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Experimental and numerical study of the peculiarities of the multicomponent gas mixtures separation under natural gravity convection

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Abstract. Experimental study of the features of separation process in ternary gas mixtures $0.6179 \text{H}_2 + 0.3821 \text{N}_2 - \text{CH}_4$, $0.7760 \text{CH}_4 + 0.2240 \text{R}_12 - n\text{-C}_4\text{H}_{10}$ is conducted. Conditions of the priority transfer of the density heaviest component of the mixture are discussed. The problem is solved by the splitting scheme by physical parameters. Numerical data on the time evolution of components concentrations at different concentrations of components of the initial mixture are obtained. Calculations have shown that for ternary systems the concentration increase of the heaviest component results to the intensity growth of convective mixing.

1. Introduction
The description of isothermal diffusion in multicomponent mixtures is described by the Stefan-Maxwell equations [1] and, in comparison with binary systems, has a number of features [2], which consist in the absence of component transfer at a nonzero concentration gradient; transferring a component with the zero value of its gradient; bidirectional (reverse) diffusion. Another manifestation of special modes of multicomponent diffusion is the appearance of convection leading to a synergistic effect associated with a significant increase in the mixing speed of the components of the system [3]. Experiments and numerical studies on the vapor diffusion of binary solutions into an inert gas [3, 4] have shown the possibility of the occurrence of convective instability in such systems. The effects described in [3, 4] are consistent with the results given in [5, 6] in which the appearance of structured convective currents is considered when changing the "diffusion-convection" regimes at different pressures and compositions.

In this paper, experimental data on the study of isothermal diffusion and convective mixing in multicomponent gas mixtures $0.6179 \text{H}_2 + 0.3821 \text{N}_2 - \text{CH}_4$, $0.7760 \text{CH}_4 + 0.2240 \text{R}_12 - n\text{-C}_4\text{H}_{10}$ are presented. By the methods of 2D modeling, the possibility of the appearance of structured convective flows in the course of diffusion at various mixing times is studied numerically.
2. Experimental study

The method of two flasks was used [5, 6] to study diffusion and convective transport. A binary mixture of light and heavy in density components was placed in the upper flask. A gas whose partial density had an intermediate value was in the lower flask. The binary mixture density was less than the density of gas in the lower flask in all experiments at any compositions, pressures and temperatures. The first part of the installation provided transportation of gases to the diffusion apparatus (see figure 1). Gas mixtures were in the cylinders (20) and (21).

The second part of the installation is a two flask apparatus. Subject to the gaseous mixture, two diffusion apparatuses with the different channels and volumes of flasks were used: 1. \( V_1 = V_2 = (76.0 \pm 0.5) \times 10^{-6} \text{ m}^3 \), the flasks were connected with vertical cylindrical channel of length \( L = (70 \pm 0.05) \times 10^{-3} \text{ m} \) and diameter \( d = (4.0 \pm 0.02) \times 10^{-3} \text{ m} \) (in the experiments with the system \( 0.6179 \text{ H}_2 (1) + 0.3821 \text{ N}_2 (2) - \text{ CH}_4 (3) \)); 2. \( V_1 = V_2 = (226.0 \pm 0.5) \times 10^{-6} \text{ m}^3 \), \( L = (165.0 \pm 0.05) \times 10^{-3} \text{ m} \), \( d = (6.1 \pm 0.02) \times 10^{-3} \text{ m} \) (in the experiments with the system \( 0.7760 \text{ CH}_4 (1) + 0.2240 \text{ R12 (2) – n-C}_4\text{H}_{10} (3) \)).

Figure 1. Block diagram of the installation of the two-flask method [5, 6]. The gas preparation block and the two-flask diffusion setup are indicated by I and II, respectively; valves (1-8); valve connected to the backing vacuum pump (9); valve connected to the interferometer or chromatograph (10); membrane dividers (11); reference pressure gages (12); equalizing tank (13); bottom flask (14); diffusion channel (15); top flask (16); fluoroplastic pellet (17); rod (18); handwheel (19); gas holders (20) and (21).

The experimental procedure was the following. The diffusion apparatus was in the constant-temperature bath. The temperature was maintained with an accuracy of \( \pm 0.1 \text{ K} \). The gases from the cylinders (20) and (21) were supplied to the upper flask (16) and the lower flask (14) up to a predetermined pressure. Then, the diffusion channel (15) was opened and the mixing start time was recorded. After some time, the channel was closed, and the gas mixture from the flasks was analyzed by a chromatograph.

2.1. Experimental results

The results of experimental studies for the system \( 0.7760 \text{ CH}_4 + 0.2240 \text{ R12} – \text{n-C}_4\text{H}_{10} \) for different mixing times are given in table 1. Experimental data were obtained at \( p = 0.22 \text{ MPa} \) and \( T = 298.0 \text{ K} \).

The dimensionless parameter \( \alpha \) was determined as the ratio of the experimental concentrations \( c_{\text{exp}} \) to the theoretical values \( c_{\text{theor}} \) calculated by using the Stefan-Maxwell equations [1] with the assumption of stable diffusion. As can be seen from table 1, the parameter \( \alpha \) of the heavy component, i.e. freon, differs significantly from 1 in the system under consideration. This indicates the presence of powerful
convective flows that substantially distort the diffusion process. This behavior of the parameter $\alpha$ is related to the fact that the diffusion coefficients of the components differ sharply.

The interdiffusion coefficient of methane into n-butane exceeds the interdiffusion coefficient of R12 into the same gas in 2.5 times ($D_{\text{CH}_4-\text{n-C}_4\text{H}_{10}} = 0.082 \cdot 10^{-4} \text{ m}^2/\text{s}$, $D_{\text{R12-\text{n-C}_4\text{H}_{10}}} = 0.0334 \cdot 10^{-4} \text{ m}^2/\text{s}$). At the initial stage of the process (of the order of a few seconds after the valve opening in the diffusion apparatus), two local regions, i.e. “enriched” by R12, and area located under it and “enriched” with methane are formed because of the greater diffusion mobility of methane, in comparison with R12. In a gravitational field, such stratified regions are unstable and there is a “flux dip” of R12, i.e. isothermal concentration convection arises. The duration of the unstable diffusion process is determined by the ratio of the composition of the light and heavy components of the mixture in the upper and lower parts of the channel. From a certain value of the concentrations, obtained as a result of convective mixing caused by instability, conditions for diffusion transfer again arise in the system. The transition to molecular diffusion is determined by comparing the experimental concentrations with those calculated from the Stefan–Maxwell equations.

Table 1. Time dependence of the parameter $\alpha$ for the system $0.7760 \text{ CH}_4 + 0.2240 \text{ R12} - \text{n-C}_4\text{H}_{10}$.

| System                                      | $\alpha_{\text{CH}_4}$ | $\alpha_{\text{R12}}$ | $\alpha_{\text{n-C}_4\text{H}_{10}}$ | $t$ (hour) |
|---------------------------------------------|------------------------|------------------------|-------------------------------------|------------|
| $0.6955 \text{ CH}_4 + 0.1614 \text{ R12} + 0.1504 \text{ n-C}_4\text{H}_{10}$ | 2.897                  | 8.000                  | 0.965                               | 1          |
| $0.0805 \text{ CH}_4 + 0.0546 \text{ R12} + 0.8496 \text{ n-C}_4\text{H}_{10}$ |                        |                        |                                     |            |
| $0.6703 \text{ CH}_4 + 0.1680 \text{ R12} + 0.1650 \text{ n-C}_4\text{H}_{10}$ | 1.321                  | 2.286                  | 1.894                               | 3          |
| $0.1057 \text{ CH}_4 + 0.0560 \text{ R12} + 0.8350 \text{ n-C}_4\text{H}_{10}$ |                        |                        |                                     |            |
| $0.6382 \text{ CH}_4 + 0.1664 \text{ R12} + 0.2061 \text{ n-C}_4\text{H}_{10}$ | 1.299                  | 7.000                  | 2.446                               | 7.2        |
| $0.1378 \text{ CH}_4 + 0.0576 \text{ R12} + 0.7939 \text{ n-C}_4\text{H}_{10}$ |                        |                        |                                     |            |

Comparison with the measured data makes it possible to classify the process as stable (diffusion) if the difference with the calculated values does not exceed the experimental error, and unstable (convective) if the divergence is sufficiently large. After a certain time, a new calculation is made subject to the prevalent concentration distribution and comparison with the experimental data.

Figure 2. Temporal evolution of dimensionless parameter $\alpha$. 1 is the calculation on the assumption of diffusion; 2 is experimental data for hydrogen; 3 is experimental data for methane; 4 is experimental data for nitrogen. $p = 2.54 \text{ MPa}$ and $T = 353.0 \text{ K}$.
As can be seen from table 1, the dimensionless parameter \( \alpha \) for all components is greater than one for a long interval of time, i.e. the unstable regime in the system under consideration takes a sufficiently long time.

The behaviour of the dimensionless parameter \( \alpha \) with the different transport time for the system \( 0.6179 \text{H}_2(1) + 0.3821 \text{N}_2(2) - \text{CH}_4(3) \) is presented in figure 2.

An elevated value of the dimensionless parameter \( \alpha \) of the heavy component is observed during the few hours of a diffusion unstable regime. This suggests that the concentration separation of the components of the examined system occurs. The effect weakens in time, but the difference in the values of \( \alpha \) remains for quite a long time. Measured and calculated according to [7] ratios \( Q_2/Q_1 \) (\( Q_1 \) and \( Q_2 \) are the partial fluxes of the light and heavy components respectively) as well as the separation coefficients for the systems under consideration are presented in table 2.

### Table 2. Ratio of partial flows at early stage of the convective mixing for diffusion-unstable systems.

| System | \( c_1 \) (mol. fractions) | \( c_2 \) (mol. fractions) | \( Q_2/Q_1 \) (exp.) | \( Q_2/Q_1 \) (theor.) |
|--------|-----------------------------|-----------------------------|----------------------|------------------------|
| \( 0.7760 \text{CH}_4 + 0.2240 \text{R12} - \text{n-C}_4\text{H}_{10} \) | 0.0985 | 0.0546 | 0.6 | 0.7 |
| \( 0.6179 \text{H}_2(1) + 0.3821 \text{N}_2(2) - \text{CH}_4(3) \) | 0.0536 | 0.0855 | 1.6 | 2.1 |

Thus, experimental studies have shown that an anomalous separation of the mixture components, when the heaviest component has the highest penetrating power, is observed under convective mixing. The main essence of this phenomenon lies in the fact that components 1 and 2 being in the upper flask enter the lower flask, not in the ratio \( c_1 I / c_2 I \), as might be expected under convection, but in such a way that \( Q_2/Q_1 \gg c_2 I / c_1 I \), i.e. there takes place the preferential transfer of the heaviest component of the mixture [7].

### 3. Formulation of the problem and numerical method

The macroscopic motion of an isothermal three-component gas mixture is described by the general system of equations involving the Navier-Stokes equations, conservation equations of the particle number of mixture and components in the Boussinesq approximation. Taking into consideration the conditions of independent diffusion during which \( \sum_{i=1}^{3} j_i = 0 \) and \( \sum_{i=1}^{3} c_i = 1 \) for an isothermal gas mixture, the system of equation by analogy with Kosov et al. [8] can be written as

\[
\rho \left[ \frac{\partial \bar{u}}{\partial t} + (\bar{u} \nabla) \bar{u} \right] = -\nabla p + \eta \Delta \bar{u} + \left( \frac{\eta}{3} + \xi \right) \text{div} \bar{u} + \rho \bar{g} \\
\frac{\partial n}{\partial t} = -\text{div}(n \bar{v}) \\
\frac{\partial c_1}{\partial t} + \nabla c_1 = \text{div} \left[ D_{11}^{*} \nabla c_1 + D_{12}^{*} \nabla c_2 \right] \\
\frac{\partial c_2}{\partial t} + \nabla c_2 = \text{div} \left[ D_{21}^{*} \nabla c_1 + D_{22}^{*} \nabla c_2 \right]
\]

Here \( \bar{u} \) is the weight-average velocity vector; \( \bar{v} \) is the number-average velocity vector; \( \rho \) is the density; \( p \) is the pressure; \( \eta \) and \( \xi \) are the coefficient of shear and bulk viscosity; \( \bar{g} \) is the gravitational acceleration vector; \( n \) is the number density; \( t \) is the time; \( c_i \) is the \( i \)-th component concentration; \( j_i \) is
the diffusion flux density of the \(i\)-th component; \(D_i^*\) is the practical diffusion coefficients, which are determined by the mutual diffusion coefficients \(D_{ij}\)

\[
D_{11}^* = \frac{D_{11} \left[ c_1 D_{32} + (c_2 + c_1) D_{12} \right]}{D} \\
D_{12}^* = -\frac{c_1 D_{23} (D_{12} - D_{13})}{D} \\
D_{22}^* = \frac{D_{23} \left[ c_2 D_{13} + (c_1 + c_3) D_{12} \right]}{D} \\
D_{21}^* = -\frac{c_2 D_{13} (D_{12} - D_{23})}{D} \\
D = c_1 D_{23} + c_1 D_{13} + c_1 D_{12}
\]

The relationship between the total flux of the \(i\)-th component and the gaseous mixture velocity can be written as

\[
\bar{v} = \sum \frac{j_i}{c_0} \quad \bar{u} = \sum \frac{m_i j_i}{\rho}
\]

where \(m_i\) is the molecular mass of the \(i\)-th component, \(\rho = \sum m_i c_i\), \(c_0 = \sum_{i=1}^{n} c_i\).

Equation (1) shall be supplemented by the equation of medium state

\[
\rho = \rho (c_1, c_2, \rho) \quad T = \text{const}
\]

Using the method of small disturbances and taking into account that \(v_i = u\) the system (1) takes the form

\[
\frac{\partial \bar{u}}{\partial t} + \bar{u} \nabla \bar{u} = -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 \bar{u} + g (\beta c_1 + \beta_2 c_2) \bar{v}
\]

\[
\text{div} \bar{u} = 0
\]

\[
\frac{\partial c_1}{\partial t} + \bar{u} \nabla c_1 = D_{11}^* \nabla^2 c_1 + D_{12}^* \nabla^2 c_2
\]

\[
\frac{\partial c_2}{\partial t} + \bar{u} \nabla c_2 = D_{21}^* \nabla^2 c_1 + D_{22}^* \nabla^2 c_2
\]

where \(\nu = \eta/\rho\) is the kinematic viscosity, \(\beta_i\) is concentration expansion coefficients.

We will write this system in the dimensionless form normalizing by the scales of length \(x^*_i = x/H\), \(x^*_z = z/H\), time \(\tau = tv/H^2\), velocity \(u^*_i = uH/D_{ij}^*\), \(u^*_z = wH/D_{zz}^*\), and pressure \(p^* = pH^2/\rho_0 \nu D_{zz}^*\) (\(\rho_0\) is a characteristic medium density corresponding to the mean values of the concentration), concentrations of the \(i\)-th component \(c^*_i = c_i/A_i H\), \(c^*_2 = c_2/A_2 H\) (omitting the dimensionless sign \(\ast\))

\[
\frac{\partial u_i}{\partial \tau} + \frac{1}{Pr_{zz}} \frac{\partial u_i}{\partial x_1} + \frac{1}{Pr_{zz}} \frac{\partial u_i}{\partial x_2} = -\frac{\partial p}{\partial x_1} + \frac{\partial^2 u_i}{\partial x_1^2} + \frac{\partial^2 u_i}{\partial x_2^2} + Ra_i c_i
\]
\[
\frac{\partial u_2}{\partial \tau} + \frac{1}{Pr_{22}} u_1 \frac{\partial u_2}{\partial x_1} + \frac{1}{Pr_{22}} u_2 \frac{\partial u_2}{\partial x_2} = -\frac{\partial p}{\partial x_1} + \frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_2^2} + Ra_c c_2
\]

\[
\frac{\partial c_1}{\partial \tau} + \frac{1}{Pr_{22}} u_1 \frac{\partial c_1}{\partial x_1} + \frac{1}{Pr_{22}} u_2 \frac{\partial c_1}{\partial x_2} = \frac{1}{Pr_{11}} \frac{\partial^2 c_1}{\partial x_1^2} + \frac{1}{Pr_{11}} \frac{\partial^2 c_1}{\partial x_2^2} + \frac{1}{Pr_{12}} \frac{\partial^2 c_1}{\partial x_1^2} + \frac{1}{Pr_{12}} \frac{\partial^2 c_1}{\partial x_2^2}
\]

\[
\frac{\partial c_2}{\partial \tau} + \frac{1}{Pr_{22}} u_1 \frac{\partial c_2}{\partial x_1} + \frac{1}{Pr_{22}} u_2 \frac{\partial c_2}{\partial x_2} = \frac{1}{Pr_{21}} \frac{\partial^2 c_2}{\partial x_1^2} + \frac{1}{Pr_{21}} \frac{\partial^2 c_2}{\partial x_2^2} + \frac{1}{Pr_{22}} \frac{\partial^2 c_2}{\partial x_1^2} + \frac{1}{Pr_{22}} \frac{\partial^2 c_2}{\partial x_2^2}
\]

\[
\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} = 0
\]

Here \( Pr_i = \frac{v}{D_i} \) is the diffusion Prandtl number, \( Ra = g \beta_i A \frac{H^4}{D_i v} \), \( Ra_v = g \beta_i A \frac{H^4}{D_v v} \).

The initial conditions and the boundary conditions for the system of equations (4) are the following:

Initial conditions:
1) For the speed of components: \( u(x, z, \tau = 0) = 0, i = 1, 2 \).
2) The process when the heavy and light gases are located in the upper part of the computational domain and the average gas is at the bottom part is studied. For the concentration in the upper computational area \( S_1 \) (figure 3b): \( c_i|_{x=0, z=S_1} = X_i \) is for the light component, \( c_i|_{z=0, x=S_1} = X_2 \) is for the heavy component, \( c_i|_{z=0, x=S_1} = 0 \) is for the middle component, where \( X_1, X_2 \) are the mole fractions of gas components.
3) For the concentration in the lower computational area \( S_0 \) (figure 3b): \( c_i|_{x=0, z=S_0} = 0 \) is for the light component, \( c_i|_{z=0, x=S_0} = 0 \) is for the heavy component, \( c_i|_{x=0, z=S_0} = 1 \) is for the middle component.

Boundary conditions:
For the speed of components: \( u_i = 0, i = 1, 2 \); for the concentration: \( \frac{\partial c_i}{\partial n} = 0, i = 1, 2 \).

Figure 3. Modelling of the studied process. (a) display of areas; (b) the initial conditions for the three-component mixture.
3.1. Numerical algorithm

As it is seen from the experimental data, mixing is carried out in the channel, which has as a rule a cylindrical shape. Heavy and light in density components of a binary mixture are in the upper part of the channel, and the gas with intermediate density in the lower part of the channel. To simplify the tasks it is considered a two-dimensional cross-section area of cylindrical sphere \( H \times d \) in the Cartesian coordinate system \((x, z)\), where \( H \) is the height of the cylindrical channel, and \( d = 2r \) is the diameter (figure 3a). To register the isoconcentrational lines characterizing the emergence and development of convection, it is sufficient to consider the part of this area \( (H/d >> 1) \), where the diffusion of components take place (figure 3b) ignoring the other areas of the two-dimensional area.

The splitting scheme by physical parameters is used for the solution of the problem of the formation of structured flows in the isothermal gas mixtures at various pressures over time in a vertical cylindrical channel. In the first stage, the momentum transfer is due to the convection and diffusion. The intermediate velocity field is determined in terms of the five-point sweep method specified by Navon [9] with the fourth order of accuracy in space and the third order of accuracy in time by means of the Adams-Bashforth explicit scheme for convective terms and the Crank-Nicolson implicit scheme for diffusion members defined by Kim and Moin [10]. In the second stage, the pressure field is defined in accordance with the found intermediate velocity field and by means of the matrix sweep method described by Abdibekova et al. [11]. At the third stage, it is assumed that the transfer is carried out only by the pressure gradient and the final velocity field is recalculated. In the fourth step, the concentration of the mixture components is calculated by means of the five-point sweep method in accordance with the Adams-Bashforth scheme subject to the found velocity fields.

3.2. Results

The calculations were carried out on a uniform rectangular staggered grid with the number of nodes \( 250 \times 250 \) along the axes \( x_1, x_2 \), respectively. The time step was selected to be 0.001. The calculations are done for actual physical parameters of geometrical characteristics of the channel. The main assumption in modeling is to limit the two-dimensional flows. In the calculations, it was assumed that the Freon concentrations had the following values of 0.3; 0.35 and 0.5 mole fractions. The pressure was assumed to be constant and equal to 0.5 MPa. The numerical results presented in figure 4 illustrate the temporal evolution of the heaviest component concentration.

![Figure 4](image-url)

**Figure 4.** Temporal evolution of the concentration in the system 0.5 CH\(_4\) + 0.5 R12 – n-C\(_4\)H\(_{10}\) at \( p = 0.5 \) MPa. (a) – \( t = 10 \); (b) – \( t = 15 \).
The isoconcentration lines shown in figure 4 are curved. With the course of time, conditions for the convective structural formations are formed and the transition from the diffusion regime to the convective regime occurs.

The calculation results show that at the starting stage the flows with small velocities arise. Then the development of more intense currents leads to a significant curvature of the isoconcentration lines and an increase in the transfer rate. The time for the stability loss of the mechanical equilibrium for a given system is tens of seconds. Then there is a rapid development of convective currents. Convective flows are realized in the form of large-scale structures.

![Diagram](image1)

![Diagram](image2)

![Diagram](image3)

**Figure 5.** Concentration-time pattern of heaviest component at $t = 17.5$. (a) $0.7 \text{CH}_4 + 0.3 \text{R}12 - \text{n-C}_4\text{H}_{10}$; (b) $0.65 \text{CH}_4 + 0.35 \text{R}12 - \text{n-C}_4\text{H}_{10}$; (c) $0.5 \text{CH}_4 + 0.5 \text{R}12 - \text{n-C}_4\text{H}_{10}$

Figure 5 shows the concentration-time pattern of components with different initial proportions of constituents. In systems with a smaller proportion of a heavy or a larger fraction of the light component, for example, in the systems $0.7 \text{CH}_4 + 0.3 \text{R}12 - \text{n-C}_4\text{H}_{10}$ and $0.65 \text{CH}_4 + 0.35 \text{R}12 - \text{n-C}_4\text{H}_{10}$, diffusion is observed. With the increase of the heaviest component fraction in the system 0.5
$\text{CH}_4 + 0.5 \text{ R}12 \rightarrow \text{n-C}_4\text{H}_{10}$, convection occurs due to the mechanical equilibrium instability of the mixture.

Thus, the results of numerical simulation showed that for ternary systems the concentration increase of the heaviest component results to the intensity growth of convective mixing.

4. Conclusion
The paper presents the results of experimental study of the peculiarities of ternary gas mixtures separations. Experimental data on the time evolution of the dimensionless parameter $\alpha$ of the heaviest component of ternary gas mixture have indicated that there is a priority transfer of the density heaviest component of the mixture. The separation coefficients for the systems $0.6179 \text{ H}_2 + 0.3821 \text{ N}_2 - \text{CH}_4$ and $0.7760 \text{ CH}_4 + 0.2240 \text{ R}12 \rightarrow \text{n-C}_4\text{H}_{10}$ have been calculated. Comparison of the experimental separation factors with the calculated has shown that the expression for the calculated factor is valid and determines the maximum value of separation of the mixture components.

The splitting scheme by physical parameters is applied in the present work to describe the a priority transfer of the density heaviest component of the mixture. It is found that the onset of instability is accompanied by a significant curvature of the isoconcentration lines and an increase in the transfer rate.

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