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**A Study of the Stability of the Diffusion Regime
in a CH₄–Ar–N₂ Ternary Gas Mixture at Elevated Pressures**

Diffusive mass transfer in multicomponent gas systems plays a key role in the design and optimization of processes in the chemical, oil and gas, and energy industries. This work presents an experimental and numerical investigation of isothermal mass transfer in the ternary CH₄–Ar–N₂ system at 295 K over a pressure range of 0.58–5.98 MPa. The system is characterized by similar diffusion coefficients of its components and relatively small density differences, which contribute to the stability of the diffusion regime. Experiments were conducted using a two-flask diffusion apparatus, with component concentration changes recorded as a function of time at different pressures. Numerical simulations were performed in ANSYS Fluent using the Species Transport model, Stefan–Maxwell diffusion formulation, and $k-\omega$ turbulence model. Good agreement between the experimental and numerical results was obtained over the entire pressure range, with discrepancies within the experimental uncertainty. At low pressures, the system exhibits a stable diffusion regime characterized by smooth, monotonic concentration kinetics. At elevated pressures, a transition to a diffusion–convection mass-transfer regime occurs, accompanied by a qualitative change in the mixing dynamics. The results demonstrate the capability of the proposed numerical approach to describe mass transfer in multicomponent gas systems under high-pressure conditions.

Keywords: multicomponent diffusion, high pressure, diffusion apparatus, mass transfer, numerical simulation, ANSYS Fluent

Introduction

Under certain conditions, diffusion mass transfer processes in multicomponent gas mixtures in a gravitational field may be accompanied by the formation of density stratification and the onset of concentration-gravity convection [1, 2]. Under such conditions, mutual diffusion of components with different molecular masses leads to a redistribution of the medium's density and may cause a disturbance in the system's mechanical equilibrium [3]. As a result, the diffusion regime of mass transfer can transition to a hybrid diffusion-convective regime, characterized by the emergence of macroscopic flows and a change in the structure of mass transfer. Such phenomena play an important role both in fundamental studies of transport processes and in various applied problems of heat and mass transfer in gaseous systems, including processes in chemical engineering, geophysics, and energy [4, 5].

The physical mechanisms underlying the formation of concentration convection in gaseous and liquid mixtures have been examined in detail in classic works on hydrodynamic stability and transport theory [1, 6, 7]. It has been shown that even in the absence of temperature gradients, mutual diffusion of compo-

nents can lead to the formation of regions with different densities, which creates conditions for the development of gravity-induced flows [8–11]. In recent years, interest in this problem has grown significantly, due to the development of high-precision experimental methods and numerical modeling of mass transfer processes in complex systems [12–16].

One of the key factors determining the nature of mass transfer in multicomponent mixtures is the difference in the diffusion coefficients of the interacting gases. If the diffusion abilities of the components differ significantly, density inversion zones may form during mutual diffusion, which can initiate the development of flows caused by the instability of the mixture's mechanical equilibrium. In this case, a noticeable discrepancy is observed between the measured and calculated values of the effective diffusion coefficients, which is considered one of the signs of the onset of diffusion instability in the system [11, 17–19]. Similar effects are observed in other types of double and triple diffusion, where the interaction of diffusion flows of various components leads to the formation of complex hydrodynamic structures [20].

At the same time, there is a whole class of multicomponent gas systems in which the difference in the diffusion coefficients of the components is relatively small. Under such conditions, the formation of pronounced density gradients is hindered, and the mass transfer process can remain steady only in the presence of a gravitational field. Selecting the initial composition of the mixture allows one to reduce the difference in densities of the interacting gases and thereby create conditions that prevent the development of convective disturbances. In such systems, mass transfer is determined primarily by molecular diffusion, and the resulting hydrodynamic disturbances prove insufficient to form flows. One of the factors that can influence the stability of the diffusion regime is pressure. An increase in pressure leads to a change in the density of the gas mixture and also affects the diffusion coefficients and other kinetic transport characteristics. As a result, with the ratios between diffusion coefficients remaining virtually unchanged, even a slight nonlinear change in the density of the components leads to a change in the density difference between the mixing gases, which can affect the nature of mass transfer in the system. One such system is the $\text{CH}_4\text{--Ar--N}_2$ ternary gas system, in which, with sufficiently wide variations in the initial composition of the components, the diffusion coefficients of methane and argon in nitrogen are similar in magnitude. With an appropriate selection of component concentrations, the density of the initial mixture turns out to be close to the density of the third gas, which creates conditions for studying both diffusion- and convection-driven mixing [21].

The study of the $\text{CH}_4\text{--Ar--N}_2$ system is motivated by both fundamental and applied considerations. Methane is the principal component of natural gas and mine gas, and its accumulation in nitrogen-rich mine atmospheres presents a well-documented safety hazard; understanding CH_4 transport in N_2 under elevated pressures is therefore relevant to ventilation and hazard assessment in underground environments. Argon, comprising approximately 0.93 % of the Earth's atmosphere, is also encountered as an inert component in various industrial gas streams. From a fundamental standpoint, the system is of particular interest because the diffusion coefficients of methane and argon in nitrogen are similar in magnitude, placing the mixture close to the stability boundary of the diffusion regime and making it sensitive to pressure-induced changes in mixture density.

Two additional aspects of the present study warrant mention. At pressures above approximately 5 MPa, methane exhibits pronounced real gas behaviour: its compressibility factor decreases to roughly 0.87–0.88 at 295 K, meaning the mixture density increases superlinearly with pressure and the effective threshold for convective onset may fall below the value predicted by ideal gas theory. This non-linearity introduces complexity into both experimental interpretation and numerical modelling, as transport coefficients and equation-of-state parameters require real gas corrections at elevated pressures [22]. At the same time, while experimental measurements of mole fractions provide reliable integral characterisation of the mass transfer process, they offer no direct insight into the spatiotemporal dynamics occurring within the diffusion channel and the flasks during the experiment—the transient formation of convective structures, the evolution of concentration fronts, and the development of density-driven instabilities remain inaccessible to end-state measurements alone. Numerical simulation addresses this limitation directly, providing full spatiotemporal resolution of the concentration and velocity fields and thereby enabling a mechanistic interpretation of phenomena that experiments cannot resolve in isolation.

This study experimentally and numerically investigates the isothermal diffusion and convective mixing of a ternary gas mixture of methane, argon, and nitrogen at various pressures (0.58–5.98 MPa) and initial compositions. The obtained values will be compared with experimental data, which will allow us to identify the effect of pressure on the nature of partial mass transfer.

Experimental

The subject of this study is the process of isothermal mass transfer in the ternary gas system $0.5504 \text{ CH}_4 + 0.4496 \text{ Ar} - \text{N}_2$, carried out in a two-flask diffusion apparatus [21]. This setup is widely used for the experimental study of the kinetics of diffusion processes in gas mixtures, as it allows for the analysis of component transport under closed-system conditions with controlled thermobarometric parameters [11, 21]. The apparatus design includes two flasks of equal volume $V_u = V_l = 55.6 \text{ cm}^3$, connected by a narrow cylindrical channel with a length $L = 64 \text{ mm}$ and a diameter $d = 4 \text{ mm}$, in which the main zone of diffusion interaction between the components is formed.

Experimental studies for this system were conducted at a temperature of 295 K over a pressure range from 0.58 to 4.02 MPa. Each experiment lasted 30 minutes, which allowed for the recording of changes in component concentrations sufficient for the subsequent determination of effective diffusion coefficients. The initial composition $0.5504 \text{ CH}_4 + 0.4496 \text{ Ar}$ was selected on the basis of prior experimental studies [23, 24]. The molar density of this mixture is lower than that of pure N_2 , placing the system in a mechanically stable configuration at low pressures. At the same time, the diffusion coefficients of methane and argon in nitrogen are similar in magnitude, which makes the system particularly sensitive to small pressure-induced changes in mixture density—conditions under which local density inversions can develop during diffusion and eventually trigger convective instability. Such a composition allows for the investigation of conditions under which the diffusion regime of mass transfer can remain stable even with significant changes in pressure.

To analyze the process under consideration, numerical simulations were performed using the ANSYS Fluent software package [23–26], which enables investigation of the spatiotemporal evolution of concentration fields in gas systems with complex geometries. The calculations utilized a three-dimensional model of the diffusion apparatus shown in Figure 1, whose geometry corresponded to the parameters of the experimental setup. This approach makes it possible to reproduce real mass transfer conditions and track changes in the distribution of components throughout the entire volume of the system.

The initial and boundary conditions of the numerical model were set in accordance with the conditions of the experiments. At the initial time, the upper flask of the diffusion apparatus contained a mixture of $0.5504 \text{ CH}_4 + 0.4496 \text{ Ar}$, while the lower flask and the diffusion channel were filled with nitrogen. This configuration fully reproduces the initial state of the system in real experiments and allows for a correct description of the mutual diffusion process of the components. The physicochemical properties of the gases were assumed to be constant and were specified based on data contained in the built-in substance library of the ANSYS Fluent 2025 R2 software package.

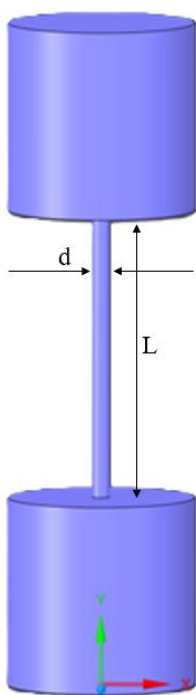


Figure 1. Three-dimensional model of a diffusion cell and the calculated simulation area

Since the diffusion apparatus is a closed system, impermeability conditions were applied to all its boundaries to prevent mass transfer across the external surfaces. To maintain isothermal conditions, the apparatus walls were modeled as a solid surface with material properties corresponding to stainless steel, which were also taken from the standard ANSYS Fluent library [26].

The computational domain was discretised, accounting for the geometric features of the apparatus. The flask volumes were approximated using an unstructured mesh, while the diffusion channel was discretised with a regular structured mesh to ensure accurate representation of concentration and velocity gradients in the primary zone of species interaction. The characteristic cell size was approximately 1 mm, with the total number of mesh elements of approximately 4.2×10^5 . This spatial resolution is consistent with mesh parameters employed in validated numerical studies of diffusion and concentration-driven convection in geometrically similar two-flask configurations [23, 25], and is considered sufficient for the accurate resolution of the transport phenomena governing mass transfer in the system under study.

Turbulence closure was provided by the standard $k-\omega$ model. Although the flow velocities in the two-flask diffusion apparatus are small and the overall Reynolds number remains low, the $k-\omega$ formulation is selected for several reasons. Unlike the $k-\varepsilon$ model, $k-\omega$ does not require wall functions and integrates directly to the wall, making it well-suited for near-wall regions where concentration and velocity gradients are steepest. In the limit of negligible turbulent kinetic energy—which prevails throughout most of the diffusion-dominated regime—the model effectively reduces to a laminar description, introducing no artificial diffusive contribution. As the pressure increases and weak convective disturbances develop, the $k-\omega$ model is capable of capturing the onset of low-intensity turbulent fluctuations without requiring a priori knowledge of the flow regime. The appropriateness of this choice is confirmed a posteriori by the close agreement between the simulated and experimental concentration profiles across all validated pressure levels.

The standard $k-\omega$ 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 . The turbulence kinetic energy k and the specific dissipation rate ω are obtained from the following transport equations [25]:

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

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_j} \left(\Gamma_\omega \frac{\partial \omega}{\partial x_j} \right) + G_\omega - Y_\omega + S_\omega + G_{\omega b}. \quad (2)$$

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_k represents the generation of k . Γ_k and Γ_ω represent 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.

The effective diffusion coefficients for $k-\omega$ model are given by the formulas

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

$$\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega} \quad (4)$$

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

$$\mu_t = \frac{\rho k}{\omega} \frac{1}{\max \left[\frac{1}{\alpha^*}, \frac{SF_2}{a_1 \omega} \right]}, \quad (5)$$

where S is the strain rate magnitude and

$$\sigma_k = \frac{1}{\frac{F_1}{\sigma_{k,1}} + \frac{1-F_1}{\sigma_{k,2}}} \quad (6)$$

$$\sigma_\omega = \frac{1}{\frac{F_1}{\sigma_{\omega,1}} + \frac{1-F_1}{\sigma_{\omega,2}}} \quad (7)$$

A transport equation is solved to determine the species concentrations in the diffusion channel. The conservation equation represents the relations for convective diffusion by which the local mass fraction Y_i of each substance i can be predicted and is defined as follows:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla(\rho \vec{v} Y_i) = -\nabla \vec{J}_i + R_i + S_i, \quad (8)$$

where ρ is the density of the mixture, $\vec{v}$ is the rate of diffusing substances, R_i is the net rate of production of species i by 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 present in the studies. $\vec{J}_i$ is the diffusion flux of a certain substance i , which for the density and temperature gradient can be calculated by the formula

$$\vec{J}_i = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc_t}\right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T}, \quad (9)$$

where μ_t is the turbulent viscosity and Sc_t is the turbulent Schmidt number calculated as $Sc_t = \mu_t/(\rho D_t)$, where D_t is the turbulent diffusion coefficient. The default value of Sc_t is 0.7. $D_{i,m}$ is the mass diffusion coefficient for substance i in the mixture, $D_{T,i}$ is the thermal diffusion coefficient for substance i in the mixture, T is the temperature. The last term in the equation was not considered, since in this work the isothermal type of mixing was considered. Also note that turbulent diffusion, as a rule, exceeds molecular diffusion, and a detailed description of the properties of molecular diffusion in turbulent flows, as a rule, is not required.

For multicomponent systems, the Stefan-Maxwell equations in the form of

$$\sum_{j=1, j \neq i}^N \frac{X_i X_j}{D_{ij}} (\vec{V}_j - \vec{V}_i) = \vec{d}_i - \frac{\nabla T}{T} \sum_{j=1, j \neq i}^N \frac{X_i X_j}{D_{ij}} \left(\frac{D_{T,j}}{\rho_j} - \frac{D_{T,i}}{\rho_i} \right), \quad (10)$$

where X is the mole fraction, $\vec{V}$ is the diffusion rate, D_{ij} is the binary mass diffusion coefficient of substance i into substance j . Since isothermal conditions are assumed, the thermal diffusion term in Eq. (10) vanishes [27, 28].

Table 1

Solution methods

Qntity	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

All simulations were performed in a transient formulation using a pressure-based coupled solver with full pressure–velocity coupling within each iteration [29]. Convective terms were discretised using the Second Order Upwind scheme, and pressure interpolation was handled by the PRESTO! scheme, which provides improved accuracy in the presence of body forces arising from density gradients. Time integration was performed with a second-order implicit scheme at a fixed time step of $\Delta t = 1$ s over a total of 1800 steps, corresponding to 30 minutes of physical process time. Convergence at each time step was assessed using residu-

al criteria of 10^{-6} for the velocity and pressure fields and 10^{-8} for species concentrations, ensuring that the solution was fully converged before advancing to the next step.

Results and Discussion

Numerical simulations of the mutual diffusion process in the $\text{CH}_4\text{--Ar--N}_2$ system were performed for a pressure range of 0.58 to 5.98 MPa under isothermal conditions. The main objective of the calculations was to reproduce the mass transfer kinetics between the flasks of the diffusion apparatus and to compare the obtained results with experimental data.

Table 2 serves as the primary validation of the numerical model. The concentration differences Δc obtained from ANSYS Fluent are compared against both the Stefan–Maxwell analytical solution and independent experimental data [21] across the full pressure range of 0.58–4.02 MPa. Agreement between simulation and experiment is consistently within experimental error at all pressures studied, confirming that the model correctly reproduces the mass transfer kinetics of the system and that the selected boundary conditions, transport coefficients, and solver settings are appropriate for this class of problems.

Table 2

Dependence of gas concentration changes in flasks on pressure

0.5504 CH_4 + 0.4496 Ar — N_2 (T = 295 K, t=30 min)									
P, MPa	Δc , mole fraction								
	Calculated according to Stefan-Maxwell theory			Experiment [21]			Ansys Fluent		
	CH_4	Ar	N_2	CH_4	Ar	N_2	CH_4	Ar	N_2
0.58	0.4172	0.3495	0.7618	0.413	0.351	0.773	0.425	0.354	0.774
1.07	0.4172	0.3495	0.7618	0.413	0.349	0.762	0.418	0.347	0.758
2.05	0.4172	0.3495	0.7618	0.416	0.353	0.768	0.421	0.351	0.764
3.04	0.4172	0.3495	0.7618	0.412	0.349	0.774	0.414	0.346	0.770
4.02	0.4172	0.3495	0.7618	0.411	0.350	0.762	0.410	0.348	0.760
5.00	0.4172	0.3495	0.7618	-	-	-	0.405	0.340	0.745
5.98	0.4172	0.3495	0.7618	-	-	-	0.328	0.276	0.604

Under these pressures, the agreement between experiment and Stefan–Maxwell theory indicates that mass transport is governed primarily by molecular diffusion. This behaviour is consistent with the physical characteristics of the $\text{CH}_4\text{--Ar--N}_2$ system: the diffusion rates of methane and argon in nitrogen are similar in magnitude, so no pronounced density inversion zones develop during mutual diffusion, and the resulting concentration gradients remain insufficient to sustain gravity-induced convective flows. Under these conditions, molecular diffusion fully accounts for the observed mass transfer kinetics.

At pressures of 5.00 and 5.98 MPa, experimental data are unavailable; however, the ANSYS Fluent results show a progressive deviation from the Stefan–Maxwell theoretical values—a deviation that grows with increasing pressure. Given that the numerical model has demonstrated reliable agreement with both experiment and theory across all lower pressures, there is reason to treat these computed values with confidence. The observed divergence between simulation and Stefan–Maxwell theory at elevated pressures suggests a qualitative change in the mass transfer mechanism: the increased mixture density appears to create conditions under which concentration-driven gravitational convection begins to contribute to the overall transport, supplementing and eventually dominating over molecular diffusion. This interpretation is consistent with the concentration dynamics discussed in relation to Figure 2.

The time dependence of the argon concentration in the lower flask (Fig. 2) reveals a clear and systematic transformation of the mass transfer mechanism as pressure increases. At $p = 0.584$ MPa, the concentration profile rises smoothly and nearly linearly over the entire 1800 s observation window, reaching approximately 0.045 at the end of the experiment with no detectable inflection points or regions of accelerated growth. This behaviour is fully consistent with a diffusion-controlled regime in which transport is governed by the concentration gradient between the flasks and the system geometry. At $p = 2.05$ MPa, the overall monotonic

trend is preserved, and the final concentration remains comparable, but starting from approximately $t \approx 600\text{--}800$ s, low-amplitude oscillations become superimposed on the mean growth curve. These perturbations do not yet alter the dominant transport mechanism, but their emergence signals that the increased mixture density is sensitising the system to local composition inhomogeneities and that the threshold of mechanical equilibrium instability is being approached.

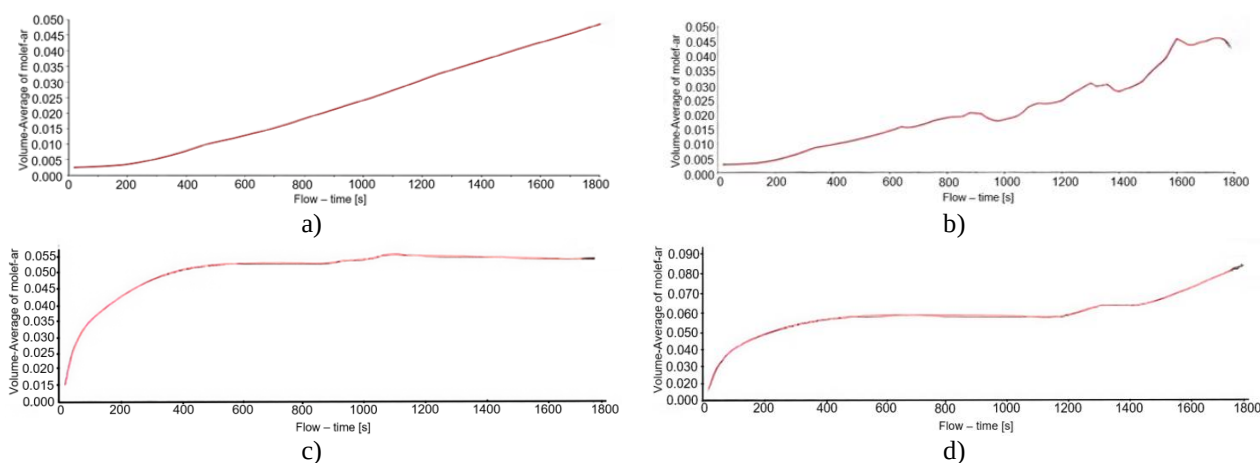


Figure 2. Time-dependent changes in Ar concentration in the lower flask as a function of pressure: a) $p=0.584$ MPa; b) $p=2.05$ MPa; c) $p=5.00$ MPa; d) $p=5.98$ MPa

At elevated pressures, the character of the concentration kinetics changes fundamentally. At $p = 5.00$ MPa, the curve exhibits a rapid initial rise reaching approximately 0.050 within the first 300–400 s, after which growth decelerates markedly, and the concentration enters an extended quasi-stationary plateau persisting through the remainder of the observation window. This two-stage profile reflects convective onset: the initial acceleration is driven by a high mixture density that lowers the threshold for gravitational instability, while the subsequent plateau indicates partial redistribution of the density field and a temporary restoration of mechanical stability. The most complex behaviour is observed at $p = 5.98$ MPa, where three distinct temporal stages can be identified. In the initial period up to approximately $t \approx 300$ s, a rapid rise occurs, after which the curve enters a deceleration phase lasting through $t \approx 1200$ s with the concentration increasing gradually from roughly 0.030 to 0.060. Beyond $t \approx 1200$ s, a pronounced secondary acceleration drives the concentration to approximately 0.085–0.090 by $t = 1800$ s—nearly twice the value observed at 0.584 MPa. This late-stage intensification reflects the accumulation of density inhomogeneities to a critical level at which mechanical equilibrium breaks down and gravity-induced macroscopic flows sustain transport well beyond diffusive rates.

The progression across the four pressure levels traces a coherent physical sequence from stable molecular diffusion through transitional perturbations to a fully developed diffusion–convective regime. Pressure acts as the governing parameter: it raises mixture density, reduces the critical gradient required for convective onset, and determines both the timing and intensity with which macroscopic flows contribute to overall mass transfer. The close agreement between computed and experimental profiles across this entire pressure range confirms that the numerical model captures not only the qualitative character of each regime but also the pressure-dependent dynamics of the transition between them.

The observed transition from diffusion-dominated to convection-influenced transport at pressures above 5 MPa is consistent with an increase in the solutal Rayleigh number $Ra = g\Delta\rho L^3/(\rho\nu D)$, where the rising mixture density at elevated pressures amplifies the buoyancy-driving term while the diffusion coefficient decreases, collectively pushing the system across the stability threshold.

The present study is subject to several limitations inherent to the adopted numerical framework. The ANSYS Fluent Species Transport model assumes ideal gas behaviour throughout; as discussed above, this assumption becomes progressively less accurate above 5 MPa, where real gas corrections to transport coefficients and mixture density are non-negligible. The simulations are performed under strictly isothermal conditions, neglecting the small temperature gradients associated with the Dufour effect; while this contribution is expected to be minor for the present system, its role at elevated pressures has not been assessed. Finally, the results reported here correspond to a single initial mixture composition (0.5504 CH_4 + 0.4496 Ar); extrapolation to other compositions is not attempted.

tion to substantially different compositions requires independent verification, as the proximity of the diffusion–convective stability boundary is sensitive to the relative densities and diffusivities of the components.

Conclusion

This study presents an experimental and numerical investigation of mass transfer processes in a ternary gas system consisting of $\text{CH}_4\text{--Ar--N}_2$ under isothermal mixing conditions at elevated pressures. By comparing the results of calculations performed in ANSYS Fluent with experimental data, it is shown that the numerical model used adequately describes the kinetics of diffusion mass transfer in the considered parameter range, and that the discrepancies between the calculated and experimental values do not exceed the experimental error margin.

An analysis of the effect of pressure on mass transfer behavior showed that at relatively low pressures, the system remains in a steady-state diffusion regime in which mass transfer is determined primarily by molecular diffusion. As pressure increases, the mixing kinetics become more complex as evidenced by changes in the shape of the time-dependent concentration curves of the components. At high pressures, signs of multistage behavior are observed, including induction phases and subsequent acceleration of mass transfer, which indicates a possible disruption of mechanical equilibrium and an increased role of gravity-induced flows.

It has been established that in a $\text{CH}_4\text{--Ar--N}_2$ system, characterized by similar diffusion coefficients for the components and a small difference in their densities, pressure is the key parameter determining the stability of the diffusion regime. Under the conditions considered, an increase in pressure does not lead to an instantaneous transition to the convective regime but contributes to the formation of conditions under which diffusion transport may be accompanied by disturbances affecting its structure and intensity.

The results advance the understanding of mass transfer mechanisms in multicomponent gas systems at elevated pressures and can be used in the development and optimization of processes involving gas separation and mixing, as well as in the construction and validation of numerical models of diffusion-convective transport.

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Жоғары қысымдағы $\text{CH}_4\text{--Ar--N}_2$ үшкомпонентті газ қоспасында диффузия режимінің тұрақтылығын зерттеу

Көпкомпонентті газ қоспаларындағы диффузиялық масса тасымалы химиялық технология, мұнай-газ өңдеу және энергетика салаларындағы инженерлік процестерді модельдеу мен жетілдірудің іргелі негізі. Осыған байланысты, жоғары қысымды ортадағы газ жүйелерінің өзара диффузиялық заңдылықтарын айқындау заманауи ғылым мен өндіріс үшін маңызды басымдыққа ие. Бұл зерттеу аясында $\text{CH}_4\text{--Ar--N}_2$ үшкомпонентті жүйесіндегі изотермиялық массаалмасу құбылысы 295 К температурада және 0,58–5,98 МПа қысым аралығында кешенді түрде зерделенді. Қарастырылып отырған жүйенің ерекшелігі компоненттердің диффузиялық коэффициенттерінің жақындығымен және тығыздық градиентінің төмендігімен айқындалады, бұл өз кезегінде диффузиялық режимнің тұрақтылық деңгейін айқындайтын шешуші фактор саналады. Тәжірибелік зерттеулер екі колбалы диффузиялық қондырғыда жүргізіліп, компоненттер концентрациясының уақыт пен қысым параметрлеріне тәуелді өзгеру динамикасы нақты тіркелді. Теориялық негіздеу мақсатында ANSYS Fluent ортасында Стефан–Максвелл теңдеулері, $k-\omega$ турбуленттілік моделі және Species Transport әдістемесі қолданылып, сандық модельдеу жүзеге асырылды. Алынған эксперименттік деректер мен

есептеу нәтижелері арасындағы сәйкестік жоғары деңгейді көрсетіп, ауытқулардың рұқсат етілген қателік шегінен аспайтыны дәлелденді. Төмен қысым жағдайында жүйеде концентрациялық кинетиканың бірқалыпты өзгеруімен сипатталатын тұрақты режим байқалды. Алайда қысым мәні жоғарылаған сайын массаалмасу механизмінің сапалық трансформациясы орын алып, диффузиялық-конвективті режимге өту процесі тіркелді. Зерттеу қорытындысы ұсынылған сандық тәсілдің жоғары қысымды көпкомпонентті жүйелердегі күрделі физикалық процестерді сипаттаудағы тиімділігін толықтай растайды.

Кілт сөздер: көпкомпонентті диффузия, жоғары қысым, диффузия аппараты, массаалмасу, сандық модельдеу, ANSYS Fluent

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Исследование устойчивости диффузионного режима в тройной газовой смеси $\text{CH}_4\text{--Ar--N}_2$ при повышенных давлениях

Диффузионный массоперенос в многокомпонентных газовых средах является фундаментальным аспектом при проектировании и модернизации технологических циклов в химической, нефтегазовой и энергетической отраслях. В данной работе представлены результаты комплексного исследования изотермического массообмена в трехкомпонентной системе $\text{CH}_4\text{--Ar--N}_2$ при температуре 295 К и давлении от 0,58 до 6,02 МПа. Специфика изучаемой системы заключается в близости коэффициентов диффузии компонентов и незначительных различиях в плотности, что выступает решающим фактором устойчивости диффузионного режима. Экспериментальная часть выполнена на двухколбовой установке, фиксирующей динамику концентрационных изменений в зависимости от времени и барических условий. Параллельно в программном комплексе ANSYS Fluent проведено численное моделирование на основе уравнений Стефана–Максвелла, модели переноса веществ (Species Transport) и $k\text{--}\omega$ модели турбулентности. Сравнительный анализ показал высокую степень корреляции между эмпирическими данными и результатами вычислений: зафиксированные отклонения не выходят за рамки допустимой погрешности. Установлено, что при низком давлении процесс характеризуется стабильным режимом с монотонной кинетикой концентраций. Однако с ростом давления наблюдается качественная трансформация механизма смешения и переход к интенсивному диффузионно-конвективному массообмену. Итоговые результаты подтверждают высокую достоверность и применимость предложенного численного алгоритма для описания сложных процессов переноса в многокомпонентных газовых системах при условиях высокого давления.

Ключевые слова: многокомпонентная диффузия, высокое давление, диффузионная установка, массоперенос, численное моделирование, ANSYS Fluent

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