E. Hála Laboratory of Thermodynamics

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RESEARCH STAFF
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Part time: JAN JIRSÁK, IVO NEZBEDA, MILAN PŘEDOTA

PHD STUDENT
KAROLINA MACHANOVÁ, STANISLAV PAŘEZ

TECHNICAL STAFF
SVATOSLAVA BERNATOVÁ

Fields of research

- Experimental determination and modelling of phase equilibria in fluid and condensed systems, including systems containing ionic liquids and systems with chemical reaction
- State and phase behaviour of fluids at superambient conditions (up to very high pressures)
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Molecular simulations of chemically reacting systems in nanoporous materials
- Mesoscale simulations of polymeric/nanoparticle systems and of energetic and reactive materials
- Development of molecular theory of polar and associating compounds (and their mixtures)
- Development of equations of state based on molecular theory
- Development and application of density functional theory for inhomogeneous fluids
- Hydrophobic interactions
- Percolation and nucleation
- Application of statistical-mechanical models to real fluids
- Thermodynamic modelling and processing of thermodynamic data

Applied research

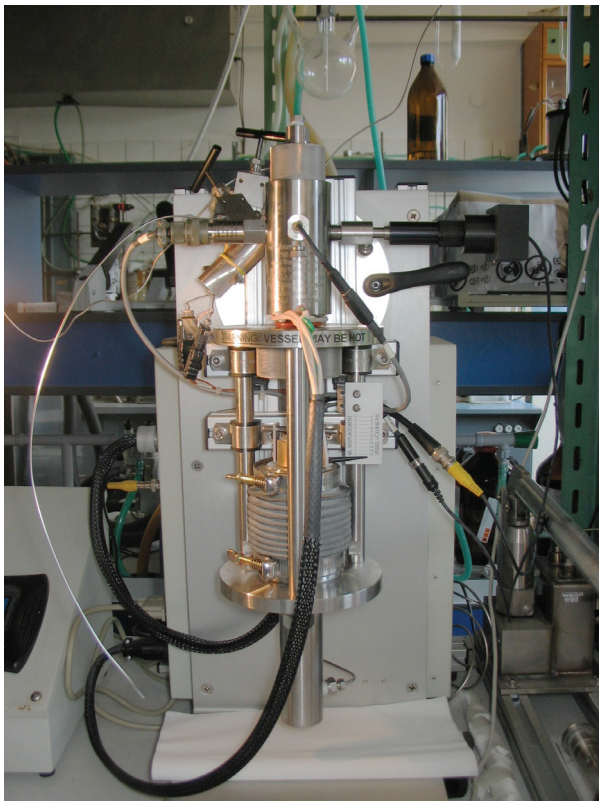
- Technology for preparation of molecularly imprinted polymeric materials

Research projects

Determination of the phase and state behaviour of fluids and fluid mixtures for processes at superambient conditions: molecular-based theory and experiment

(K. Aim, joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

Research was focused on application of results obtained in the framework of perturbation methods. The use is made of the finding that the inclusion of a short-range part of the total attractive interaction into a reference system allows a natural extension of the traditional first-order perturbation theory of simple fluids to practically all thermodynamic states. Research continued also on applications of the perturbation theory using a reference system based on the short-range part of intermolecular interactions to describe the thermodynamic behaviour of systems containing carbon dioxide + alkanols. Vapour pressures of a set of aliphatic alcohols were determined experimentally. The measurements of liquid-liquid equilibria in binary systems of 1-ethyl-3-methylimidazolium ethyl sulphate + C7 hydrocarbons were completed and the data obtained were successfully represented by polymer-solution models. [Refs. 1, 4-6, 8, 10, 15, 29, 32, 34, 38, 45, 51-54]



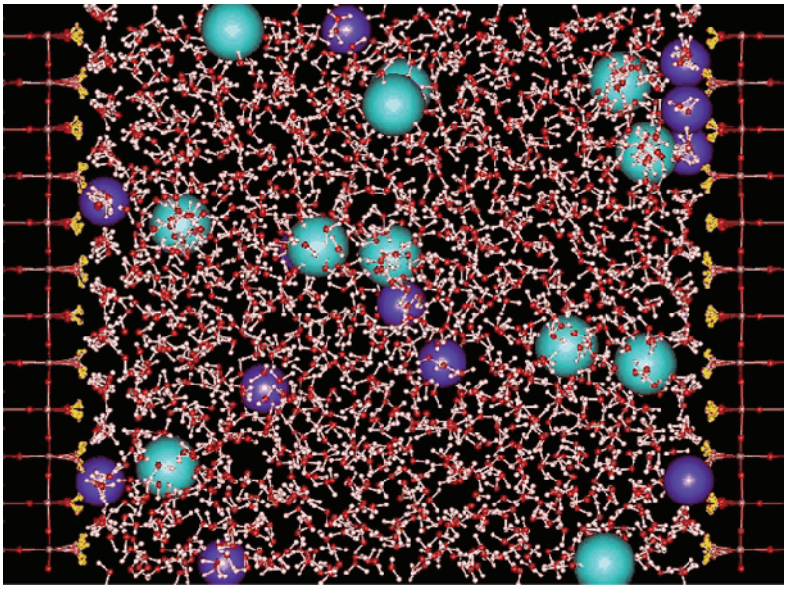
Variable-volume view cell (Super Phase Monitor SPM 20, Thar Technologies) for the determination of phase equilibria at high pressures

Computer modelling of structural, dynamical and transport properties of fluids in nanospace

(M. Lísal, joint project with University of South Bohemia in Ceske Budejovice, supported by GACR, grant No. GA203/08/0094)

Behaviour of fluids in the nanospace, solid-liquid interfaces (metal oxide-aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) is studied by equilibrium and nonequilibrium molecular simulations to provide structural, dynamical and

transport properties of fluids in nanoconfinement. At solid-liquid interfaces, the simulation results for dynamics of water molecules are linked with quasielastic neutron scattering; the space-dependent shear viscosity and the dielectric properties are linked with electrophoretic data. We are also developing a method for the determination of local, space-dependent permittivity in inhomogeneous systems. In the case of nanoporous carbons, we adopt the methods for calculating local, space-dependent diffusivity and shear viscosity of pure fluids to slit and cylindrical nanopores, develop a method for the determination of space-dependent shear viscosity of fluid mixtures from computer simulations, and simulate the structural, dynamical and transport properties of industrially important fluid mixtures in carbon nanopores. [Refs. 11, 18-20, 22, 23, 26, 28, 35, 39, 46, 47]



Ions-water system in nanoslit with TiO_2 walls

EFCE Working Party "Fluid Separations"

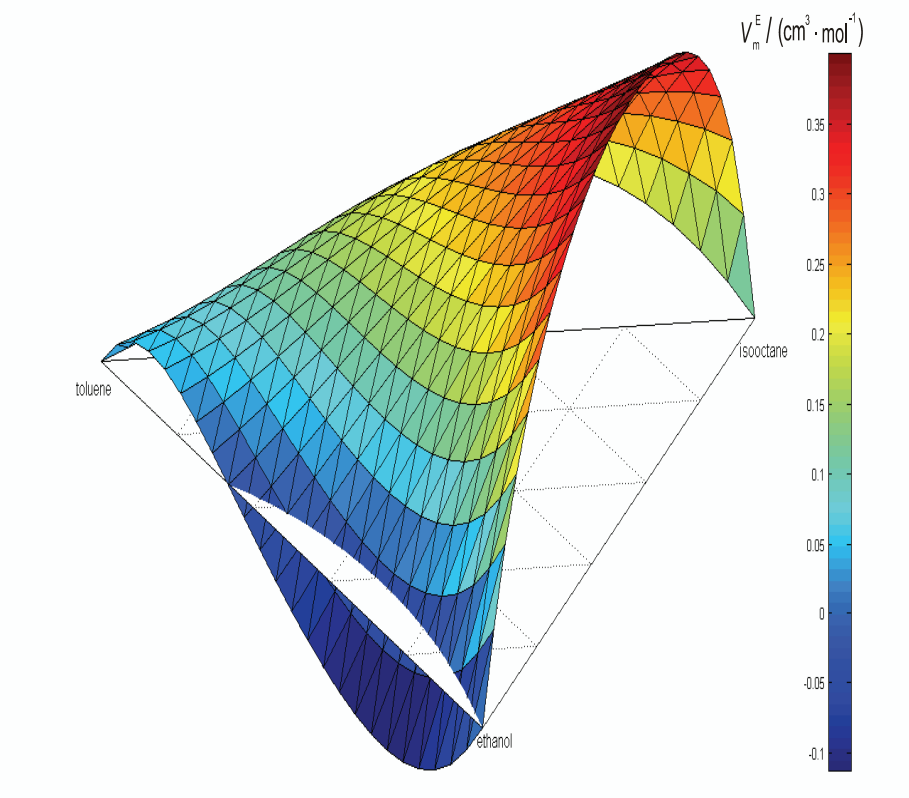
(M. Bendova, supported by MEYS, programme INGO project No. LA320)

Activities connected with membership of M. Bendova in EFCE Working Party on "Fluid separations". On behalf of M. Bendova, K. Machanova took part in the International Symposium on Solubility Phenomena in Leoben on July 25–30, 2010. [Ref. 31]

P-V-T behaviour of liquid mixtures constituting engine biofuels – experimental determination, correlation and prediction

(J. Linek, supported by GACR, grant No. GA104/09/0666)

Densities and sound velocities for binary systems composed of isooctane, toluene, and MTBE were measured at four temperatures within the range of 298.15 to 328.15 K at atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes. Volumetric properties of pyridine, 2-picoline, 3-picoline, and 4-picoline at temperatures from 298.15 K to 328.15 K and at pressures up to 40 MPa were experimentally determined. Volumetric behaviour of ternary liquid system composed of ethanol, isooctane, and toluene at temperatures from 298.15 K to 328.15 K was also measured and correlated to determine the necessary number of ternary constants to fit the experimental data within experimental errors. [Refs. 13, 14, 41, 42]



Excess molar volumes (V^E_m) plotted against mole fraction of components (ethanol/isooctane/toluene) at T = 298.15 K and atmospheric pressure

Simple and complex models of aqueous solutions: The effect of nonadditive interactions

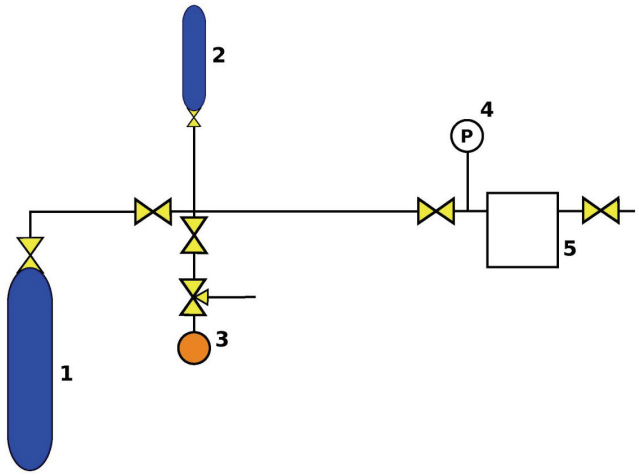
(I. Nezbeda, supported by ASCR, grant No. IAA400720802)

The multi-particle move Monte Carlo (MPM-MC) method developed in 2008 has been further extended and fully reviewed. An analysis of the behaviour of metastable water was carried out with two contradicting results, one from molecular simulations and the other from available equations of state. Exact expressions for the description of interaction of fluids at solid surface of variable curvature have been derived. [Refs. 7, 12, 15, 16, 21, 24, 25, 36, 37, 43, 44]

High-pressure phase equilibrium and p-V-T behaviour

(Z. Sedláková, supported by GACR, grant No. GP203/09/P141)

A new apparatus for measurement of high-pressure phase equilibria by synthetic method was assembled, based on Thar Technologies Super Phase Monitor. Accuracy of the apparatus was first checked by measuring the solubilities of supercritical CO_2 in ethanol, butanol, and 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl] imide ([EMIM][TFSI]). New ternary high-pressure data have been obtained for system CO_2 + 1-butanol + [EMIM][TFSI]. For easy recyclability of ionic liquids, binary systems of amines and ionic liquids are investigated for use in carbon dioxide capture; solid-liquid and liquid-liquid equilibria in system diethylamine + [EMIM][TFSI] have therefore been studied. Experimental data were correlated by using the Redlich-Kister equation and compared with calculated ideal solubilities. Density and viscosity of ammonium-based ionic liquid were determined. [Refs. 14, 30, 31, 40-42, 48-50]

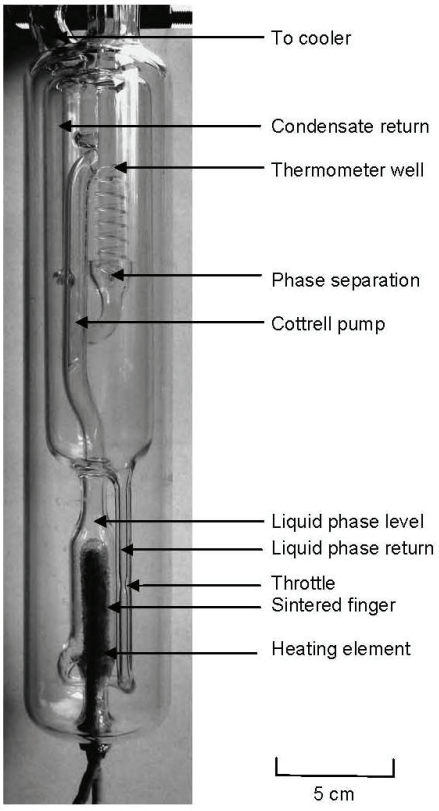


Assembly for the measurement of high-pressure phase equilibria: 1 - gas cylinder, 2 - CO_2 reservoir, 3 - vacuum pump, 4 - external pressure gauge, 5 - Super Phase Monitor SPM 20

Phase equilibria for the design of energy efficient separation processes

(I. Wichterle, supported by ICPF)

Vapour–liquid equilibrium data have been measured in binary and ternary systems of compounds with selected functional groups. New microebulliometer for total pressure measurement was developed, tested and used to measure the component activities in mixtures of polymers with organic solvents. A collection of data on miscibility and phase behaviour of binary polymer blends based on styrene, 2,6-dimethyl-1,4-phenylene oxide and their derivatives was published. [Refs. 2, 3, 9, 17, 27, 33]



New microebulliometer for total pressure measurement

International co-operations

INA, Research and Development, Zagreb, Croatia: Properties of polymer solutions
Institute of Condensed Matter, Ukrainian Academy of Sciences, Lviv, Ukraine: Modelling of molecular fluids at extreme conditions: Theory and applications
Institute of Physical Chemistry Ilie Murgilescu, Romanian Academy of Sciences, Bucharest, Romania: Phase properties of systems containing ionic liquids
Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems
Pennsylvania State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behaviour of model proteins on surface
Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid-liquid phase equilibria in systems of ionic liquids
Technical University of Vienna, Austria: Colloids and theory of fluids
Université François Rabelais, Tours, France: Liquid-liquid phase equilibria in systems of ionic liquids
University of Ljubljana, Ljubljana, Slovenia: Water and hydration of nonpolar and ionic solutes
University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids
U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale simulations of energetic and reactive materials

Visits abroad

M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)
M. Lísal: Pennsylvania State University, State College, PA, USA (1 month)
K. Machanová: Laboratoire PCMB, Université François Rabelais, Tours, France (2 weeks)
A. Malijevský: Imperial College, London, UK (3 months)
Z. Sedláková: Laboratoire PCMB, Université François Rabelais, Tours, France (2 weeks)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

D. Gheorghe Chiscan, Institute of Physical Chemistry Ilie Murgilescu, Romanian Academy of Sciences, Bucharest Romania
J. Jacquemin, Laboratoire PCMB, Université François Rabelais, Tours, France
D. Lemordant, Laboratoire PCMB, Université François Rabelais, Tours, France
R. Melnyk, Institute of Condensed Matter Physics, Lviv, Ukraine
A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine
V. Vlachy, University of Ljubljana, Ljubljana, Slovenia

Teaching

K. Aim: ICT, Faculty of Chemical Engineering, postgraduate courses "Experimental methods of determination of phase equilibria in fluid systems" and "Applied statistical analysis and processing of data"

M. Bendová: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
J. Jirsák: UJEP, Faculty of Science, courses "Physical Chemistry Seminar", "Essential of programming languages"
M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"
M. Lísal: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
M. Lísal: UJEP, Faculty of Science, courses "Parallel programming", "Numerical Mathematics I" and "Numerical Mathematics II"; tutorials "Molecular Simulations I"
I. Nezbeda: UJEP, Faculty of Science, courses "Molecular simulations I", "Principles of Scientific Communication" and "Statistical Physics"
I. Nezbeda, K. Aim: ICT, Faculty of Chemical Engineering, postgraduate course "Applied statistical thermodynamics of fluid systems"
M. Předota: University of South Bohemia, Ceske Budejovice, courses "Lectures from physics oriented to particle and nuclear physics" and "Selected lectures from physics"

Publications

Original papers

[1] Ahlström P., Aim K., Dohrn R., Elliott J.R., Jackson G., Jaubert J.-N., Macedo E.A., Pokki J.-P., Reczey K., Victorov A., Fele-Žilnik L., Economou I.G.: A Survey of the Role of Thermodynamics and Transport Properties in ChE University Education in Europe and the USA. Chem. Eng. Edu. 44(1), 35-43 (2010).
[2] Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapor-Liquid Equilibria in the Two Binary and the Ternary Systems Composed of tert-Amyl Methyl Ether, tert-Butanol and Isooctane. J. Chem. Eng. Data 56(4), 783-788 (2011).
[3] Bogdanić G., Wichterle I.: Vapor–Liquid Equilibrium in Diluted Polymer + Solvent Systems. J. Chem. Eng. Data 56(4), 1080-1083 (2011).
[4] Čenský M., Roháč V., Růžička K., Fulem M., Aim K.: Vapor Pressure of Selected Aliphatic Alcohols by Ebulliometry. Part 1. Fluid Phase Equilib. 298(2), 192-198 (2010).
[5] Černá I., Klusoň P., Bendová M., Floriš T., Pelantová H., Pekárek T.: Intensification of the use of ionic liquids as efficient reaction co-solvents in asymmetric hydrogenations. Chem. Eng. Process. 50(3), 264-272 (2011).
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[7] Jirsák J., Nezbeda I.: A Note on Scenarios of Metastable Water. Collect. Czech. Chem. Commun. 75(5), 593-605 (2010).
[8] Krejčí J., Nezbeda I., Melnyk R., Trokhymchuk A.: EXP6 Fluids at Extreme Conditions Modeled by Two-Yukawa Potentials. J. Chem. Phys. 133(9), 094503-1 -8 (2010).
[9] Kuzmić A.E., Bogdanić G., Wichterle I.: Znanstveni projekt "Nova tehnologija dobivanja molekulski tiskanih polimernih materijala". (Cro) . Kem. Ind. 59(10), 499-502 (2010).
[10] Malijevský A.: Microscopic Density Functional Theory for Dendrimers. Phys. Rev. E 80(4), 042801-1-4 (2009).
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[14] Morávková L., Wagner Z., Sedláková Z., Linek J.: Volumetric Behaviour of the Ternary Liquid System Composed of Methyl tert-Butyl Ether, Toluene, and Isooctane at Temperatures from (298.15 to 328.15) K. Experimental Data and Correlation. J. Chem. Thermodyn. 42(7), 920-925 (2010).
[15] Moučka F., Nezbeda I.: The multi-particle sampling method in Monte Carlo simulations on fluids and its efficient implementations. Mol. Simul., 36(7-8), 526-534 (2010).
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[21] Předota M., Nezbeda I., Pařez S.: Coarse-Grained Potential for Interaction with a Spherical Colloidal Particle and Planar Wall. Collect. Czech. Chem. Commun. 75(5), 527–545 (2010).
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[26] Setničková K., Wagner Z., Noble R., Uchytil P.: Semi-Empirical Model of Toluene Transport in Polyethylene Membrane Based on the Data of New Type of Apparatus for Gas Permeability, Diffusivity and Solubility Grant. Eur. Polym. J., submitted.

Books and monographs

[27] Bogdanić G., Wichterle I., Erceg Kuzmić A.: Collection of Miscibility Data and Phase Behavior of Binary Polymer Blends Based on Styrene, 2,6-Dimethyl-1,4-Phenylene Oxide and of Their Derivatives. 124pp., Research Signpost, Trivandrum 2010.

Chapters in books

[28] Chennamsetty N., Bock H., Lísal M., Brennan J.K.: Chapter 2: An Introduction to Coarse-Graining Approaches: Linking Atomistic and Mesoscales. In: Molecular Systems Engineering. (Pistikopoulos, E. - Georgiadis,M. - Dua, V., Ed.), pp. 43-84, Wiley-VCH Verlag, Weinheim 2010.

International conferences

[29] Aim K., Wichterle I.: Two-Phase Reactive Systems: Transesterification and Esterification Reactions Coupled with Vapour-Liquid Equilibria in Quaternary Systems. 20th International Conference on Properties and Phase Equilibria for Product and Process Design PPEPPD 2010, Book of Abstracts, p. 210, Suzhou, China, 16-21 May 2010.
[30] Bendová M., Sedláková Z., Aim K., Klusoň P., Černá I.: Liquid-Liquid Equilibrium in Ternary System 1-Butyl-3-Methylimidazolium Hexafluorophosphate + 1-Chlorobutane + 1-Methylimidazole. EUCHEM Conference on Molten Salts and Ionic Liquids 2010, Book of Abstracts, p. 318 (LMP 22), Bamberg, Germany, 14-19 March 2010.
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[37] Jirsák J., Škvor J., Smith W.R., Nezbeda I.: Molecular-Level Simulation of Electrolyte System Solubility and Chemical Speciation. International Workshop "Molecular Modeling and Simulation for Industrial Applications", Book of Abstracts, p. P 13, Würzburg, Germany, 22-23 March 2010.
[38] Lísal M., Předota M., Aim K.: Chemical Reaction Equilibrium and Space-Dependent Self-Diffusion for Dimerization Reactions in Carbon-like Slit and Cylindrical Nanopores: Insight from Molecular-Level Simulations. 20th International Conference on Properties and Phase Equilibria for Product and Process Design PPEPPD 2010, Book of Abstracts , p. 110, Suzhou, China, 16-21 May 2010.
[39] Lísal M., Předota M., Aim K.: Molecular Simulations of Chemical Reaction Equilibrium and Space-Dependent Self-Diffusion of Dimerization Reactions in Carbon-like Slit and Cylindrical Nanopores. 19th International Congress of Chemical and Process Engineering CHISA 2010 and 7th European Congress of Chemical Engineering ECCE-7, Summaries 2, p. 623 (2 pp. full text on CD-ROM), Prague, Czech Republic, 28 August - 1 September 2010.
[40] Machanová M., Bendová M., Sedláková Z., Wagner Z., Aim K.: Solubility of Ionic Liquids in Binary Systems with Water and Pseudobinary Systems with Solution Methanol/Water (1:1 Proportion of Weight). 19th International Congress of Chemical and Process Engineering CHISA 2010 and 7th European Congress of Chemical Engineering ECCE-7, Summaries 2, p. 668, Prague, Czech Republic, 28 August - 1 September 2010.
[41] Morávková L., Wagner Z., Sedláková Z., Linek J.: Volumetric Properties of Ternary Liquid System Composed of Methyl tert-Butyl Ether, Toluene, and Isooctane at Temperatures from 298.15 K to 328.15 K. Experimental Data and Their Correlation. 19th International Congress of Chemical and Process Engineering CHISA 2010 and 7th European Congress of Chemical Engineering ECCE-7, Summaries 2, p. 673, Prague, Czech Republic, 28 August - 1 September 2010.
[42] Morávková L., Wagner Z., Sedláková Z., Linek J.: Volumetric Behaviour of Ternary Liquid System Composed of Methyl tert-Butyl Ether, Toluene, and Isooctane at Temperatures from 298.15 K to 328.15 K. Experimental Data and Correlation. 37th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 66 (11 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 24-28 May 2010.
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[45] Nold A., Pereira A., Malijevský A., Kalliadasis S.: Statistical Mechanics of a Thin Film on a Solid Substrate. Euromech Fluid Mechanics Conference EMFC - 8, Abstracts, p. S8-22, Bad Reichenhall, Germany, 13-16 September 2010.
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Slovak Society of Chemical Engineering, Proceedings, p. 171, Tatranské Matliare, Slovakia, 24-28 May 2010.

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[48] Sedláková Z., Bendová M, Wagner Z., Aim K.: High-Pressure Measurements in Binary System Containing Supercritical CO_2 and 1-Butanol. 19th International Congress of Chemical and Process Engineering CHISA 2010 and 7th European Congress of Chemical Engineering ECCE-7, Summaries 2, p. 650 (5 pp. full text on CD-ROM), Prague, Czech Republic, 28 August - 1 September 2010.

[49] Sedláková Z., Bendová M., Wagner Z., Aim K.: Supercritical CO_2 Solubility in Ethanol, 1-Butanol, and [EMIM][NTf_2]. 14th International Symposium on Solubility Phenomena ISSP 2010, Abstract Volume, p. 66, Leoben, Austria, 25-30 July 2010.

[50] Sedláková Z., Rotrekl J., Bendová M., Vrbka P., Morávková L., Aim K.: Solid - Liquid Equilibrium in Binary System N,N-diethylamine + Ionic Liquid. 37th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 72, Tatranské Matliare, Slovakia, 24-28 May 2010.

[51] Setničková K., Wagner Z., Noble R., Uchytil P.: Toluene Transport Model Based on Data from New Type of Permeation Apparatus. International Conference on Inorganic Membranes (ICIM11), Book of Abstracts, pp. 1-2, Washington, DC, USA, 17-22 July 2010.

[52] Zíková N., Wagner Z., Schwarz J., Smolík J., Ždímal V.: One-year SMPS Measurements at Background Station Košetice - Basic Statistics. International Aerosol Conference IAC 2010, Registration Handbook, P3LP12, Helsinki, Finland, 29 August - 3 September 2010.

[53] Zíková N., Wagner Z., Schwarz J., Smolík J., Ždímal V.: Diurnal Cycles of Aerosol Particle Number Size Distributions in Relation to Meteorology and Gaseous Pollutants. EUCAARI Annual Meeting 2010, Presentation Abstracts, Helsinki, Finland, 22-26 November 2010.

[54] Zíková N., Wagner Z., Schwarz J., Smolík J., Ždímal V.: Rozdělení velikosti aerosolových částic na stanici Košetice - základní statistika roční řady měření spektrometrem SMPS. (Czech) Aerosol Number Size Distribution in Košetice Observatory – Basic Statistic of One-Year SMPS Measurement . XI. Konference České aerosolové společnosti, Sborník konference, pp. 29-30, Praha, Czech Republic, 18-19 November 2010.