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NUMERICAL RESEARCH OF THE CHANGE OF REGIME FOR UNSTABLE MASS TRANSFER IN A TERNARY GAS MIXTURE HYDROGEN- NITRIC OXIDE-NITROGEN

Kalimov A.B. [1], *Fedorenko O.V.* [2], *Kossov V.N.* [1]

[1]*Abai Kazakh National Pedagogical University, Almaty, Kazakhstan*
[2]*Al-Farabi Kazakh National University, Almaty, Kazakhstan*

Abstract

On the basis of the software package "MathCad", by solving the Stefan-Maxwell diffusion equations, the evolution of the features of mass transfer in a three-component gas mixture, depending on pressure changes, has been numerically studied. In this analysis, the mixing process is studied in a vertical cylindrical channel of a finite size and at the isothermal conditions. The governing equations are solved at the boundary conditions assuming the absence of matter transfer through the walls of diffusion channel. Through the Rayleigh partial numbers, the influence of the pressure change on the behaviour of diffusion and convective flows is examined.

The numerical results reveal that an increase in the pressure leads to a change of modes in ternary gas mixture. The present results are in good agreement with the existing experimental data.

Keywords: isothermal molecular diffusion, diffusion instability, gravitational concentration convection, mechanical equilibrium, linear theory of stability.

Аңдатпа

А.Б. Калимов[1], *О.В. Федоренко*[2], *В.Н. Косов*[1]
[1]*Абай атындағы Қазақ ұлттық педагогикалық университеті, Алматы қ., Қазақстан*
[2]*әл-Фараби атындағы Қазақ ұлттық университеті, Алматы қ, Қазақстан*

ҮШ КОМПОНЕНТТІ ГАЗ ҚОСПАСЫНДАҒЫ ТҰРАҚСЫЗ МАССА АЛМАСУ КЕЗІНДЕ РЕЖИМДЕРДІҢ ӨЗГЕРУІН САНДЫҚ ЗЕРТТЕУ СУТЕГІ- АЗОТ ОКСИДІ-АЗОТ

«MathCad» бағдарламалық пакетінің негізінде Стефан-Максвеллдің диффузиялық теңдеулерін шешу әдісі қысымның өзгеруіне байланысты үш компонентті газ қоспасындағы масса алмасу сипаттамаларының эволюциясы сандық зерттелген. Негізгі теңдеулер диффузиялық каналдың қабырғалары арқылы заттың тасымалданбауы туралы болжаммен шекаралық жағдайларда шешіледі. Рэлейдің парциалды сандарының көмегімен қысымның өзгеруінің диффузиялық және конвективті ағындардың әрекетіне әсері зерттеледі.

Сандық нәтижелер қысымның жоғарылауы үштік газ қоспасындағы режимдердің өзгеруіне әкелетінін көрсетеді. Ұсынылған нәтижелер қолданыстағы тәжірибелік мәліметтермен жақсы үйлеседі.

Түйін сөздер: изотермиялық молекулалық диффузия, диффузиялық тұрақсыздық, гравитациялық концентрациялық конвекция, механикалық тепе-теңдік, сызықтық тұрақтылық теориясы.

Аннотация

А.Б. Калимов[1], *О.В. Федоренко*[2], *В.Н. Косов*[1]
[1]*Казахский национальный педагогический университет имени Абая, г.Алматы, Казахстан*
[2]*Казахский национальный университет имени аль-Фараби, г.Алматы, Казахстан*

ЧИСЛЕННЫЕ ИССЛЕДОВАНИЯ СМЕНЫ РЕЖИМОВ ПРИ НЕУСТОЙЧИВОМ МАССОПЕРЕНОСЕ В ТРЕХКОМПОНЕНТНОЙ ГАЗОВОЙ СМЕСИ ВОДОРОД-ОКСИД АЗОТА-АЗОТ

На основе программного пакета «MathCad», методом решения уравнений диффузии Стефана-Максвелла численно исследована, эволюция особенностей массопереноса в трехкомпонентной газовой смеси в зависимости от изменения давления. В представленном анализе процесс смешения исследуется в вертикальном цилиндрическом канале конечных размеров при изотермических условиях. Основные уравнения решаются при граничных условиях в предположении отсутствия переноса вещества через стенки диффузионного канала. С помощью парциальных чисел Рэлея исследуется влияние изменения давления на поведение диффузионных и конвективных потоков.

Численные результаты показывают, что повышение давления приводит к смене режимов в тройной газовой смеси. Представленные результаты хорошо согласуются с существующими экспериментальными данными.

Ключевые слова: изотермическая молекулярная диффузия, диффузионная неустойчивость, гравитационная концентрационная конвекция, механическое равновесие, линейная теория устойчивости.

Introduction

The process of diffusion instability (i.e. the onset of convective flows in multicomponent liquid and gaseous systems) depends on certain conditions and parameters, for example, concentration, temperature, pressure, the difference in diffusion components, geometry of diffusion channel and etc. [1-5].

However, some experiments showed that a change in the mass transfer regime from molecular diffusion to concentration convection is to be characterized a different sign of the density gradient [6]. This made it possible to reveal the evolution of some characteristic features of the mass transfer regime in ternary gas mixtures in the course of transition from molecular diffusion to the diffusion instability and the ordinary convective mixing. Application of stability theory [7] allowed formulating an approach to revealing common regularities in determining the transition from the diffusion regime to the gravitational concentration convection.

The aim of this study is to examine the transition from the state of diffusion to the regime of concentration gravitational convection (diffusion instability) in a channel of finite size in the absence of mass-transfer through its wall in the framework of the stability theory. In addition, to compare the obtained data with the experiments presented in [6], where the transition from the state of diffusion to the regime of convection is studied at different pressures.

Mathematical Model of Diffusion Instability

The macroscopic flow of the isothermal ternary gas mixture is described by the general system of the hydrodynamic equations, that includes the Navier – Stokes equations, equations for conservation of the number of particles in the mixture and the components. Taking into account the conditions of independent diffusion, for which the $\sum_{i=1}^{3} \vec{j}_i = 0$ and $\sum_{i=1}^{3} c_i = 1$ are valid, the system of equation takes the following form [7, 8]:

$$\rho\left[\frac{\partial \vec{u}}{\partial t} + \left(\vec{u}\nabla\vec{u}\right)\right] = -\nabla p + \eta\nabla^2\vec{u} + \left(\frac{\eta}{3} + \xi\right)\nabla div\vec{u} + \rho\vec{g}, \quad \frac{\partial n}{\partial t} + div\left(n\vec{v}\right) = 0,$$

$$\frac{\partial c_i}{\partial t} + \vec{v}\nabla c_i = -div\vec{j}_i, \quad \vec{j}_i = -\left(D_{ii}^*\nabla c_i + D_{ij}^*\nabla c_j\right), \tag{1}$$

where D_{ij}^* is the practical diffusion coefficient.

The equations (1) are supplemented with the environmental state equation

$$\rho = \rho\left(c_1, c_2, p\right), \; T = const$$

interrelating the thermodynamic parameters entering Eqs. (1).

The method of small perturbations [7] has been used by solution of the system of equations (1). Taking into account that at $L » r$ (L, r are the length and radius of diffusion channel accordingly) the differences between perturbations of the average $\vec{v}$ and weight-average $\vec{u}$ velocities in the Navier – Stokes equation will be inconsiderable, then the final system of equation of gravitational concentration convection for perturbation values in dimensionless quantities takes the form:

$$P_{22}\frac{\partial c_1}{\partial t} - \left(\vec{u}\vec{\gamma}\right) = \tau_{11}\nabla^2 c_1 + \frac{A_2}{A_1}\tau_{12}\nabla^2 c_2,$$

$$P_{22}\frac{\partial c_2}{\partial t} - \left(\vec{u}\vec{\gamma}\right) = \frac{A_1}{A_2}\tau_{21}\nabla^2 c_1 + \nabla^2 c_2, \tag{2}$$

$$\frac{\partial \vec{u}}{\partial t} = -\nabla p + \nabla^2\vec{u} + \left(R_1\tau_{11}c_1 + R_2 c_2\right)\vec{\gamma},$$

$$div\vec{u} = 0,$$

where $P_{ii} = \nu / D_{ii}^*$ is the Prandtl diffusion number, $R_i = g\beta_i A_i d^4 / \nu D_{ii}^*$ is the Rayleigh partial number [4, 8], $\tau_{ij} = D_{ij}^* / D_{22}^*$ denotes the parameters, which determine the relationship between the "practical" diffusion coefficients.

It is necessary to define exactly the boundary conditions for the solution of the system of equations (2). Therefore, we have considered the unstable diffusion mixing problem in the cylindrical channel of a finite size, which is distinct from the infinite case.

The equation system (2) is solved by the method given in [7-9]. As a result, we determine the concentration distribution along the length of the cylindrical channel of finite dimensions *L*, *r* [8]:

$$c_i = \frac{11K_i\left(h^2 - z^2\right)\left(5h^2 - z^2\right)\cos n\varphi}{248\alpha^2\left(k^2+\alpha^2\right)} \times \left[\alpha^2 \frac{J_n(kr)}{J_n(k)} + \frac{I_n(\alpha r)}{\alpha I_n(\alpha)}\left\{n\left(\alpha^2+k^2\right) - \alpha^2 k \frac{J_n'(k)}{J_n(k)}\right\} - \left(k^2+\alpha^2\right) r^n\right], \quad (3)$$

where $K_1 = \frac{\left(1 - \frac{A_2}{A_1}\tau_{12}\right)}{(\tau_{11} - \tau_{12}\tau_{21})}$, $K_2 = \frac{\left(\tau_{11} - \frac{A_1}{A_2}\tau_{21}\right)}{(\tau_{11} - \tau_{12}\tau_{21})}$, $\alpha^2 = \frac{153}{62h^2}$, J_n and I_n are the n-order Bessel functions of the first kind, and the parameter *k* can be found from the equation $kJ_n''(k) = (n+1)J_n'(k)$.

In order to determine the monotonous stability boundary of the problem under consideration, the third equation of the system (2) can be scalarly multiplied by the vector $\vec{u}$ and integrated all over the volume *V* of the diffusion channel. This can be done under the conditions, that $\nabla p = 0$, $\frac{\partial \vec{u}}{\partial t} = 0$. Then we have:

$$\int \vec{u}\nabla^2\vec{u}dV + R_1\tau_{11}\int u_z c_1 dV + R_2\int u_z c_2 dV = 0. \quad (4)$$

This equation in the coordinates (R_1, R_2) gives a straight line MM dividing the region of molecular transport and the region of the diffusion instability. Figure 1 shows the location of the neutral line of monotonic instability for the system $0.4163H_2 + 0.5837N_2O - N_2$ for $n = 1$. The region that lies below the line M_1M_1 corresponds to diffusion.

From the condition of zero density gradient of the mixture and with allowance for the determined values of partial Rayleigh numbers (2), we obtain the following equation for the line in the plane (R_1, R_2):

$$\tau_{11}R_1 = -R_2. \quad (5)$$

The mutual position of the line of monotonic instability M_1M_1 (Eq. (4)) and the line $\nabla\rho = 0$ (Eq. (5)) for $n = 1$ is shown in Fig. 1. As follows from figure, there exists a region on the plane (R_1, R_2) where the line MM is situated below the line (5). In this region, the mixture appears to be unstable.

Results of Numerical Experiment

Analysis of Experimental Data

Assessment of the pressure influence on the intensity of unstable process is given in [6]. The following system $0.4163H_2 + 0.5837N_2O - N_2$ was examined. The experiments described in [6] were conducted in a two-flask diffusion setup comprising the upper and lower vessels with equal volumes $V_1 = V_2 = 55$ cm^3 and a diffusion channel with a diameter of 4.0 mm and a length of 7.0 mm. The temperature in all experiments was 298.0 K. The experiments lasted 20 min that made it possible to obtain the full information about the character of the examined mass transfer.

The binary gas mixture $0.4163H_2 + 0.5837N_2O$ was always charged into the upper flask and the nitrogen was admitted to the lower flask. The process of gas mixing in the system was studied at various pressures. The experimental data allowed the characteristic transition regimes to be revealed. In the interval of pressures from atmospheric to about 0.4 MPa, behaviour of the component concentration is characteristic of the molecular diffusion. The further increase in the pressure leads to the development of instability in the mechanical equilibrium of the gas mixture. The subsequent increase in the pressure from 1.5 to 3.0 MPa leads to a change in the sign of the density gradient, which is accompanied by competition of the convective flows caused both by the diffusion instability and by the traditional convective mixing.

Analysis of Calculation Results

To compare the numerical results identifying the areas of stability and instability with the experimental data shown in [6] we represent them in the form of partial Rayleigh numbers. The partial Rayleigh numbers in accordance with (2) can be written as follows:

$$R_1 = \frac{gnr^4 \Delta m_1}{\rho \nu D_{11}^*} \cdot \frac{\partial c_1}{\partial z}, R_2 = \frac{gnr^4 \Delta m_2}{\rho \nu D_{22}^*} \cdot \frac{\partial c_2}{\partial z} \quad , \tag{6}$$

where m_i is the molecular mass of the *i*-th component, $\Delta m_1 = m_1 - m_3$, $\Delta m_2 = m_2 - m_3$. If conditions of the experiment are known (pressure, temperature, composition of mixtures in each of the flasks, the size of the diffusion channel), then according to Eq. (6) we can find R_1 and R_2 and thus determine the point representing this experiment on the plane (R_1, R_2). From experiment, we know what the regime (diffusion or convection) occurs under the given conditions.

Figure 1 shows the experimental data in terms of the Rayleigh numbers for the system $0.4163H_2$ + $0.5837N_2O$ – N_2 obtained by varying the pressure. The full circles correspond to the convective mixing process while the open circles conform to the diffusion one. The lines M_1M_1, M_2M_2 are drawn for first and third modes of the disturbances characterizing the change of convective mass transfer type.

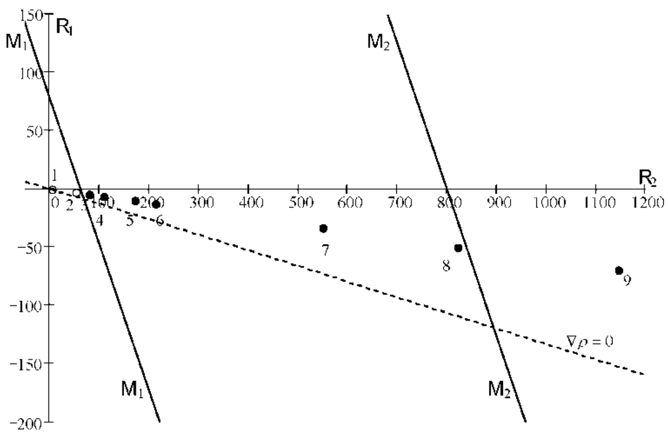

Fig.1. Boundary lines of monotonic instability MM and zero density gradient $\nabla\rho = 0$ *for the system $0.4163H_2 + 0.5837N_2O – N_2$. Symbols ● correspond to data that determine unstable state. The calculation is carried out at the pressure values: p = 0.093 (1), 0.323 (2), 0.400 (3), 0.471 (4), 0.588 (5), 0.659 (6), 1.059 (7), 1.294 (8), 1.529 (9) MPa.*

As it is seen from the experimental data represented in [6], the change of the passed hydrogen or nitrous oxide concentration subject to the pressure is the curve with the maximum. If we suppose that the areas connecting with the abrupt changes of the process intensity correspond to the transfer mode change, then the experimental partial Rayleigh numbers determining at pressures of the intensity jump should be near the critical Rayleigh numbers fitting with the change of disturbances modes *n*.

As is seen, in Fig. 1 that at the pressure from 0.093 to 0.323 MPa the system $0.4163H_2$ + $0.5837N_2O$ – N_2 is in the area of stable diffusion. It is conformed to the data given in [6]. According to Fig. 1 point 3 corresponds to the pressure 0.4 MPa is situated practically near the curve of monotonic disturbances M_1M_1. That indicates the instable process observes at the considered pressure, i.e. first regime change (or the transition from the molecular diffusion to the diffusion instability) happens at this pressure.

At the pressure above $p \approx 1.294$ MPa the change of the disturbance scale to the formed flow regime occurs and the next convective regime $n = 3$ arises. A more detailed description of the features of the appearance of structured flows at various pressures and mixture compositions in the convective instability regime was proposed in [10].

Thus, the results reveal that ternary gas mixture exhibits various types of mixing and the transition regimes depending on the pressure.

Conclusion

In this article, a numerical investigation has been performed to comprehend the evolution of the mass transfer regime in three-component gas mixture hydrogen- nitric oxide-nitrogen in a vertical cylindrical channel of a finite size for the pressure range from atmospheric (0.093 MPa) to 3.0 MPa. Moreover, we can see that ternary gas mixture exhibits various types of mixing and the transition regimes depending on the pressure. The comparison of theoretical results with the experimental data for the study of the pressure dependence of the diffusion mixing of ternary gas mixture $0.4163H_2 + 0.5837N_2O - N_2$ indicates qualitative and quantitative agreement.

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References:

1 Ruev G.A., Fedorov A.V., Fomin V.M.(2009) Description of the anomalous Rayleigh-Taylor instability on the basis of the model of dynamics of a three-velocity three-temperature mixture. J. Applied Mech. and Tech. Phys. Vol. 50, No. 1.49-57. (In English)

2 Ryzhkov I.I., Shvetsova V.M. (2009) Long-wave instability of a multicomponent fluid layer with the Soret effect. Phys. Fluids. Vol. 21, 014102. (In English)

3 Aleksandrov O.E., Seleznev V.D. (2016) Pressure dependence of the mixing rate for the free convection of a binary gas mixture in a two-flask apparatus. Tech. Phys.Vol 61, No. 7.982-986. (In English)

4 Kossov V., Fedorenko O., Zhakebayev D. (2019) Features of multicomponent mass transfer in gas mixtures containing hydrocarbon components. Chem. Eng. Technol. Vol. 42, No. 4, 896-902. (In English)

5 Sankar M. (2010) Younghae Do. Numerical simulation of free convection heat transfer in a vertical annual cavity with discrete heating. Intern. Commun. in Heat and Mass Transfer. Vol. 37,600-606. (In English)

6 Zhavrin Yu.I., Kosov V.N., Kul'zhanov D.U., Karataeva K.K. (2000) Effect of the pressure on the type of mixing in a three-component gas mixture containing a component possessing the properties of a real gas. Tech. Phys. Letters. Vol. 26, No. 12, 1108-1109. (In English)

7 Gershuni G.Z., Zhukhovitskii E.M. (1976) Convective Stability of Incompressible Fluids.Jerusalem, Israel: Keter Publishing House, 392. (In English)

8 Kossov V., Krassikov S., Fedorenko O. (2017) Diffusion and convective instability in multicomponent gas mixtures at different pressures. Eur. Phys. J. Special Topics. Vol. 226, 177-1187. (In English)

9 Kosov V., Fedorenko O.V., Mukamedenkyzy V., Kalimov A.B. (2020) Special modes of diffusion mass transfer in isothermal triple gas mixtures. Journal of Physics: Conference Series. Vol. 1565, 012061. (In English) doi:10.1088/1742-6596/1565/1/012061

10 Kosov V.N., Krasikov S.A., Fedorenko O.V., Kalimov A.B. (2020) Convective mixing in an inclined channel caused by ternary diffusion under condition of increasing density of the mixture with height. Abai University bulletin Ser. Physics & Mathematical Sciences № 1(69), 229-234. (In English)