordered, but small distortions of isoconcentration lines occur near the contact region of the components (Fig. 4a). These disturbances reflect the emergence of concentration fluctuations caused by the instability of density stratification and indicate a violation of the pure diffusion transport mechanism. As the process develops, the spatial disturbances intensify, covering the entire cross-section of the channel and leading to a pronounced deformation of the isoconcentration surfaces (Fig. 4b). At this point, diffusion transport is no longer able to compensate for the emerging density inhomogeneities, which leads to a sustained growth of convective motions.

As the process continues, the concentration field acquires a stable spatially heterogeneous structure, reflecting the formation of a developed convective mass transfer regime (Fig. 4c). Convective flows ensure intensive redistribution of components throughout the diffusion channel, and the subsequent evolution of the system is accompanied by complex circulation and maintenance of the quasi-stationary nature of the concentration field.

4. Conclusions

This paper presents a numerical study of mass transfer in a binary gas system *N_2–He* under conditions of isothermal mixing at varying pressure. It is shown that pressure is one of the key parameters determining the stability of mechanical equilibrium and the spatial organization of the concentration field of the gas mixture.

A critical pressure value of $p \approx 0.52$ MPa has been established, at which the diffusion mode of mass transfer loses stability and concentration-driven convection is initiated in the system. In the region of elevated pressures, a developed convective regime is formed, accompanied by an intense spatial redistribution of components and the formation of stable convective structures.

Numerical results obtained using component transport equations and the k–ω turbulence model show good agreement with experimental data and correctly reproduce both the transition from diffusion mode to convection and the subsequent evolution of convective flows. Analysis of the spatiotemporal dynamics of the concentration field revealed the characteristic stages of the process—from the emergence of small concentration perturbations to the formation of stable spatial structures.

The results obtained clarify the physical mechanisms of mechanical equilibrium instability in gas mixtures and can be used in modeling diffusion-convection processes in systems with controlled density stratification.

Conflict of interest statement
The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

CRediT author statement
Mukamedenkyzy V.: Conceptualization, Validation, Supervision, Writing - Review & Editing; **Akberdiyev B.E.:** Methodology, Software, Formal analysis, Writing - Original Draft.
The final manuscript was read and approved by all authors.

Statement on the use of Artificial Intelligence.
During the preparation of this manuscript, artificial intelligence tools were used solely for language editing and grammatical improvement.

Data Availability Statement
The data are available upon reasonable request from the authors.

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