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Numerical modelling of multi-component mass transfer regimes in four-component gas systems

For argon and carbon dioxide, which are part of the tetra-component gas mixture He + Ar + CO2 – N2 and are the heaviest compared to other components, graphs of the behavior of the concentration of these components at different points of the diffusion channel and time intervals are presented. To simulate convective flows in the four-component mixture under consideration, the Flow Simulation computer package included in the SolidWorks engineering design system was used. The equations are solved by the finite volume method using the standard k – ε turbulence model and with initial and boundary conditions. Indicated, that obtained distributions change nonlinearly both in time and along the length of the diffusion channel. In this case, there is a change in the diffusion process to a convective one, which is due to the nonlinearity in the distribution of the components concentration, which is connected with the imbalance of mechanical equilibrium. It was found that the most significant change in the behavior of the concentrations of heavy-weight components occurs within 120 s. This time interval coincides with the appearance of two contrasting areas on the graphs, namely, the formation of a developed convective flow. An enhancement in the time of the numerical experiment showed that the concentration of the component with the maximal molar mass remains practically unchanged. This behavior of the concentration of heavy-weight components is characteristic of the effect when the mixture is enriched in the heavy-weight component. An analysis of the streamlines on the plots of concentration distributions showed that vortices of various scales interacting with each other and leading to a pulsating mixing regime are formed along the length of the channel. It has been established that the presence of large-scale vortices determines the preferential migration of the components with the maximal molar mass.

Keywords: gas mixtures, diffusion, instability, convection, concentration distribution, anomalous component separation, numerical modeling, finite volume method.

Introduction

Multicomponent diffusion in gas systems differs from ordinary binary diffusion occurring under isothermal conditions in that new phenomena arise in multicomponent mixtures due to the mutual influence of the components on each other and confirmed by experimental studies and from the analysis of the Stefan-Maxwell equations [1]. There are the following phenomena (special mixing modes), such as a reverse diffusion, osmotic diffusion and diffusion barrier [2], as well as the onset of the mechanical equilibrium instability of the mixture, which is caused by the distinction in the interdiffusion coefficients of the miscible components [3, 4]. An essential nonlinearity along the channel length of the distributions of the concentrations of heavy components can lead to the appearance of convective instability under isothermal conditions, which follows from the results of numerical studies [5]. As a further matter, if some conditions are formed in the system, then nonmonotonicity with both a minimum and a maximum is also possible in the mixture density distribution, which can cause gravitational convection that is not observed during diffusion at a constant temperature [6].

Analysis of the stability of isothermal ternary gas mixtures carried out within the bounds of the Boussinesq approximation [7] showed that the transfer from the diffusion mode to the convection one is possible in both situations when the mixture density reduces with altitude and when the density gradient has the opposite direction [8]. Nevertheless, the proposed approach has a number of limitations that do not allow one to describe the onset time of the unstable regime and the evolution of convection currents.

Experimental research on the diffusion of steam mixtures of solutions into an inactive gas [3], as well as blending in ternary gaseous mixtures at various compounds and pressures [4, 9], showed that convection currents are observed. These currents cause a synergistic effect, resulting in an essential acceleration of the mixing process of the system's components. Also in [4, 9], the preferred migration of the component with the maximal molar mass was found, which is an unusual phenomenon for diffusion processes. Sometimes, the

pulsating nature of the mixing was also recorded. The results obtained in [3, 4, 9], which showed the possibility of enriching the resulting mixture with a constituent having the maximal molar mass, are also of practical importance since they can be implemented in combined approaches relating to the growth of the selective features of a given component [10, 11]. Including those based on the use of membranes [12, 13] and convective separation mechanisms [14, 15]. At the same time, experimental and numerical studies of combined mass transfer in isothermal four-component systems are episodic. Consequently, it is extremely important to conduct studies aimed at clarifying the separation mechanisms in gas mixtures consisting of several components, as well as correctly assessing the parameters that determine the transition from one mixing mode to another. These issues play a significant role in both applied and fundamental problems related to mass carry.

The main objective of this paper is to create a numerical model for the analysis of various modes of multicomponent mass transfer in a tetra-component gaseous mixture He + Ar + CO_2 – N_2. A feature of this system is the selected composition, which approximately provides the condition of the zero density gradient of the mixture. The distributions of concentrations of argon and carbon dioxide over time and along the length of a vertical flat diffusion channel at elevated pressure under isothermal conditions have been obtained and analyzed.

Mathematical description of the occurrence of convective flows in a quaternary gas mixture

The study of mass transfer in systems consisting of more than two components is possible due to the use of the Navier-Stokes equation, as well as equations describing the conservation of energy, momentum, and mass in a given medium. Moreover, when modeling mass transfer in multicomponent gas systems, not only the equations of state of the fluid components are taken into account, but also empirical relationships that consider the dependence of the viscosity and thermal conductivity of each component on temperature. Averaging the effect of turbulence on flow parameters on a small time scale is used in modeling convective flows in the Navier-Stokes equation. In addition, the introduction of the corresponding time derivatives makes it possible to take into account large-scale temporal changes averaged over a small time scale of the components of the gas-dynamic parameters of the flow [16]. The Navier-Stokes equations, which are used to represent convective flows, have extra variables that describe Reynolds stresses. Additional equations that describe the transport of turbulence kinetic energy and its dissipation in the framework of the *k-ε* turbulence model are utilized to completely close this system of equations [17]. This set of equations, which takes into consideration unsteady spatial flow, comprises mass, momentum, and energy conservation equations [16], can be presented as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0, \quad i = 1, 2, 3 \tag{1}$$

$$\frac{\partial\left(\rho u_i\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j - \tau_{ij}\right) + \frac{\partial p}{\partial x_i} = S_i, \quad j = 1, 2, 3, i \neq j \tag{2}$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x_i}\left(\left(\rho E + p\right)u_i + q_i - \tau_{ij}u_j\right) = S_i u_i, \tag{3}$$

$$E = U + \frac{u^2}{2}, \tag{4}$$

where ρ is the fluid density, u_i or u_j is the flow rate, t is the time, p is the fluid pressure, q_j is the diffusion heat flux, τ_{ij} is the viscous shear stress tensor (the subscripts mean the summation in three coordinate directions), E is the total energy of unit mass of current medium, U is the specific internal energy of the medium, S_i is the external mass forces due to the gravitational action $S_i = S_i^{gravity}$ ($S_i^{gravity} = -\rho g_i$) acting on unit mass of the current medium along the coordinate directions x_i, g_i is the component of the gravitational acceleration in the x_i coordinate direction.

The viscous shear stress tensor for Newtonian fluids is calculated as:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right) - \frac{2}{3}\rho k\delta_{ij}, \tag{5}$$

where k is the kinetic energy of turbulence, δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ at $i = j$; $\delta_{ij} = 0$ at $i \neq j$), $\mu = \mu_l + \mu_t$, μ_l is the dynamic viscosity coefficient, and μ_t is the turbulent viscosity coefficient. When using the $k - \varepsilon$ turbulence model, the turbulent viscosity coefficient μ_t is determined through the parameters of the kinetic energy of turbulence k and the dissipation rate of this energy ε:

$$\mu_t = f_\mu \frac{C_\mu \rho k^2}{\varepsilon}, \tag{6}$$

where $C_\mu = 0.09$ is the empirical constant defining the turbulent viscosity, $f_\mu = \left[1 - \exp\left(-0.025R_y\right)\right]^2\left(1 + \frac{20.5}{R_T}\right)$ is the damping function, $R_y = \frac{\rho\sqrt{k}y}{\mu_l}$ is the Reynolds number, where y is the distance from the wall surface, $R_T = \frac{\rho k^2}{\mu_l \varepsilon}$ is the turbulent Reynolds number.

The following equations make it possible to determine the parameters of the turbulent kinetic energy k and the dissipation rate of this energy ε:

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j k\right) = \frac{\partial}{\partial x_j}\left(\left(\mu_l + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right) + S_k, \tag{7}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j \varepsilon\right) = \frac{\partial}{\partial x_j}\left(\left(\mu_l + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right) + S_\varepsilon, \tag{8}$$

where $S_\varepsilon = C_{\varepsilon 1}\frac{\varepsilon}{k}\left(f_1 \tau_{ij}^R \frac{\partial u_i}{\partial x_j} + \mu_t C_B P_B\right) - C_{\varepsilon 2} f_2 \frac{\rho \varepsilon^2}{k}$, $S_k = \tau_{ij}^R \frac{\partial u_i}{\partial x_j} - \rho\varepsilon + \mu_l P_B$, $P_B = -\frac{g_i}{\sigma_B}\frac{1}{\rho}\frac{\partial \rho}{\partial x_i}$ is the generation of turbulent kinetic energy due to repulsive force, $\tau_{ij}^R = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right) - \frac{2}{3}\rho k\delta_{ij}$, $\sigma_R = 0.9$ is the turbulent Prandtl constant for energy, $C_R = 1$ is the constant determining the degree of impact of the repulsive force on ε at $P_R \succ 0$ and $C_R = 0$ at $P_R \leq 0$, $f_1 = 1 + \left(\frac{0.05}{f_\mu}\right)^3$, $f_2 = 1 - \exp\left(-R_T^2\right)$, $C_{\varepsilon 1} = 1.44$ is the empirical constants of the model for the generation term of the equation for ε, $C_{\varepsilon 2} = 1.92$ is the empirical constants of the model for the dissipation term of the equation for ε, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.3$ are the Prandtl numbers for the turbulent kinetic energy k and the energy dissipation rate ε.

To simulate the diffusion heat flow, an equation is used that has the following form:

$$q_i = -\left(\frac{\mu_l}{\mathrm{Pr}} + \frac{\mu_t}{\sigma_c}\right)c_p \frac{\partial T}{\partial x_i}, \qquad i = 1, 2, 3 \tag{9}$$

where T is the temperature of the fluid medium, c_p is the specific heat capacity at constant pressure, Pr is the Prandtl number, $\sigma_c = 0.9$ is the Prandtl turbulence number.

To study the diffusion of components in multicomponent gas mixtures, equations are used that describe the change in the concentration of each component in space:

$$\frac{\partial \rho c_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j c_i\right) = \frac{\partial}{\partial x_j}\left(\left(D_{ij} + D_{ij}^t\right)\frac{\partial c_i}{\partial x_j}\right),\ i, j = 1, 2, \ldots N, \tag{10}$$

where D_{ij}, D_{ij}^t is the molecular and turbulent diffusion coefficients, which according to the Fick's law, so that $D_{ij} = D \cdot \delta_{ij}$, $D_{ij}^t = \delta_{ij} \cdot \frac{\mu_t}{\sigma}$, where D is the interdiffusion coefficient, σ is the turbulent Schmidt number, c_i is the concentration of the i-th component of mixture $\left(\sum_{i=1}^{N} c_i = 1\right)$, N is the number of components in mixture.

To find a solution to the system of equations (1)-(10), the following boundary conditions are taken into account, which complement the problem posed and ensure the accuracy of the result obtained:

$$u_i\big|_n = 0,\ u_i\big|_t = 0,\ \left.\frac{\partial u_i}{\partial x_i}\right|_n = 0,\ \left.\frac{\partial c_i}{\partial x_j}\right|_n = 0, \tag{11}$$

where n and t are the normal and tangent directions in relation to the wall.

To study the processes in a separating diffusion apparatus, the system of equations (1)–(10) is solved using the finite volume method and a special Flow Simulation package built into the SolidWorks engineering design system. The formulation of the problem included setting the initial and boundary conditions, which ensured the accuracy and reliability of the results obtained.

To confirm the effectiveness of the described mathematical model, the results of a numerical simulation of convective flows in a binary gas mixture at different inclination angles of the diffusion channel are presented in [18]. The calculation results are in qualitative agreement with the experimental data for isothermal binary gas mixtures.

The outcomes of the numerical simulations conducted on a quaternary gaseous mixture

Figure 1 shows a model of a representative two-flask apparatus simulated using SolidWorks [19]. This model for various forms of the diffusion channel can be used to simulate diffusion and convective mass transfer, as well as various features that arise when gases are mixed. The calculations were carried out for a flat vertical channel. The considered flat channel had the following characteristics: length L = 0.165 m, thickness $a = 6 \cdot 10^{-3}$ m, and width $b = 30 \cdot 10^{-3}$ m. A non-dimensional mesh with the following dimensions 8 × 34 × 8 was used in the computations.

Our focus is on studying the mixing process for a system that consists of helium, argon, and carbon dioxide that is diffusing into pure nitrogen. During the numerical simulation, the top flask of the diffusion cell was stocked with a mixture comprising of 0.36 He + 0.33 Ar + 0.31 CO_2, whereas the bottom flask was stocked with pure nitrogen. Before the chemical element, its concentration in mole fractions is indicated. The pressure and temperature of the experiment were p_{abs} = 0.6 MPa and T = 298.0 K, and the mixing time interval was 0 – 180 s.

For argon in the quasi-stationary mixing mode, at integrated relationship is obtained that describes the change in its concentration with time. This dependence is shown in Figure 2. In accordance with Figure 2, the amount of argon diffused for 120 s is maximum. During this time, the amount of transferred argon has changed by more than 8 times that is not observed during diffusion. Apparently, under these conditions, the mechanism of the preferential migration of the components with the maximal molar mass is implemented. Subsequent growth of the mixing time does not lead to a synergistic increase in the transfer intensity, which allows assuming that the current has a convective type of flow. A similar behavior is observed for carbon dioxide.

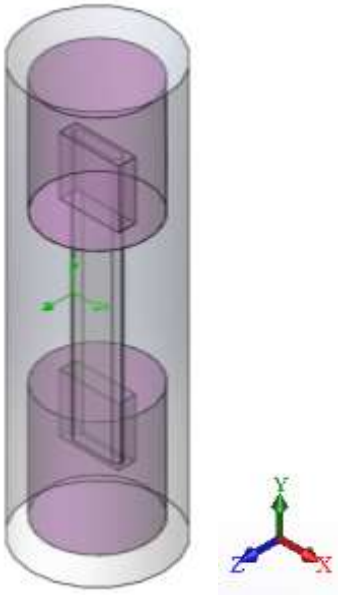


Figure 1. Pattern of a diffusive unit

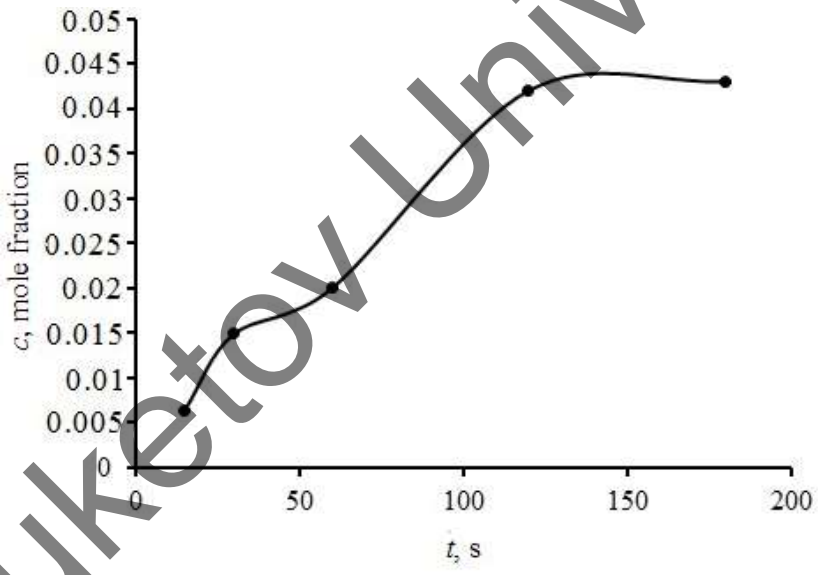
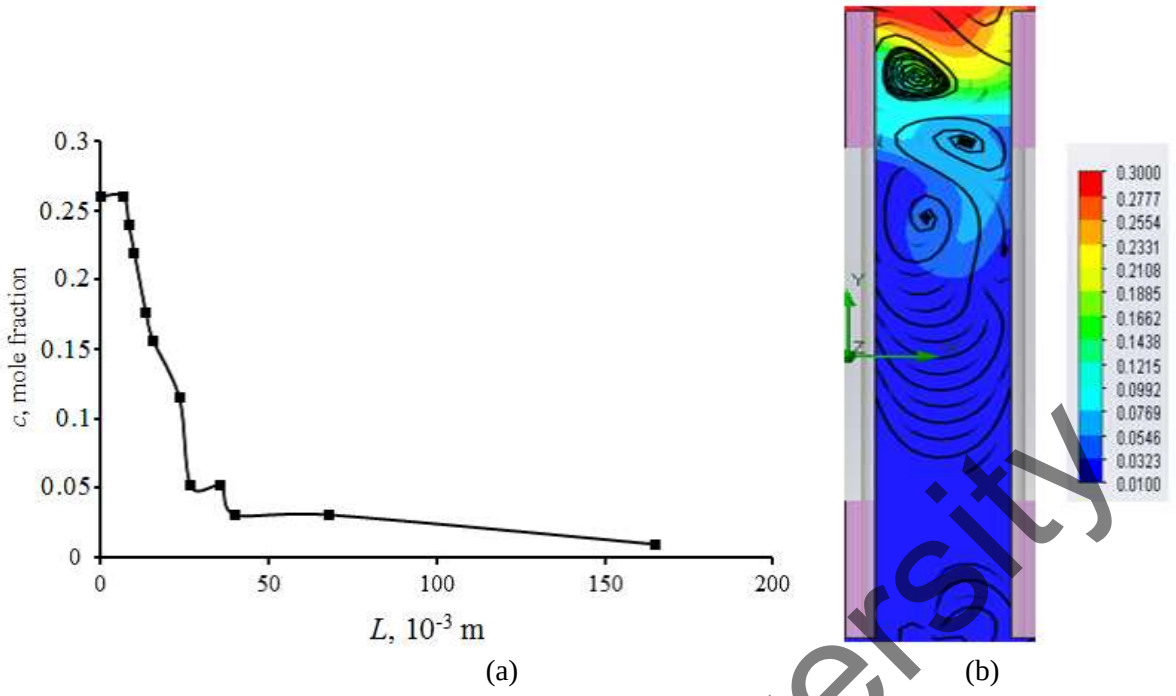


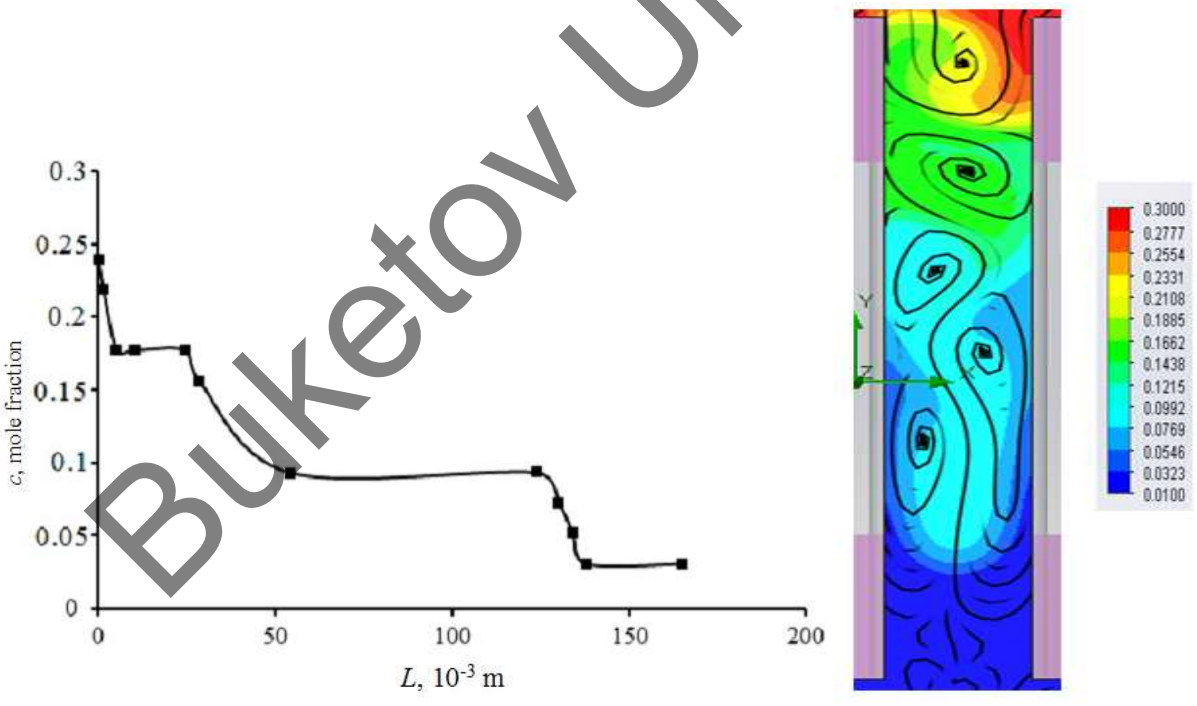
Figure 2. Time-dependence of the amount of argon diffused into nitrogen

Figures 3-7 display how the average concentration of carbon dioxide varies according to the channel altitude and how the concentrations are distributed at different times. Calculations have shown that an analogous picture is realized for argon.



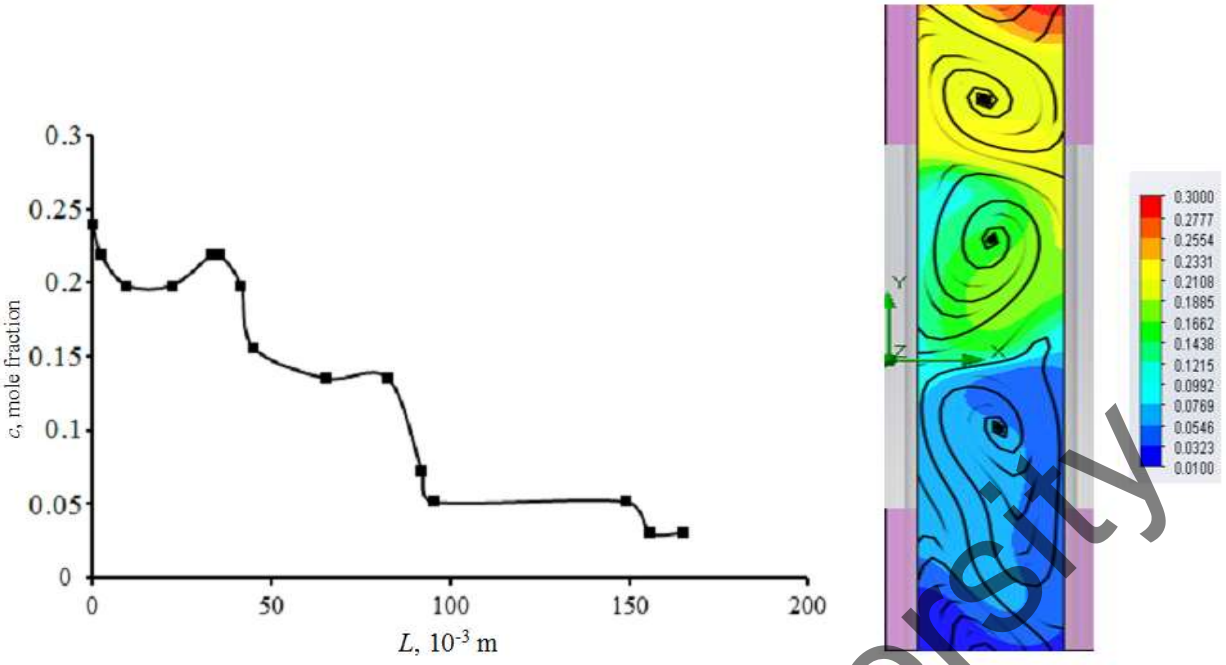
(a) (b)

Figure 3. Length-dependence of the amount of carbon dioxide (a) and pattern displaying the behavior of carbon dioxide (b) for the time moment of 15 s



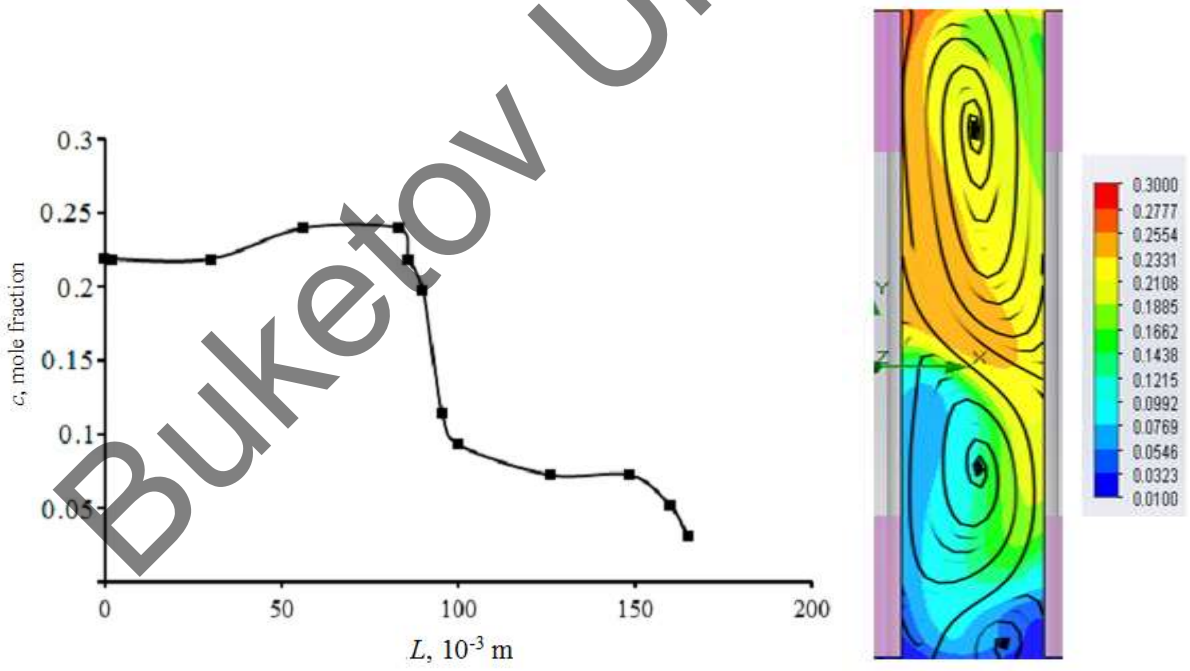
(a) (b)

Figure 4. Length-dependence of the amount of carbon dioxide (a) and pattern displaying the behavior of carbon dioxide (b) for the time moment of 30 s



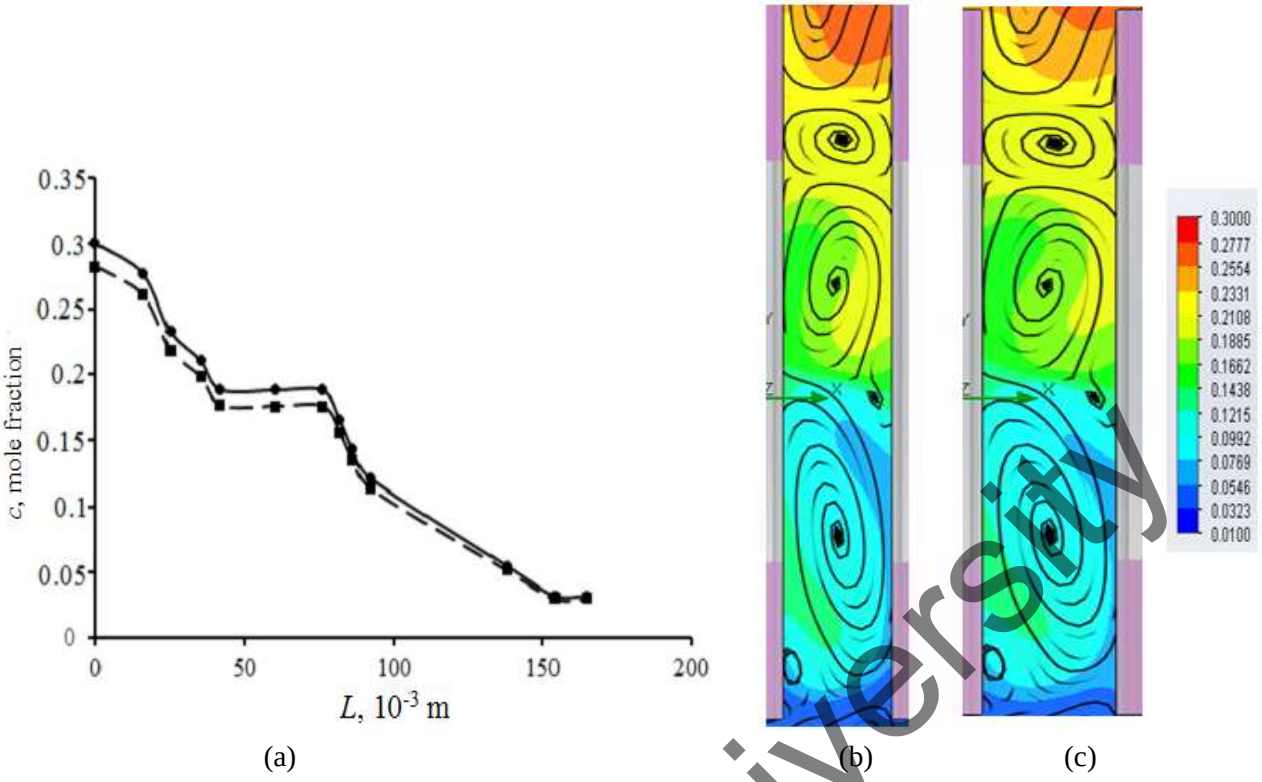
(a) (b)

Figure 5. Length-dependence of the amount of carbon dioxide (a) and pattern displaying the behavior of carbon dioxide (b) for the time moment of 60 s



(a) (b)

Figure 6. Length-dependence of the amount of carbon dioxide (a) and pattern displaying the behavior of carbon dioxide (b) for the time moment of 120 s



(a) (b) (c)

Figure 7. Length-dependence (a) of the amount of carbon dioxide (■) and argon (●), and pattern displaying the behavior of carbon dioxide (b) and argon (c) for the time moment of 180 s

According to Figure 3, at a length of 0.0268 – 0.0357 m of the diffusion channel, there is a region in which the CO_2 concentration is 0.051 mole fractions. On the diagram, this concentration corresponds to the formation of a vortex, which is blurred along the channel length. An increase in time to t = 30 s (Fig. 4) and t = 60 s (Fig. 5) corresponds to the situation when several regions with a constant content of CO_2 concentration are formed in the channel. In this case, the number of vortices formed along the length of the channel decreases from four to two. At the time t = 120 s (Fig. 6), at a length of the diffusion channel of 0.056 – 0.083 m, the greatest transfer of carbon dioxide concentration is observed, which corresponds to the formation of two competing regions on the diagrams, i.e., developed convective flow. A further increase in time to t = 180 s (Fig. 7) is characterized by the behavior of the concentrations of heavy components similar to that shown in Figure 3. However, the difference lies in the fact that the concentrations remain constant at a greater distance along the length of the diffusion channel. The appearance of a new convective regime is indicated by an increase in vortices along the length of the channel.

The following unique features of convective mass transfer that occur in a quaternary gaseous system can be discovered through the study of the obtained data:

1 The non-linear distribution of the concentrations of the components with the maximal molar mass in a quaternary gaseous system indicates the possibility of an instability of the mechanical equilibrium of the system, which leads to a transition from the diffusion mode of mixing to the convective one.

2 The appearance of closed streamlines should be taken into account to determine if the mixing mode has changed. A chaotic formation structure is observed during the initial stages of mixing. Vortices of different sizes gradually develop, and their interaction can lead to the appearance of a pulsating mixing mode.

3 The initial stage of mixing results in the preferential migration of components, which is explained by an increase in the concentration of gases with the maximal molar mass. This process can be due to the presence of large-scale vortices, which facilitate the forward movement of these components. Their subsequent disappearance leads to the stabilization of the transfer.

Conclusions

Numerical modeling of the partial mass transfer of the four-component mixture 0.36 He + 0.33 Ar + 0.31 CO_2 – N_2 at elevated pressure and room temperature showed that the variation in the diffusion coefficients of the components might cause a shift in the "diffusion – convection" modes in the system. Convective instability in the mixture arises because the distribution of concentrations of components with higher molecular weight along the diffusion channel is not linear. The main indicator of the transfer through the separation boundary of kinetic regimes is the appearance of closed streamlines. In their presence, the diffusion regime loses stability. For the considered mixture under given thermophysical conditions, the time of stability loss is estimated to be on the order of a second. Priority transmission of the component with the largest molar mass is feasible with unstable mixing. The emergence of large-scale vortices is connected with this regime.

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Төрт компонентті газ жүйелеріндегі көп компонентті масса тасымалдау режимдерін сандық модельдеу

Төрт компонентті He + Ar + CO2 – N2 газ қоспасының құрамына кіретін және басқа компоненттермен салыстырғанда ең ауыр болып табылатын аргон және қостотықты көміркышқыл газы үшін диффузиялық каналдың әртүрлі нүктелерінде және уақытша аралықтардағы осы компоненттердің концентрациясы тәртібінің өзгеру графиктері берілген. Қарастырылып отырған төрт компонентті қоспадағы конвективті ағындарды модельдеу үшін *SolidWorks* инженерлік жобалау жүйесіне енгізілген *Flow Simulation* компьютерлік пакеті пайдаланылды. Теңдеулер стандартты $k-\varepsilon$ турбуленттілік моделін қолданып, сондай-ақ бастапқы және шекаралық шарттарды белгілей отырып, ақырлы көлем әдісімен шешілді. Алынған үлестірулер уақыт бойынша да, диффузиялық каналдың ұзындығы бойынша да сызықтық емес өзгеретіні көрсетілген. Концентрацияны үлестірудің бұл сызықтық емес әрекеті механикалық тепе-теңдіктің тұрақсыздығымен байланысты, бұл өз кезегінде жүйенің диффузиялық процестен конвективті процеске ауысуына әкеледі. Қарастырылып отырған ауыр компоненттер үшін концентрацияның ең үлкен өзгерісі 120 с ішінде байқалады, бұл эпюраларда екі бәсекелес аймақтың пайда болуына, яғни дамыған конвективті ағынға сәйкес келеді. Сандық эксперимент ұзақтығының одан әрі ұлғаюы ең үлкен молекулалық салмағы бар компоненттердің концентрациясының шамалы өзгеруіне әкеледі, бұл қоспаны ауыр компонентпен байыту эффектісіне сәйкес. Концентрациялардың үлестіру эпюраларындағы тік сызықтарын талдау, каналдың ұзындығы бойынша әр түрлі масштабтағы өзара әрекеттесетін құйындар түзіліп, пульсациялық араластыру режиміне әкелетінін көрсетті. Кең ауқымды құйындардың болуы ең үлкен молекулалық салмағы бар компоненттің басым тасымалдануына әкелетіні анықталды.

Кілт сөздер: газ қоспалары, диффузия, тұрақсыздық, конвекция, концентрацияның үлестіруі, компоненттердің қалыптан тыс бөлінуі, сандық модельдеу, ақырлы көлем әдісі.

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Численное моделирование режимов многокомпонентного массопереноса в четырехкомпонентных газовых системах

Для аргона и двуокиси углерода, входящих в состав четырехкомпонентной газовой смеси He + Ar + CO_2 – N_2 и являющихся наиболее тяжелыми по сравнению с другими компонентами, приведены графики изменения поведения концентрации этих компонентов в различных точках диффузионного канала и временных интервалах. Для моделирования конвективных течений в рассматриваемой четырехкомпонентной смеси использовался компьютерный пакет Flow Simulation, входящий в систему инженерного проектирования SolidWorks. Уравнения решаются методом конечных объемов с использованием стандартной *k–ε* модели турбулентности и с заданием начальных и граничных условий. Показано, что полученные распределения изменяются нелинейно как по времени, так и по длине диффузионного канала. Такое нелинейное поведение распределений концентраций связано с неустойчиво-

стью механического равновесия, что, в свою очередь, приводит к переходу системы от диффузионного процесса к конвективному. Установлено, что для рассматриваемых тяжелых компонентов наибольшее изменение концентрации наблюдается в течение 120 с, что соответствует образованию на эпюрах двух конкурирующих областей, то есть развитому конвективному течению. Дальнейшее увеличение продолжительности численного эксперимента приводит к незначительному изменению концентрации компонентов с наибольшим молекулярным весом, что соответствует эффекту обогащения смеси тяжелым компонентом. Анализ линий тока на эпюрах распределений концентраций показал, что по длине канала образуются взаимодействующие между собой вихри различных масштабов, приводящие к пульсационному режиму смешения. Установлено, что наличие крупномасштабных вихрей обусловливает приоритетный перенос компонентов с наибольшим молекулярным весом.

Ключевые слова: газовые смеси, диффузия, неустойчивость, конвекция, распределение концентрации, аномальное разделение компонентов, численное моделирование, метод конечных объемов.

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