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SOME FEATURES OF RAYLEIGH-TAYLOR CONVECTION IN THE MIXING OF IDEAL GAS MIXTURES

The paper deals with computer modeling of convective structures formation at isothermal mixing of three-component gas system on the basis of numerical experiments using ANSYS Fluent. The research aims to study the transition of the system from a diffusion regime to a convective regime and to analyze the stability of mechanical equilibrium in multicomponent gas systems.

The scientific and practical significance lies in understanding mass transfer processes, which are crucial for applied tasks in thermophysics, energy, and environmental sciences. Investigating the characteristics of transitional processes enables the clarification of diffusion-convection interaction mechanisms and the development of recommendations for process optimization. The research methodology includes numerical modeling of mass transfer processes using the k-ω turbulence model and Stefan-Maxwell equations. Boundary conditions, computational grids, and modeling parameters were adapted to adequately describe the structural features of mixing and convective flows. The main results confirmed the effectiveness of ANSYS Fluent in modeling convective flows. The numerical data demonstrated good agreement with experimental results, indicating the model's ability to account for the influence of convective flows. The value of this study lies in developing a numerical approach that enables a quantitative description of kinetic transitions between diffusion and convection. The practical significance of the work is its applicability to the study of mixing processes in complex gas systems, making it useful for technological and scientific advancements.

Keywords: diffusion, convection, computational modeling.

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Идеал газ қоспаларының араласуы кезіндегі Рэлей-Тейлор конвекциясының кейбір ерекшеліктері

Мақалада ANSYS Fluent көмегімен сандық эксперименттер негізінде үш компонентті газ жүйесінің изотермиялық араласуы кезінде конвективті құрылымдардың қалыптасуын компьютерлік модельдеу қарастырылады. Зерттеудің мақсаты – жүйенің диффузиялық режимнен конвективтік режимге өту процесін зерттеу және көпкомпонентті газ жүйелеріндегі механикалық тұрақтылығын талдау. Зерттеудің ғылыми және практикалық маңыздылығы массаалмасу үдерістерін түсінумен байланысты, бұл жылуфизикасы, энергетика және экология саласындағы қолданбалы міндеттерде маңызды рөл атқарады. Өтпелі процестердің сипаттамаларын зерттеу диффузиялық-конвективтік өзара әрекеттесу механизмдерін нақтылауға және технологиялық процестерді оңтайландыру бойынша ұсыныстар әзірлеуге мүмкіндік береді. Зерттеудің әдістемесі массаалмасу үдерістерін сандық модельдеуді, турбуленттілік үшін *k-ω* моделін және Стефан-Максвелл теңдеулерін қолдануды қамтиды. Шекаралық шарттар, есептеу торлары және модельдеу параметрлері араласудың құрылымдық ерекшеліктері мен конвективті ағындарды дұрыс сипаттау үшін бейімделген. Негізгі нәтижелер ANSYS Fluent бағдарламасының конвективті ағындарды модельдеуде тиімділігін растады. Сандық мәліметтер эксперименттік нәтижелермен жақсы үйлесетіні анықталды. Бұл модельдің конвективті ағындардың әсерін ескере алатындығын көрсетеді. Зерттеудің құндылығы – диффузия мен конвекция арасындағы кинетикалық өтулерді сандық сипаттауға мүмкіндік беретін тәсілді әзірлеу. Жұмыстың практикалық мәні – күрделі газ жүйелерінде араласу процестерін зерттеу үшін әзірленген әдістердің қолданбалы және ғылыми зерттеулерде қолданылу мүмкіндігінде.

Түйін сөздер: диффузия, конвекция, компьютерлік модельдеу.

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Некоторые особенности конвекции Рэлея-Тейлора при смешении идеальных газовых смесей

В статье рассматривается компьютерное моделирование формирования конвективных структур при изотермическом смешении трёхкомпонентной газовой системы на основе численных экспериментов с использованием ANSYS Fluent. Цель работы заключается в изучении перехода системы из диффузионного режима смешения в конвективный и анализе устойчивости механического равновесия многокомпонентных газовых систем. Научная и практическая значимость исследования связана с пониманием сложных процессов массопереноса, которые играют важную роль в прикладных задачах теплофизики, энергетики и экологии. Изучение характеристик переходных процессов позволяет уточнить механизмы диффузионно-конвективного взаимодействия и разработать рекомендации для оптимизации технологических процессов.

Методология исследования включает численное моделирование процессов массопереноса с использованием модели турбулентности *k-ω* и уравнений Стефана-Максвелла. Настройки граничных условий, расчетные сетки и параметры моделирования были адаптированы для адекватного описания структурных особенностей смешения и конвективных потоков. Основные результаты подтверждают эффективность использования ANSYS Fluent для моделирования конвективных течений. Было установлено, что численные данные хорошо согласуются с экспериментальными результатами, что свидетельствует о способности модели учитывать влияние конвективных потоков. Ценность проведенного исследования заключается в разработке численного подхода, позволяющего количественно описать кинетические переходы между диффузией и конвекцией. Практическое значение работы заключается в применимости разработанных методов для изучения процессов смешения в сложных газовых системах, что может быть использовано в технологических и научных разработках.

Ключевые слова: диффузия, конвекция, компьютерное моделирование.

Introduction

In multicomponent gas systems, a great variety of mixing regimes is observed. The intensity of mass transfer in such systems is usually determined by a combination of molecular (diffusion) and convective processes [1]. In practice, it is often underestimated that molecular diffusion can lead to a violation of mechanical equilibrium and initiate the development of convective motions. These motions significantly enhance mass transfer, which plays a key role in many industrial and scientific applications.

Particular attention is paid to the emergence and development of concentration convection, which is associated with the distribution of gas components and a significant enhancement of mass transfer. Such phenomena are important both for fundamental problems of Rayleigh-Taylor theory and for applied studies related to the mixing of different gases under stratified conditions. In particular, the study of the stability and dynamics of multicomponent systems allows a better understanding of the physical processes that determine their behavior and transport characteristics [2-3]. Practical problems related to the study of diffusive and convective regimes are particularly relevant in the context of the development of efficient technological processes, as well as in the modeling of natural phenomena. For example, complex convective structures can arise in multicomponent gas mixtures, which significantly change the mass transfer conditions and lead to the enhancement or suppression of individual mixing processes [4-5].

The study of transitions from diffusive to convective modes of mixing requires the use of modern numerical methods and experimental approaches. Numerical modeling allows us to identify critical parameters at which mechanical equilibrium is broken and stable convective flows are formed. Experiments in real conditions confirm the data of numerical calculations, providing a comprehensive understanding of the ongoing processes [6-8]. Thus, the study of the interaction between diffusion and convection mechanisms in multicomponent gas systems is an important step toward a deeper understanding of mass transfer processes and the creation of new effective technological solutions.

Under isothermal conditions, the instability of mechanical equilibrium of the system is determined solely by the contribution of partial gradients of components, which allows us to isolate the role of diffusion mechanisms in pure form. The peculiarities of instability occurrence in multicomponent diffusion under isothermal conditions are considered in detail in the review [9]. In [10-13] the evolution of mixing in multicomponent systems caused by equilibrium disturbance was studied. It was shown that the arising convective currents promote synergetic amplification of partial fluxes of components, which is not characteristic for ordinary diffusion. In addition, the parameters of the transition from the diffusive regime to convective mixing were revealed. Experimental studies [10], carried out using the two-flask method [14-15], demonstrated that with increasing mixing time, the probability of transition between the diffusion-convection modes decreases, and the observed kinetic transitions are characterized by lower mixing intensity compared to the initial stage of the process. However, the presented experimental data do not provide a complete answer to this question, since under the given conditions for the studied mixtures the time of registration of partial fluxes is of the order of thousands of seconds. By this time, the transition "diffusion-convection" in the systems studied in [10-13] could already be completed, and developed convective flows were recorded in the experiment.

The purpose of this study is to numerically simulate the transition of the system from the diffusive state to the convective state for a multicomponent system, where the instability of mechanical equilibrium is observed, using the ANSYS Fluent software package [16]. Comparison of the numerical simulation results with experimental data is planned. It is expected that the analysis will provide a better understanding of the mechanisms of transition between diffusive and convective regimes and provide recommendations for a more detailed description of mixing processes in multicomponent systems.

Problem statement and basic equations

Accurate determination of the moments of change of convective mixing modes plays a key role in assessing the influence of partial flows of components on the overall mass transfer process. The ANSYS Fluent software package, which allows modeling of mass transfer processes in gas media, was used for the numerical study. The main advantages of this package include the ability to perform three-dimensional calculations in models of diffusion channels, as well as visualization of physical processes described by the selected system of mathematical equations.

Figure 1 shows the scheme of the diffusion cell (DC) used in the two-flask apparatus, where concentration measurements were performed to analyze diffusive and convective types of mixing [10]. The experimental technique allowed us to record shadow images of structural formations as shown in [16], which made it possible to promptly determine the mixing type and compare it with the results of computer modeling. In the process of numerical modeling, it was assumed that at the initial moment of time the upper chamber of the apparatus was filled with a gas mixture differing in chemical composition from the gas in the lower chamber. It was also taken into account that at the initial moment the density of the triple mixture decreases with height. The investigated region of the model consists of three main parts: the upper and lower cylinders and the diffusion channel located between them. The cylinder volumes were assumed to be the same $V_{up} = V_{lower} = 55.6 \times 10^{-6}\, m^3$ and the dimensions of the diffusion channel are as follows: d=4 $\times 10^{-3} m$ – diameter, $L = 64 \times 10^{-3}\, m$ – height.

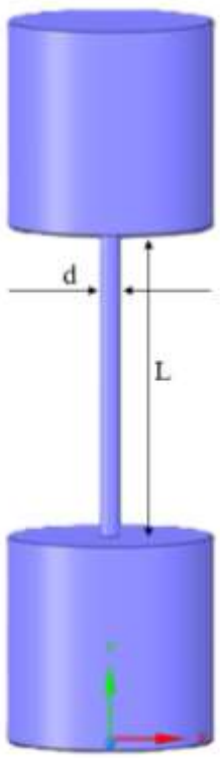

Figure 1 – 3D model of the diffusion cell and the simulation area under study

Within the framework of this study, a combined mesh model was used: the upper and lower cylinders were discretized using triangular elements, and the

diffusion channel was discretized using square elements. This approach provides an efficient adaptation to different geometrical features of the system components.

The grid element size was chosen equal to 1 mm, which is due to the need for a detailed description of the geometry and to ensure convergence of the numerical solution. The total number of grid elements amounted to 402489, which confirms the high resolving power of the model and allows to reproduce reliably the key physical processes occurring in the system.

The use of a combination of triangular and square elements in the grid model allows achieving a balance between modeling accuracy and computational costs. Triangular elements applied in cylindrical regions provide flexibility in adapting to curved surfaces, while square elements in the channel simplify calculations in regions with simpler geometry. This approach is in line with modern standards of computational mesh design, where the choice of element type and size is determined by the complexity of geometry and modeling accuracy requirements.

Convective flows arising at disturbance of mechanical equilibrium in the investigated system constantly evolve. Moreover, the formation of emerged flows can go through several stages of development associated with: the growth of small convective disturbances; nonlinear interaction of disturbance modes; turbulent stage of instability realization determined by the complex type of flow and the appearance of vortex structures of different scale; other features. To calculate partial fluxes of components in the presence of convective currents of different intensity, it is possible to apply a numerical approach in the framework of the k - ω model of turbulence [15].

The standard k - ω model, is a semi-empirical model based on the model transport equations of turbulence kinetic energy (k) and specific dissipation rate (ω), which can also be viewed as the ratio of ε to k [16]. The turbulence kinetic energy k and the specific dissipation rate ω are obtained from the following transport equations:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}(\Gamma_k \frac{\partial k}{\partial x_j})+G_k-Y_k+S_k+G_b \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \omega)+\frac{\partial}{\partial x_i}(\rho \omega u_i)=\frac{\partial}{\partial x_j}(\Gamma_\omega \frac{\partial \omega}{\partial x_j})+G_\omega-Y_\omega+S_\omega+G_{\omega b}$$

In these equations, G_k represents the generation of turbulence kinetic energy due to mean velocity gradients, ρ is the density, and u_i is the velocity component along x_i. G_ω represents the generation of ω. Γ_k and Γ_ω represents the effective diffusivity of k and ω, respectively. Y_k and Y_ω define the dissipation of k and ω, respectively. S_k and S_ω are initial parameters defined by the user [16].

Effective diffusion coefficients for k - ω model are given by the formulas

$$\Gamma_k=\mu+\frac{\mu_t}{\sigma_k}$$
$$\Gamma_\omega=\mu+\frac{\mu_t}{\sigma_\omega} \tag{2}$$

where σ_k and σ_ω is turbulence Prandtl numbers for k and ω, respectively, characterizes the effective diffusion behavior of turbulent kinetic energy diffusion (k) and its dissipation rate (ω). In this model, they were set to fixed values: $\sigma_k=2$ and $\sigma_\omega=2$. μ is molecular viscosity, and turbulent viscosity μ_t, is calculated by combining k and ω as follows:

$$\mu_t=\alpha^*\frac{\rho k}{\omega}. \tag{3}$$

where α^* is coefficient damping turbulent viscosity and having constant value $\alpha^*=1$ [16].

The addition of a transport equation is required to determine the mixing parameters in the DC. The conservation equation represents the relations for convective diffusion, with which the local mass fraction Y_i of each substance i can be predicted, and is defined as follows:

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla\bullet(\rho\vec{v}Y_i)=-\nabla\bullet\vec{J_i}+R_i+S_i. \tag{4}$$

In which ρ is mixture's density, $\vec{v}$ is velocity of diffusing substances, R_i is rate of formation of n as a result of a chemical reaction, and S_i represents any sources defined by the user. The last two terms in the right-hand side were not considered in this work

because chemical reactions and additional sources were not available in the studies [10 - 13]. J_i is is the diffusion flux of a particular substance *i*, which for the density and temperature gradient can be calculated by the formula,

$$\overrightarrow{J_i} = -(\rho D_{i,m} + \frac{\mu_t}{Sc_t})\nabla Y_i - D_{T,i}\frac{\nabla T}{T}. \quad (5)$$

where μ_t is turbulence viscosity, but Sc_t is turbulent Schmidt number, calculated as $Sc_t = \frac{\mu_t}{\rho D_t}$, where D_t is turbulence diffusion coefficient. Sc_t default value is 0,7. $D_{i,m}$ is the mass diffusion coefficient for substance *i* in the mixture, $D_{T,i}$ is thermal diffusion coefficient for substance *i* in the mixture, T is temperature. The last term in the equation was not considered, since the isothermal type of mixing was considered in this paper. We also note that turbulent diffusion generally outperforms molecular diffusion, and a detailed description of molecular diffusion properties (e.g., the concentration dependence of the diffusion coefficient D_{ij}) in turbulent flows is generally not required.

For multicomponent systems the Stefan-Maxwell equations [16] will be used in the form of

$$\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{X_i X_j}{D_{ij}}(\overrightarrow{V_j} - \overrightarrow{V_i}) = \overrightarrow{d_i} - \frac{\nabla T}{T}\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{X_i X_j}{D_{ij}}(\frac{D_{T,j}}{\rho_j} - \frac{D_{T,i}}{\rho_i}), \quad (6)$$

where X is mole fraction, $\vec{V}$ is diffusion rate, D_{ij} is binary mass diffusion coefficient of substance i to substance j. By the same way as equation (5), the calculations were performed under the assumption of isothermality, so the temperature gradient is zero and, accordingly, the last term in equation (6) was not taken into account.

The binary diffusion coefficient D_{ij} is determined within the framework of the Chapman-Enskog kinetic approximation [16]:

$$D_{ij} = 0.00186\frac{[T^3(\frac{1}{M_{w,i}} + \frac{1}{M_{w,j}})]^{1/2}}{p_{abs}\sigma_{ij}^2\Omega_D} \quad (7)$$

where, M_w is molar weight (g/mole), T is temperature (K), p_{abs} is absolute pressure (atm), Ω_D is dimensionless integral of diffusion collision, which is a measure of interaction of molecules in the system.

Setup algorithm

The pressure-based coupled algorithm handles the momentum and pressure-based continuity equations together as a single system. Unlike the segregated approach, where solving momentum equations and updating pressure corrections are separate steps, the coupled method combines these into a single operation. The remaining equations are still solved independently, similar to the segregated approach [16].

With the coupled algorithm, each iteration consists of the steps outlined below:

1. Update the fluid properties, such as density, viscosity, and specific heat, based on the current solution state. This also includes recalculating turbulent viscosity (or diffusivity) to ensure accurate simulation of flow dynamics.

2. Solve the momentum equations, one after another, using the recently updated values of pressure and face mass fluxes.

3. Solve the pressure correction equation using the recently obtained velocity field and the mass-flux.

4. Correct face mass fluxes, pressure, and the velocity field using the pressure correction obtained from Step 3.

5. Solve the equations for additional scalars, if any, such as turbulent quantities, energy, species, and radiation intensity using the current values of the solution variables.

6. Update the source terms arising from the interactions among different phases (for example, source term for the carrier phase due to discrete particles).

7. Check for the convergence of the equations.

Ansys Fluent provides several methods for interpolating pressure values at the cell faces. By default, the Second Order scheme is used. However, for mixture or VOF multiphase simulations, the default changes to PRESTO! for improved accuracy. The Second Order scheme reconstructs the face pressure using a central differencing scheme. The pressure values at the faces are given by:

$$P_f = \frac{1}{2}(P_{c_0} + P_{c_1}) + \frac{1}{2}(\nabla P_{c_0}\bullet\vec{r}_{c_0} + \nabla P_{c_1}\bullet\vec{r}_{c_1}). \quad (8)$$

The SIMPLE algorithm establishes a connection between velocity and pressure corrections to ensure mass conservation, allowing for the accurate calculation of the pressure field.

If the momentum equation is solved using an initial guessed pressure field, the resulting face flux

may be inaccurate and require corrections to achieve mass conservation and accurate flow predictions.

$$J_f^* = J^*_f + d_f(p^*_{c_0} - p^*_{c_1}). \quad (9)$$

To address this issue, a correction term is added to the face flux. This adjustment ensures that the corrected face flux satisfies the continuity equation, maintaining mass conservation in the flow simulation.

$$J_f = J_f^* + J'_f. \quad (10)$$

The SIMPLE algorithm assumes that the corrected face flux can be expressed as a combination of the initial flux and a correction term:

$$J'_f = d_f(p'_{c_0} - p'_{c_1}). \quad (11)$$

The SIMPLE algorithm inserts the flux correction equations (10)-(11) into the discrete continuity equation. This process leads to a discrete equation that solves for the pressure correction in each cell, ensuring that mass conservation is satisfied throughout the domain [16].

$$a_p p' = \sum_{nb} a_{nb} p'_{nb} + b. \quad (12)$$

where the source term is the net flow rate into the cell:

$$b = \sum_{f}^{N_{faces}} J_f^* A_f. \quad (13)$$

The pressure-correction equation (11) can be efficiently solved using the algebraic multigrid (AMG) method outlined in the Algebraic Multigrid (AMG) section. After obtaining the solution, corrections are applied to both the cell pressure and face flux to improve the accuracy of the flow field and ensure mass conservation.

$$p = p^* + \alpha_p p', \qquad J_f^* = J_f^* + d_f(p'_{c_0} - p'_{c_1}). \quad (14)$$

The parameter α_p represents the under-relaxation factor for pressure, which helps stabilize the solution process. With this correction, the face flux ensures that the discrete continuity equation is fully satisfied at each iteration, improving convergence and solution accuracy.

When working with ANSYS Fluent program it is necessary to adjust all parameters so that the program works both efficiently and accurately enough. For this purpose, below are the steps in which the settings were changed.

- Physics: – Energy (on)
  - Turbulence (Standard k-ω model)
  - Create or edit materials (add *He*, *Ar*, N_2)
  - Species (Species Transport)
  - Boundaries (Operating pressure, temperature and density; define wall as a *steel*)
- Solutions: – Residuals (set all to 10^{-6})
  - Methods (Scheme – Simple)
  - Initialize (patch pressure, temperature, mole fractions)
  - Report definitions – creating plot of mole fractions depending on time
- Results: Contours (creating heavy element's contour of mixing)

Following these parameters, it is possible to model the mixing of multicomponent gas mixtures with sufficiently high accuracy at a given geometry and thermophysical parameters.

Let us analyze the mixing conditions corresponding to the positive density gradient of the mixture (Fig. 1), assuming the location of the heavier in density binary mixture in the upper chamber of the diffusion cell, and the lighter (in density) gas is in the lower flask. This configuration fully corresponds to the conditions used in real experiments. All physical and chemical parameters of the gases used were considered constant and were taken from the ANSYS 2024 R2 chemical library [16].

Since the apparatus is a closed system, the boundary conditions were set as impermeability conditions, which eliminates the possibility of mass transfer across the system boundaries. This ensures that there is no inflow or outflow of components from or into the external environment. Thermal boundary conditions were applied to create isothermal mixing conditions and the boundaries of the apparatus were defined as a solid stainless steel surface. The material properties were taken from the ANSYS 2024 R2 library [16].

A pressure-based solver was used for all models. The relationship between pressure and velocity was provided using the simple scheme specified earlier. Within the framework of spatial discretization, the computational fluid dynamics (CFD) equations were solved using the methods presented in Table 1, which have been shown to be highly effective in [11].

Table 1 - Solution methods

Quantity	Discretization
Gradient	Least Square Cell Based
Pressure	Second order
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

These parameters refer to the numerical solution settings in the ANSYS Fluent software package and describe the discretization methods, approximation and algorithms used to solve the equations during the calculations. Each of these methods is aimed at minimizing numerical errors in the simulation of diffusive and turbulent flows, including cases with significant partial gradients and complex geometry of diffusion channels. The chosen combination of methods and discretization parameters provides an optimal balance between calculation accuracy and computational efficiency, which is especially important for problems related to the joint influence of diffusion and convection. This makes them the most suitable for solving the problem at hand.

Computer modeling results

Table 2 shows experimental and calculated values of component concentrations obtained under the assumption of diffusive transport, as well as partial concentrations calculated using the ANSYS Fluent program for the case of combined transport. The table shows that the results of numerical simulation are in good agreement with the experimental data, which confirms the ability of the program to take into account the influence of convective processes on the system. At the same time, theoretical calculations performed within the diffusion model based on the Stefan-Maxwell formula do not reflect such effects.

Table 2 – Amount of diffusing gas from one flask to another as a function of experimental pressure

0.232 He + 0.768 Ar – N_2 (T=298 K, t=20 min)									
	Stefan-Maxwell analysis			**Experiment** [8]			**Ansys Fluent**		
Pressure, MPa	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**
0.829	0.0117	0.0094	0.0211	0.0680	0.1234	0.1944	0.081	0.113	0.1894
1.074	0.0092	0.0073	0.0164	0.0588	0.1850	0.2438	0.037	0.157	0.188
2.055	0.0049	0.0038	0.0087	0.1352	0.2089	0.3441	0.1090	0.2653	0.3393
0.098 He + 0.902 Ar – N_2 (T=298 K, t=20 min)									
	Stefan-Maxwell analysis			**Experiment** [8]			**Ansys Fluent**		
Pressure, MPa	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**
0.829	0.0050	0.0128	0.0178	0.0869	0.1840	0.2709	0.017	0.2096	0.2367
1.074	0.0038	0.0098	0.0132	0.0368	0.2472	0.2840	0.0217	0.2376	0.2455
2.055	0.0021	0.0052	0.0072	0.0565	0.2411	0.2975	0.0289	0.2856	0.3125
0.299 He + 0.701 Ar – N_2 (T=298 K, t=20 min)									
	Stefan-Maxwell analysis			**Experiment** [8]			**Ansys Fluent**		
Pressure, MPa	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**	**He**	**Ar**	**N_2**
0.829	0.0151	0.0079	0.0230	0.0252	0.0692	0.1927	0.0262	0.0608	0.0399
1.074	0.0118	0.0061	0.0179	0.0465	0.1462	0.2594	0.0270	0.0910	0.1391
2.055	0.0063	0.0032	0.0095	0.0866	0.1924	0.2790	0.0497	0.1395	0.1881

The average deviation between numerical and experimental data for all gases is about 21%. But if you look at each number clearly, you can see that individual measurements exceed 40% in some places. This is especially repeated for the light component in the mixture - this may be due, of course, to the non-ideality of the program calculation, as well as to the fact that the molecular weight, viscosity and other parameters of the component differ from the real values. But, nevertheless, this table and calculations testify to the possibility of quantitative estimation of partial fluxes of components arising at violation of mechanical equilibrium of the system. At the same time, the discrepancy between experimental data and calculations performed within the diffusion model can reach hundreds of percent and more, which confirms the presence of convective currents in the system.

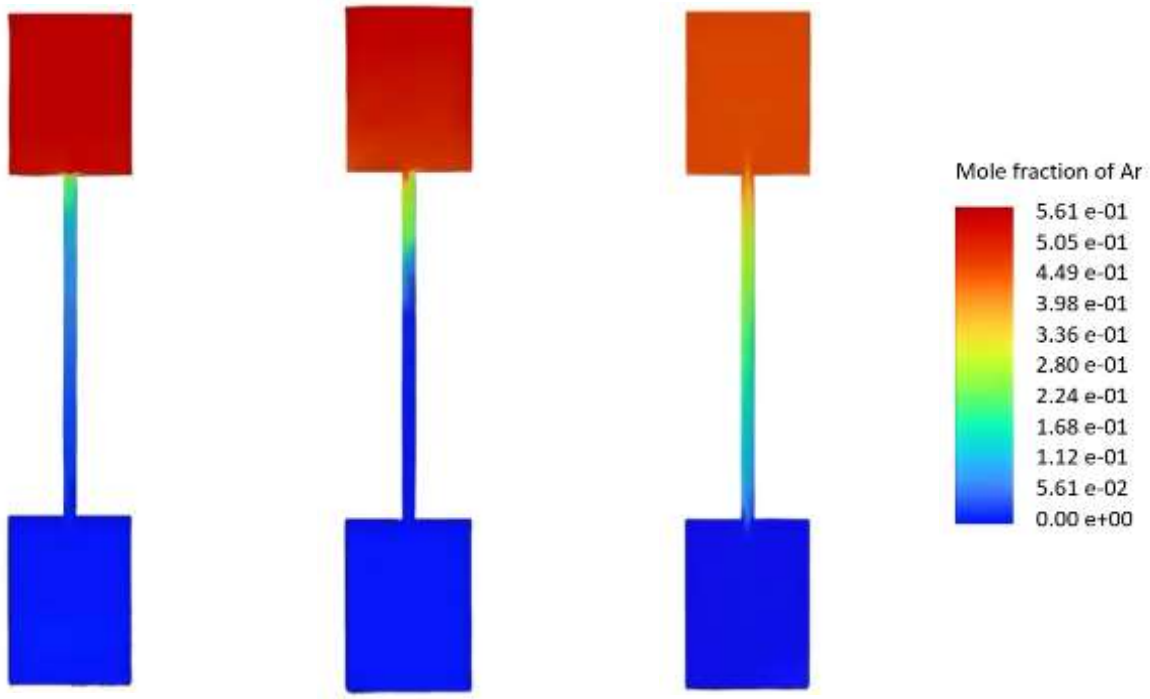

Figure 2 – Convective structures formed in the diffusion channel for the system 0.232 He + 0.768 Ar – N_2 at p=1.074 MPa, T=298 K, t=20 min: a) t=6 min; b) t=9 min; c) t=18 min; d) Concentration scale for cases (a), (b) and (c) describing numerical values of colors

One can also observe the evolution of the formation of convective structures at mixing of this system in Figure 2. As can be seen in Figure 2a clearly shows the beginning of instability of mechanical equilibrium, at which the bending of isoconcentration line appears. Figure 2b shows the beginning of intensive transition of the heavy component from the upper flask to the lower flask through the diffusion channel. And on Figure 2c already established convective flow in the form of convective thread connecting the two flasks, through which the gas is transferred.

Conclusion

Based on the experimental study of convective mixing of an isothermal ternary mixture of helium-argon-nitrogen, numerical studies using ANSYS Fluent were carried out. These studies showed high accuracy in describing the processes of combined mass transfer. Comparison of calculated data with experimental data confirmed the adequacy of the used model for complex systems of multicomponent mixing.

The studies have shown the possibility of quantitative determination of kinetic transitions between different types of convective mixing. Characteristic times for a new type of mixing were determined. The identified stages, including diffusion, formation of convective flows and their further evolution, confirm the existence of complex dynamics of mass transfer processes. The application of ANSYS Fluent allows effective modeling of structural features of flows, such as upward and downward convective flows, and their interaction. This makes this software package a promising tool for the study of combined mass transfer processes under isothermal conditions.

Numerical results show that, with proper adjustment of initial and boundary conditions, ANSYS Fluent can account for the effects of all key parameters, including density gradients, initial composition, pressure, temperature, and geometric characteristics of the diffusion channel, which is confirmed by adequate reproduction of experimental data. The proposed approaches and models can be recommended for applied research aimed at optimizing technological processes related to convective and diffusive mechanisms of mass transfer.

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References

1 Banerjee A. Rayleigh–Taylor instability: A status review of experimental diagnostics and measurements // Journal of Fluids Engineering. – 2020. – Vol. 142, No. 12. – P. 120801. DOI: 10.1115/1.4048349.

2 Kallepalli S., Johnson L., Mattson B. Graham's Law of Diffusion: A Classroom Demonstration of Gas Diffusion and Effusion // Journal of Chemical Education. – 2021. – Vol. 98, No. 10. – P. 3258–3262. DOI: 10.1021/acs.jchemed.1c00657.

3 Kossov V., Fedorenko O., Zhakebayev D. Features of multicomponent mass transfer in gas mixtures containing hydrocarbon components // Chemical Engineering & Technology. – 2019. – Vol. 42, No. 4. – P. 896–902. DOI: 10.1002/ceat.201800604.

4 Федоренко О.В. и Поярков И.В. Устойчивость механического равновесия в неидеальных газовых смесях // Вестник. Серия Физическая. – 2024. - № 90(3). – С. 116–124. https://doi.org/10.26577/RCPh.2024v90i3-014.

5 McLaren C.P., Kovar T.M., Penna A., Müller C.R., Boyce C.M. The role of microstructural heterogeneity in the mechanical behavior of materials: A multiscale approach // Proceedings of the National Academy of Sciences of the United States of America. – 2019. – Vol. 116, No. 19. – P. 9263–9268. DOI: 10.1073/pnas.1820820116.

6 Tang Y., Li Z., Wang R., Cui M., Wang X., Lun Z., Lu Y. Experimental study on the density-driven carbon dioxide convective diffusion in formation water at reservoir conditions // ACS Omega. – 2019. – Vol. 4, No. 6. – P.11082–11092. DOI: 10.1021/acsomega.9b00627

7 Ortiz de Zárate J.M., Kirkpatrick T.R., Sengers J.V. Nonequilibrium Casimir pressures in liquids under shear // The European Physical Journal E. – 2019. – Vol. 42. – P. 399–404. DOI: 10.1140/epje/i2019-11803-2.

8 Kossov V., Fedorenko O., Zhakebayev D., Mukamedenkyzy V., Kulzhanov D. Numerical study of the interaction of vortex ring and shock wave in a supersonic flow // ZAMM – Journal of Applied Mathematics and Mechanics. – 2022. – Vol.102, No. 1. – P.e201900197. DOI: 10.1002/zamm.201900197.

9 Kossov V., Altenbach H. Asymptotic long-wave model for a high-contrast two-layered elastic plate // ZAMM – Journal of Applied Mathematics and Mechanics. – 2023. – Vol. 103, No. 1. – P. e202300080. DOI: 10.1002/zamm.202300080.

10 Hu Z.C., Zhang X.R. An experimental study on the transient runback characteristics of wind-driven film/rivulet flows // Physics of Fluids. – 2021. – Vol. 33, No. 11. – P. 112103. DOI: 10.1063/5.0049247.

11 Peixoto M.L.R., Brito M.S.C.A., Santos R.J., Vilar V.J.P. Evaluation of the performance of a novel photocatalytic reactor for the degradation of emerging contaminants in water // Chemical Engineering Research and Design. – 2024. – Vol.210. – P. 150–162. DOI: 10.1016/j.cherd.2024.08.030.

12 Abd Halim M.A., Nik Mohd N.A.R., Mohd Nasir M.N., Dahalan M.N. The evaluation of k-ε and k-ω turbulence models in modelling flows and performance of S-shaped diffuser // International Journal of Automotive and Mechanical Engineering. – 2018. – Vol. 15, No. 2. – P. 5161–5177. DOI: 10.15282/ijame.15.2.2018.2.0399.

13 Kossov V., Fedorenko O., Asembaeva M., Moldabekova M., Zhaneli M. Diffusion instability in three-component gas mixtures containing greenhouse gas // International Journal of Thermofluids. – 2023. – Vol. 20.– Article 100495. DOI: 10.1016/j.ijft.2023.100495.

14 Молдабекова М.С., Мукамеденкызы В., Асембаева М.К. и Толепберген А.Г. Исследование диффузии двух газов, в равной степени разбавленных различными балластными газами // Вестник. Серия Физическая (ВКФ). – 2024. - № 89(2). – С. 57–61. https://doi.org/10.26577/RCPh.2024v89i2-08

15 Kosov V.N., Fedorenko O.V., Asembaeva M.K., Mukamedenkyzy V. Changing diffusion–convection modes in ternary mixtures with a diluent gas // Theoretical Foundations of Chemical Engineering. – 2020. – Vol. 54, No. 2. – P. 289–296. DOI: 10.1134/S0040579520020136.

16 ANSYS Inc. ANSYS Fluent User's Guide. Release 2024. Canonsburg,

References

1 A. Banerjee, Journal of Fluids Engineering 142, 12-29 (2020). https://doi.org/10.1115/1.4048349.

2 S. Kallepalli, L. Johnson and B. Mattson, Journal of Chemical Education 98, 10, 3258-3262 (2021). https://doi.org/10.1021/acs.jchemed.1c00657.

3 V. Kossov, O. Fedorenko and D. Zhakebayev, Chemical Engineering & Technology, 42, 896-902 (2019). https://doi.org/10.1002/ceat.201800604.

4 O.V. Fedorenko and I.V. Poyarkov, Recent Contributions to Physics. 90, 3, 116–124 (2024). https://doi.org/10.26577/RCPh.2024v90i3-014 (in Russ.)

5 C.P. McLarena, T.M. Kovarb, A.Penna, C.R. Müllera and C.M. Boycea, PNAS, 116, 9263-9268 (2019). doi/10.1073/pnas.1820820116.

6 Y. Tang, Z. Li, R. Wang, M. Cui, X. Wang, Z. Lun and Y. Lu, ACS Omega 4, 11082−11092 (2019). https://doi.org/10.1021/acsomega.9b00627.

7 J.M. Ortiz de Zarate, Eur. Phys. J. E 42, 399–404 (2019). https://doi.org/10.1140/epje/i2019-11803-2.

8 V. Kossov, O. Fedorenko, D. Zhakebayev, V. Mukamedenkyzy and D. Kulzhanov, ZAMM- J. Appl. Math. Mech., 102, (2022). https://doi.org/10.1002/zamm.201900197.

9 V. Kossov and H. Altenbach, Z Angew Math Mech. 103, (2023). https://doi.org/10.1002/zamm.20230080

10 Z.C. Hu and X.R. Zhang, Phys. Fluids 33, 5 (2021). https://doi.org/10.1063/5.0049247.

11 M.L.R. Peixoto, M.S.C.A. Brito, R. J. Santos and V.J.P. Vilar, Chemical Engineering Research and Design, 210, 150–162 (2024). https://doi.org/10.1016/j.cherd.2024.08.030

12 M. A. Abd Halim, N. A. R. Nik Mohd, M. N. Mohd Nasir and M. N. Dahalan, International Journal of Automotive and Mechanical Engineering, 15, 5161-5177 (2018). https://doi.org/10.15282/ijame.15.2.2018.2.0399

13 V. Kossov, O. Fedorenko, M. Asembaeva, M. Moldabekova and M. Zhaneli, International Journal of Thermofluids, 20, (2023). https://doi.org/10.1016/j.ijft.2023.100495

14 M.S. Moldabekova, V. Mukamedenkyzy, M.K. Asembaeva and A.G. Tolepbergen, Recent Contributions to Physics, 89, 2, 57–61 (2024). https://doi.org/10.26577/RCPh.2024v89i2-08 (in Russ)

15 V. Kosov, O.V. Fedorenko, M.K. Asembaeva and V. Mukamedenkyzy, Changing diffusion-convection modes in ternary mixtures with a diluent gas, Theor. Found. Chem. Eng., 54, 2, 289-296 (2020).

16 ANSYS Fluent User's Guide, Release 2024. ANSYS Inc., Canonsburg, PA, USA. Available at: https://www.ansys.com/

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