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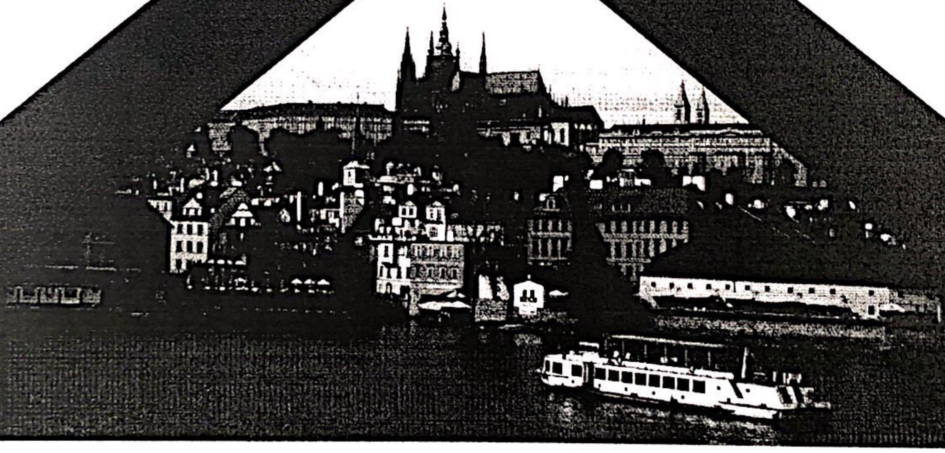

# PROGRAM

## Plenary Lectures Summaries
## 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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Thermokinetic parameter determination of RAFT polymerization reaction of methacrylate monomers using real-time reaction calorimetry. ***I. Lahoud, N. Brodu, I. Ben Talouba, L. Balland, N. Mouhab** (Univ. Rouen, FR) [1109]

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Production of butyl levulinate from fructose and butanol over thermostable acidic ion-exchange resins. **G. Gordillo, E. Ramírez, *R. Bringué, M. Iborra, F. Cunill, J. Tejero** (Univ. Barcelona, ES) [794]

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Regeneration of spent denitration catalyst by carbon reduction. ***T. Kato, Y. Sato, H. Okawa, K. Sugawara** (Akita Univ., JP) [1132]

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Gas-phase oxidation of piperidine with nitrous oxide to 2,3.4.5-tetrahidropyridine. **I. T. Nagieva, N. I. Ali-zadeh, *T. M. Nagiev[1]** (Inst. Catal. Inorg. Chem., Baku, AZ; [1]Baku State Univ., AZ) [451]

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Green and efficient Knoevenagel condensation of 1,3-thiazolidin-2,4-dione with aromatic aldehydes in choline-chloride/urea deep eutectic solvent. ***M. Molnar, M. Komar, M. Lončarić, V. Bušić** (Bestprojekt, Zagreb, HR) [1108]

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High-pressure calorimetry: measurement of thermophysical properties at pressures of up to 3000 bar. ***J. Nowotny, M. Busch** (Tech. Univ., Darmstadt, DE) [1042]

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Performance of caffeine removal by using different AOPs technologies. **X. W. Yu, F. Audino, J. M. Toro Santamaria[1], M. Graells, *M. Pérez-Moya** (Univ. Politéc. Cartagena , ES; [1]Frauenhofer Inst., Stuttgart, DE) [1103]

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Experimental investigation of the effect of pipe inclination on the hydrodynamic behaviour of slug flow using electrical capacitance tomography. **M. Abdulkadir, *N. Makwashi[1], D. Zhao[1], L. A. Abdulkareem[2]** (Sch. Eng. Eng. Technol., Minna, NG; [1]London South Bank Univ., UK; [2]Univ. Zakho, IR) [1088]

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Electroflocculation of green microalga Chlorella vulgaris. ***M. Zednikova, I. Branyikova, S. Lucakova[1], M. C. Ruzicka, T. Branyik[1]** (Inst. Chem. Proc. Fundam., Praha, CZ; [1]Univ. Chem. Technol. Prague, Praha, CZ) [1110]

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Scientific process simulation cluster. ***A. Fricke, M. Ul Mosaid, J. Schöneberger** (Chemstations Europe GmbH, Berlin, DE) [1022]

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Nucleation of $H_2SO_4$-$H_2O$ in laminar co-flow tube: CFD simulations and analytical modelling. ***T. Travnickova, J. Havlica[1], J. Hrubý[2], V. Ždímal** (Inst. Hydrodyn., Praha, CZ; [1]Purkinje Univ., Usti n/L, CZ; [2]Inst. Thermomech., Praha, CZ) [1067]

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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]

**P1.65**

Numerical simulation of metal ions sensing with nanofluidic diodes. ***C.-H. Lo, Y.-T. Chiou, L. H. Yeh** (Nat. Yunlin Univ. Sci. Technol., Yunlin, TW) [463]

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Weakly charged nanochannels can generate high nanofluidic salinity gradient power. ***Y.-T. Chiou, F. Chen, Y. S. Su, L. H. Yeh** (Nat. Yunlin Univ. Sci. Technol., Yunlin, TW) [490]

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Experimental and computational study of turbulent bed contactor hydrodynamics. ***A. Pourverdi, B. Hashemi Shahraki** (Petrol. Univ. Technol., Ahwaz, IR) [1001]

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IBM-DEM predicting of drag force for particles clusters in a riser. ***Y. Y. Wu, X. G. Shi, X. Y. Lan, J. S. Gao** (China Univ. Petrol., Beijing, CN) [324]

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Analysis of the evolution of bed expansion and correlation development in turbulent bed contactor. ***B. Bensebia, O. Bensebia[1], F. Bentahar[1], S. Kouadri Moustefai**

# About the possibility of the emergence of diffusion instability in isothermal mixing of multicomponent gas mixtures

V. N. Kossov, [1]O. Fedorenko, V. Mukamedenkyzy, [2]D. Zhakebayev
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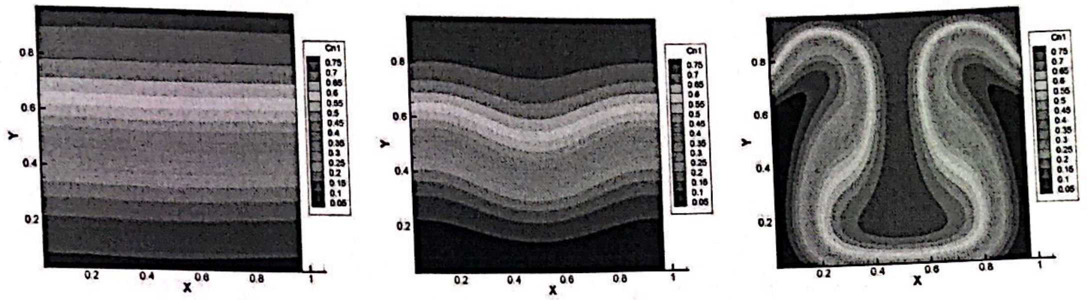
In multicomponent gas mixtures, there is a wide variety of mixing regimes. The molecular, convective, and most often the joint action of the listed regimes determine the intensity of mass transfer in them. In this case, the fact that the process of molecular diffusion can lead to instability of the mechanical equilibrium of the mixture with subsequent occurrence of natural convection is practically not taken into account [1]. Moreover, the emergence and development of concentration convection occurs not only within the framework of traditional representations of the Rayleigh thermal problems [2, 3], but also for situations in which motions arise with stable stratification of the mixture [4]. The experiments were recorded convective flow leading to the synergistic effect associated with a significant increase in the rate of mixing of system components. The paper presents a computational model for the study of mass transfer in three-component gas mixtures at different pressures over time at the boundary of the regime change "diffusion-concentration gravitational convection" in a vertical cylindrical channel of finite dimensions.

Numerical 2D-simulation of the process is based on the Navier-Stokes equation, the continuity equation and the equations of the concentration. We study the process when a binary mixture 0.8 Ar + 0.2 He, located at the top of a vertical cylindrical channel and the pure gas ($N_2$) - at the bottom, in which, provided the condition of the occurrence of instability. For physical quantities are specified the following boundary conditions: on all borders of the cylinder condition of solid wall $u_i\big|_{x_i=0,x_i=L_i} = 0, i = 1,2$, and for the concentration components we use boundary conditions $\partial C/\partial n\big|_{x_i=0,x_i=L_i} = 0, i = 1,2$.

For the numerical solution of the problem of gas motion in the cylinder area is used the splitting scheme by physical parameters:

$$
\begin{aligned}
&1.\quad \frac{\overline{u}^{*}-\overline{u}^{n}}{\tau} = -\overline{u}^{n}\nabla\overline{u}^{*} + \Delta\overline{u}^{*} + \tau_{11}Ra_1C_1 + Ra_2C_2,\\
&2.\quad \Delta p = \frac{\nabla\overline{u}^{*}}{\tau}, \qquad 3.\quad \frac{\overline{u}^{n+1}-\overline{u}^{*}}{\tau} = -\nabla p, \qquad\qquad (1)\\
&4.\quad \frac{\overline{C}_1^{n+1}-\overline{C}_1^{n}}{\tau} = -\left(\overline{u}^{n+1}\nabla\right)\overline{C}_1^{*} + \frac{1}{\mathrm{Pr}_{11}}\Delta\overline{C}_1^{*} + \frac{1}{\mathrm{Pr}_{12}}\Delta\overline{C}_2^{*},\\
&5.\quad \frac{\overline{C}_2^{n+1}-\overline{C}_2^{n}}{\tau} = -\left(\overline{u}^{n+1}\nabla\right)\overline{C}_2^{*} + \frac{1}{\mathrm{Pr}_{21}}\Delta\overline{C}_1^{*} + \frac{1}{\mathrm{Pr}_{22}}\Delta\overline{C}_2^{*}.
\end{aligned}
$$

At the first stage, the Navier-Stokes equation is solved without considering pressure. At the second stage, the Poisson equation obtained from the continuity equation with allowance for the velocity field of the first stage is solved. The obtained pressure field in the third stage is used to recalculate the final velocity field. The fourth stage is the concentration with the use of finite velocity fields.



a) b) c)

Figure 1. Dynamics of changes in concentration over time at different pressures in the system 0.8 Ar + 0.2 He – $N_2$ at $T = 298.0$ K and $t = 12.5$ s. a) $p = 0.3$ MPa; b) $p = 0.5$ MPa; c) $p = 1.5$ MPa.

The concentrations of the components calculated according to scheme (1) at different pressures and mixing times are shown in Fig. 1. For $p = 0.3$ MPa, diffusion is observed in the system. A similar picture in the distribution of concentrations is characteristic for any mixing times. Increasing the pressure to $p = 0.5$ MPa in the system, the nonlinearity in the concentration distribution is noted (Fig. 1b), which is the reason for the nonlinear distribution of the mixture density in the vertical cylindrical channel. In turn, the nonlinearity in the density distribution can lead to an instability of the mechanical equilibrium of the mixture. Later on, conditions arise in the system for the formation of convective structures, consisting mainly of the heaviest component in the density (Fig. 1c). Apparently this type of flow corresponds to the results of [1, 4].

Thus, numerical studies of the effect of pressure on diffusion mass transfer in systems with a significant difference in the diffusion coefficients have shown that non-linear isoconcentration distributions can arise in such mixtures. Unusual distribution of concentrations leads to a nonmonotonic density distribution in the channel, followed by the appearance of convective currents that significantly increase the mixing rate.

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