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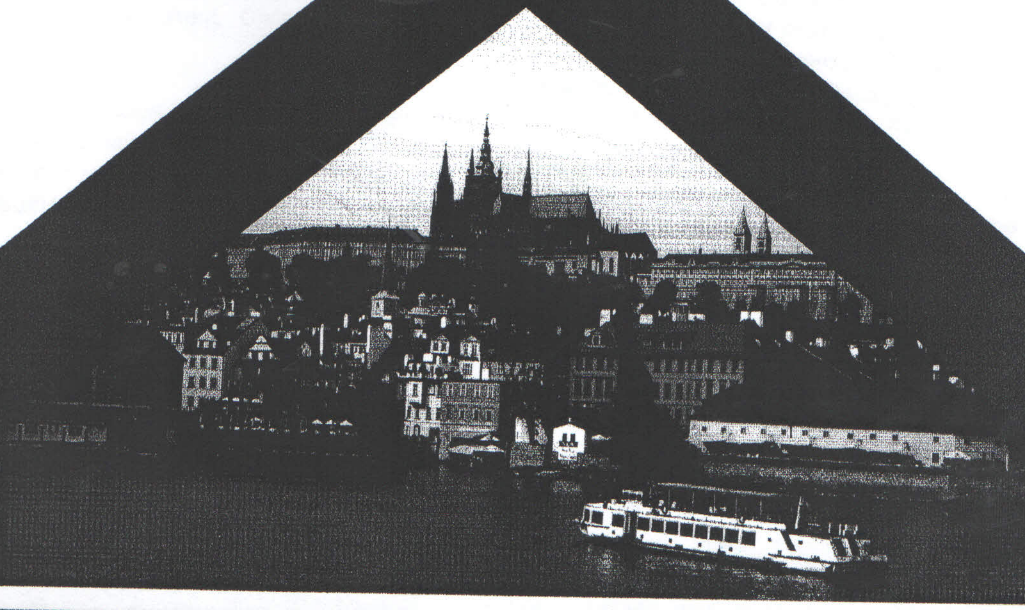

# PROGRAM

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## List of Participants

25 August - 29 August 2018
Prague, Czech Republic

organized by
ČSCHI ČESKÁ SPOLEČNOST CHEMICKÉHO INŽENÝRSTVÍ CZECH SOCIETY OF CHEMICAL ENGINEERING

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About the possibility of the emergence of diffusion instability in isothermal mixing of multicomponent gas mixtures. ***V. N. Kossov, O. Fedorenko**[1]**, V. Mukamedenkyzy, D. Zhakebayev**[2] (Kaz. Nat. Pedag. Univ., Almaty, KZ; [1]Inst. Exp. Theor. Physics, Almaty, KZ; [2]Al-Farabi Kaz. Nat. Univ., Almaty, KZ) [171]

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Features of multicomponent mass transfer at the boundary of change in the "diffusion - concentration gravitational convection" regime in gas mixtures containing hydrocarbon components. ***V. N. Kossov, O. Fedorenko**[1]**, D. Zhakebayev**[2] (Kaz. Nat. Pedag. Univ., Almaty, KZ; [1]Inst. Exp. Theor. Physics, Almaty, KZ; [2]Al-Farabi Kaz. Nat. Univ., Almaty, KZ) [172]

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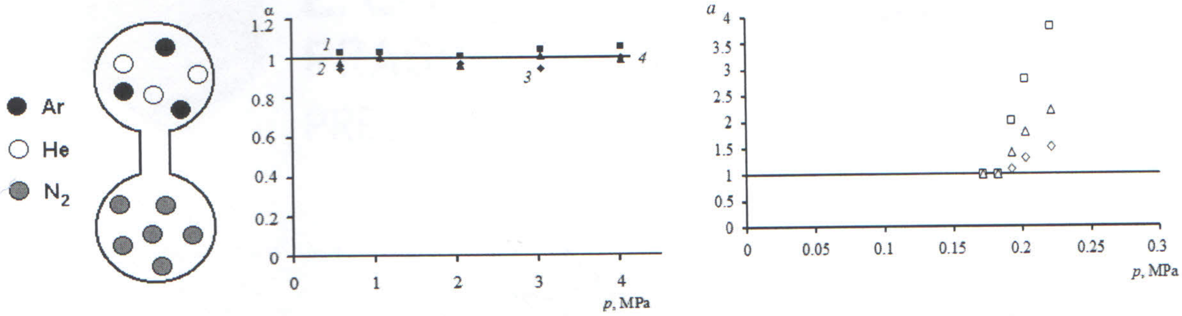
# Features of multicomponent mass transfer at the boundary of change in the "diffusion - concentration gravitational convection" regime in gas mixtures containing hydrocarbon components

V. N. Kossov, [1]O. Fedorenko, [2]D. Zhakebayev
Abai Kazakh National Pedagogical University, 13 Dostyk Ave., 050010 Almaty, Kazakhstan; tel./fax: +7727 291 1022, e-mail: kosov_vlad_nik@list.ru; [1]Institute of Experimental and Theoretical Physics, 71 Al-Farabi Ave., 050040 Almaty, Kazakhstan; tel.+7727 377 3191, e-mail: fedor23.04@mail.ru; [2]Al-Farabi Kazakh National University, 71 Al-Farabi Ave., 050040 Almaty, Kazakhstan; tel.+7727 377 33 33, e-mail: dauren.zhakebayev@gmail.com.

The study of the vapours diffusion of liquid binary solutions into the receiving gas has shown that convective mechanisms, which significantly intensify the total mass transfer during evaporation, can arise in such systems [1]. Similar mixing modes also arise in systems containing hydrocarbon components. If the receiving gas is a multicomponent mixture, then the transition of the system from the diffusion mode to the convective one will be determined not only by the difference in the partial transport coefficients, but also by parameters such as the pressure, the mixture composition. In this paper, isothermal diffusion is studied experimentally and numerically at different pressures and compositions in a system of two flasks connected by a vertical channel (Fig. 1a) [2].

For the study, two systems $CH_4$ (1) + Ar (2) – $N_2$ (3) and $CH_4$ (1) + R12 (2) – n-$C_4H_{10}$ (3) were chosen. A binary mixture of methane and argon (or methane and dichlorodifluoromethane) was located in the upper flask of the apparatus, and nitrogen (or n-butane) was in the lower one. Then, the channel connecting both flasks was opened. The mixing time was simultaneously recorded. At the end of the experiment, the channel was blocked and the gas mixture from each flask was analyzed on a chromatograph. The initial composition of the systems was chosen so that the density of the binary mixture at a given pressure interval did not exceed the density of nitrogen or n-butane. We will assume that the direction of the density gradient of the mixture in this case is negative ($\nabla\rho < 0$). The studied systems have one more feature. In the first mixture, the interdiffusion coefficients $D_{ij}$ [3] are approximately the same ($D_{12} \approx D_{13} \approx D_{23}$), and in the second the diffusion coefficients differ almost by three times ($D_{12} \approx D_{13} >> D_{23}$).

Experimental data for the systems 0.5504 $CH_4$ (1) + 0.4496 Ar (2) – $N_2$ (3) and 0.8366 $CH_4$ (1) + 0.1634 R12 (2) – n-$C_4H_{10}$ (3) are shown in Fig. 1b, c as the dependence of the parameter $\alpha$ on the experiment pressure. The parameter $\alpha = c_{exp}/c_{theor}$ was obtained by normalizing the experimental values of concentrations $c_{exp}$ to the calculated $c_{theor}$ from the Stefan-Maxwell equations [3] under the assumption of diffusion. For the mixture $CH_4$ (1) + Ar (2) – $N_2$ (3), the experimental values of the component concentrations within the experimental error agree with those calculated. The parameter $\alpha \approx 1$ is observed throughout the investigated pressures range. A completely different picture is observed in the system 0.62 $CH_4$ (1) + 0.38 R12 (2) – n-$C_4H_{10}$. As is seen in Fig. 1c the parameter α begins to significantly exceed unity at a certain pressure. A further increase in pressure leads to a sharp growth of the dimensionless parameter $\alpha$, which is atypical for diffusion. In this pressure range, the experimental values of concentrations $c_{iexp}$ significantly exceed the calculated values obtained under the assumption of ternary diffusion. Intensification of mass transfer is associated with the occurrence of convective mechanisms of components mixing caused by the instability of mechanical equilibrium of the gas mixture. The reason for the instability of mechanical equilibrium is the inversion of the density gradient, which arises from the difference in the diffusion coefficients.




a) b) c)

Figure 1. a) Diagram of the two-flask apparatus; b) Dependence of $\alpha$ on pressure. The line is the calculation on the assumption of diffusion. The points correspond to: 1 – methane, 2 – argon, 3 – nitrogen; c) The points correspond to: □ – freon; Δ – butane; ◊ – methane.

The observed convective mechanism is similar to the Rayleigh-Benard problem for an inhomogeneous temperature field and other manifestations of instability, where it is necessary to take into account the dependence of the medium properties on composition, temperature, and cross effects [4]. Therefore, the formalism of stability theory was used to determine the characteristic conditions defining the occurrence of convective flows under diffusion [4]. The transition parameters that determine the change in the "diffusion-convection" regimes can be obtained from the joint solution of the equations of continuum mechanics and the equation of medium state recorded for ternary systems. Linearizing the system of hydrodynamics equations with respect to small perturbations, we obtain a homogeneous system of linear differential equations with time-independent coefficients that have solutions of the type $exp\left(-i\omega t\right)$. If among those found $\omega = \omega_0 + i\omega_1$ there are those for which $\omega_1 > 0$, then the state will be unstable. The boundaries of change in the diffusion and convection regimes determined in terms of the Rayleigh numbers $Ra_i$ show that under certain conditions the mechanical equilibrium of the mixture can be unstable that causes the appearance of convection in the region $\nabla\rho < 0$, which was recorded experimentally. The isoconcentration distributions of components along the channel length and the mean velocity profile obtained by numerical modeling have a non-planar front, which indicates the presence of ascending and descending convective flows in the diffusion channel.

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REFERENCES

1. Dil'man, V.V., Lipatov, D.A., Lotkhov, V.A. and Kaminskii, V.A., 2005. "Instability in unsteady-state evaporation of binary solutions into an inert gas". *Theor. Found. Chem. Eng.* Vol. 39. No. 3. pp. 566 - 572.

2. Zhavrin, Yu. I., Kosov, V.N., Fedorenko, O.V. and Akzholova, A.A., 2016. "Some features of isothermal multicomponent mass transfer in the convective instability of gas mixture" *Theor. Found. Chem. Eng.* Vol. 50. No 2. pp. 171 - 177.

3. Bird, R.B., Stewart, W.E. and Lightfoot, E.N., 2007. *Transport Phenomena* (Revised Second ed.). John Wiley & Sons, New York.

4. Gershuni, G.Z. and Zhukhovitskii, E.M., 1976. *Convective Stability of Incompressible Fluids*, Keter, Jerusalem.