E. Hála Laboratory of Thermodynamics

HEAD
KAREL AIM

DEPUTY
MARTIN LÍSAL

RESEARCH STAFF
MAGDALENA BENDOVÁ, GROZDANA BOGDANIĆ, JAN LINEK, ALEXANDR MALIJEVSKÝ, LENKA MORÁVKOVÁ, JAN PAVLÍČEK, ZUZANA SEDLÁKOVÁ, LUKÁŠ VLČEK, ZDENĚK WAGNER, IVAN WICHTERLE
Part time: JAN JIRSÁK, IVO NEZBEDA, MILAN PŘEDOTA

PHD STUDENT
KAROLINA MACHANOVÁ, STANISLAV PAŘEZ

TECHNICAL STAFF
ADÉLA ANDRESOVÁ, SVATOSLAVA BERNATOVÁ

Fields of research

- Experimental determination and modeling of phase equilibria in fluid and condensed systems, including systems containing ionic liquids, polymers, 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 modeling and processing of thermodynamic data

Applied research

- Technology for the 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, kaim@icpf.cas.cz; joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

The research continued on applications of results obtained in the framework of perturbation methods. Further use was 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. A feasibility study on the use of non-Lorentz-Berthelot combining rules for water-methanol mixtures has been performed. New applications of DFT (density functional theory), in particular for studying the behavior of model colloidal fluids and phenomena at the gas-liquid interface on curved substrates, have been developed. Thermophysical properties of alkylammonium-based ionic liquids were experimentally studied over a range of conditions. [Refs. 1, 6, 7, 10, 11, 16, 18-20, 39]

Thermodynamic properties of mixtures of ionic liquids and molecular solvents for use in two-phase catalysis

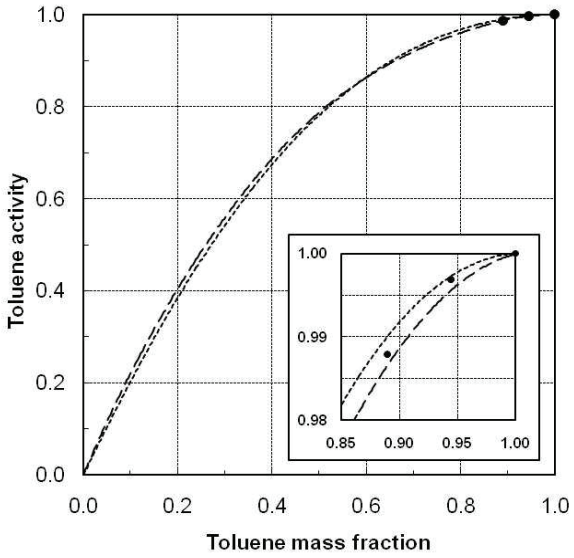
(M. Bendová, bendova@icpf.cas.cz; joint project with Institute of Microbiology of the ASCR; Zentiva Group, a.s., Prague; supported by MEYS, project No. MEB021009)

Noyori-type Ru-BINAP catalytic complexes may be used to a great advantage in syntheses of highly pure optically active compounds. Pseudo-immobilization of the catalyst by means of ionic liquid provides good contact between the catalyst and substrates. However, the contamination of ionic liquid by trace amounts of impurities may negatively affect the catalytic activity of the complex. The work is therefore aimed at optimizing the process of ionic liquids purification and their subsequent use in model asymmetric hydrogenation of methyl-3-oxobutanoate to methyl-3-hydroxyoxobutanoate in a reversibly biphasic mixture of ethanol / 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6]. Phase behaviour of mixtures [bmim][PF_6] with the precursors 1-chlorobutane and 1-methylimidazole as well as the efficiency of the individual purification steps were determined. [Refs. 5, 34]

Phase equilibria in the polymer-solvent systems for the design of energy-efficient separation processes

(G. Bogdanić, bogdanic@icpf.cas.cz; joint project with INA, Research and Development, Zagreb, Croatia; supported by ICPF)

Isothermal vapour–liquid equilibrium data were determined for polymer + toluene systems. Due to their importance as flow improvers for crude oil, the polymers studied were copolymers and terpolymers of octadecyl acrylate, acrylic acid, 1-vinyl-2-pyrrolidone, and styrene. Two group-contribution models (the Entropic-FV activity coefficient model, and the GC-Flory EOS) were used to predict the phase behaviour of the systems. Very good agreement with experimental data was achieved, as illustrated in the graph for poly($ODA_{0.79}$–$AA_{0.11}$–$VP_{0.10}$) terpolymer solution. Also, a new method for the estimation of porous structure parameters of crosslinked macroporous copolymers was developed. The method enables the estimation of specific pore volumes of poly(GMA-co-EGDMA) copolymers within experimental errors. Preliminary results for quick determination of liquid–liquid equilibrium in polymer solutions by the turbidimetric method were obtained for the polystyrene–methyl-cyclohexane system. [Refs. 4, 27, 29, 30, 32, 33]



Activity of toluene in poly(ODA$_{0.79}$–AA$_{0.11}$–VP$_{0.10}$) at 353.15 K; • experimental data; (- - -) prediction by the Entropic-FV model; (– – –) prediction by the GC-Flory model

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

(J. Linek, linek@icpf.cas.cz; supported by GACR, grant No. 104/09/0666)

The density and speed of sound in ethanol + isooctane, ethanol + toluene, and ethanol + isooctane + toluene systems were measured by Anton Paar instrumentation at four temperatures over the range from 298.15 to 328.15 K and the respective values of excess volumes V_m^E and adiabatic compressibility κ_S were calculated. The V_m^E and κ_S values for the binary systems were fitted to Redlich-Kister equation. The respective ternary data together with corresponding binary data were then fitted to the modified Redlich–Kister equation considering various numbers of ternary model parameters. It was found that even for the systems containing self-associating alcohol, only one ternary parameter is sufficient to describe well the ternary system. [Refs. 14, 36, 37, 38, 41, 42, 43]

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

(M. Lísal, lisal@icpf.cas.cz; joint project with University of South Bohemia in České Budějovice; supported by GACR, grant No. 203/08/0094)

Behavior of fluids in the nanospace, solid-liquid interfaces (metal oxide - aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) was further 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 were 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. Numerical integration schemes based upon the Shardlow-splitting algorithm were presented for dissipative particle dynamics approaches at various fixed conditions. [Refs. 9, 12, 15, 21, 40, 47, 51, 52]

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

(I. Nezbeda, IvoNez@icpf.cas.cz; supported by ASCR, grant No. IAA400720802)

In 2011 a brand new and fundamental result has been obtained: It was shown that by introducing non-additive repulsive interactions it is possible to extend the excluded volume concept to systems with association, i.e. to systems whose behavior has not yet been fully understood and explained. It was shown that the augmented van der Waals equation of state based on a Yukawa reference provides better results than the SAFT-VR (statistical associating fluid theory for potentials of variable attractive range) equation of state. An invited perspective-review on the modeling of water, which also contains new results for the Henry's law constant and its anomaly, was published. Finally, the scope of the research has been extended by studies on cluster formation and its relation to Fisher-Widom lines. [Refs. 8, 10, 11, 13, 17, 18, 23, 25, 35, 44-46]

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

(Z. Sedláková, sedlakova@icpf.cas.cz; supported by GACR, grant No. 203/09/P141)

New experimental high-pressure binary and ternary data on phase equilibria and phase behaviour of systems containing hydrocarbons, carbon dioxide and ionic liquid were determined by Anton Paar densitometry and by Thar Technologies Super Phase Monitor SPM 20 apparatus. Binary data were compared both to the previously measured data by another verified apparatus in our laboratory and to the literature data. Both comparisons demonstrated good agreement within the experimental errors. High-pressure data of binary systems containing carbon dioxide and ionic liquid of imidazolium type with bistriflate anion were correlated by the Soave-Redlich-Kwong equation of state. Solid-liquid and liquid-liquid equilibria in system organic solvent + [emim][NTf_2] have also been studied. [Refs. 14, 36-38, 42, 43, 48, 49]

Phase equilibria for the design of energy-efficient separation processes (measurement and data processing)

(I. Wichterle, wichterle@icpf.cas.cz; supported by ICPF)

Isothermal vapour−liquid equilibrium (VLE) data were measured in binary and ternary systems containing alcohol, hydrocarbon and (ether or ketone), namely: *tert*-butanol, 2-propanol, isooctane, *tert*-amyl methyl ether, 4-methyl-2-pentanone or 2,4-dimethyl-3-pentanone. The binary VLE data were correlated using the Wilson and NRTL (nonrandom two-liquid) equations by means of a new algorithm and resulting parameters were used for the calculation of phase behavior in the ternary system and for subsequent comparison with experimental data. [Refs. 2, 3, 22, 28, 31]

All glass recirculation still for VLE measurement

International co-operations

INA, Research and Development, Zagreb, Croatia: Novel technology of molecularly imprinted polymeric materials preparation

Institute of Condensed Matter, Ukrainian Academy of Sciences, Lviv, Ukraine: Modeling of molecular fluids at extreme conditions: Theory and applications

Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, 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

A. Andresová: Université François Rabelais, Tours, France, and Institut de Chimie du CNRS, Clermont-Ferrand, France (2 weeks)
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: Université François Rabelais, Tours, France, and and Institut de Chimie du CNRS, Clermont-Ferrand, France (2 weeks)
A. Malijevský: Imperial College, London, UK (2 months)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

D. Gheorghe Chiscan, Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, Romania
T. Abdallah, Laboratoire PCMB, Université François Rabelais, Tours, France
B. Montigny, 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 course “Experimental methods of determination of phase equilibria in fluid systems”
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, České Budějovice, courses “Lectures from physics oriented to particle and nuclear physics” and “Selected lectures from physics”
Z. Sedláková: UJEP, Faculty of Science, course “Chemical analysis”

Publications

Original papers

[1] Archer J.A., Malijevský A.: On the Interplay between Sedimentation and Phase Separation Phenomena in Two-Dimensional Colloidal Fluids. *Mol. Phys.* 109(7-10, SI), 1087-1099 (2011).

[2] Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2,2,4-Trimethylpentane, 2-Methyl-1-Propanol, and 4-Methyl-2-Pentanone. *Fluid Phase Equilib.* 307(1), 66-71 (2011).

[3] 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).

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[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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[9] Kolafa J., Lísal M.: Time-Reversible Velocity Predictors for Verlet Integration with Velocity-Dependent Right-Hand Side. *J. Chem. Theory Comput*. 7(11), 3596-3607 (2011).

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[11] Krejčí J., Nezbeda I., Melnyk R., Trokhymchuk A.: Mean-Spherical Approximation for the Lennard-Jones-like Two Yukawa Model: Comparison against Monte Carlo Data. *Condens. Matter Phys*. 14(3), 33005 (2011).

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[13] Melnyk R., Nezbeda I., Trokhymchuk A.: Vapour/Liquid Coexistence in Long-Range Yukawa Fluids Determined by Means of an Augmented van der Waals Approach. *Mol. Phys*. 109(1, Sp.I:Sl), 113-121 (2011).

[14] Morávková L., Wagner Z., Sedláková Z., Linek J.: Volumetric Behaviour of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from (298.15 to 328.15) K. Experimental Data and Correlation. *J. Chem. Thermodyn*. 43(12), 1906-1916 (2011).

[15] Moučka F., Lísal M., Škvor J., Jirsák J., Nezbeda I., Smith W.R.: Molecular Simulation of Aqueous Electrolyte Solubility. 2. Osmotic Ensemble Monte Carlo Methodology for Free Energy and Solubility Calculations and Application to NaCl. *J. Phys. Chem. B* 115(24), 7849–7861 (2011).

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[17] Nezbeda I., Jirsák J.: Water and Aqueous Solutions: Simple Non-Speculative Model Approach. *Phys. Chem. Chem. Phys.* 13(44), 19689-19703 (2011).

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[25] Škvor J., Nezbeda I.: Percolation Line and Response Functions in Simple Supercritical Fluids. *Mol. Phys*. 109(1, Sp.I:Sl), 133-139 (2011).

[26] Ždímal V., Smolík J., Eleftheriadis K., Wagner Z., Housiadas Ch., Mihalopoulos N., Mikuška P., Večeřa Z., Kopanakis I., Lazaridis M,.: Dynamics of Atmospheric Aerosol Number Size Distributions in the Eastern Mediterranean During the "SUB-AERO" Project. *Water Air Soil Pollut.* 214(1-4), 133-146 (2011).

International conferences

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[28] Bernatová S., Pavlíček J., Wichterle I.: Vapour–Liquid Equilibria in Alcohol + Hydrocarbon + Ketone Systems. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, p. 303, Saint Petersburg, Russia, 24-27 June 2011.

[29] Bogdanić G., Jovanović S. M.: Estimation of the Porous Structure Parameters of the Crosslinked Macroporous Copolymers Based on Methacrylates. 36th International Invention Show (bronze medal awarded), Katalog, p. 127, Zagreb, Croatia, 09-12 November 2011.

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[33] Bogdanić G., Wichterle I.: Vapor–Liquid Equilibrium in Diluted Polymer + Toluene Systems. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 5 pp. full text on CD-ROM, p. 149 (V22), Srní, Šumava, Czech Republic, 24-27 October 2011.

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[35] Jirsák J., Nezbeda I.: Towards a Molecular Theory of Hydrophobic Hydration: Hard Spheres in Primitive Water. 8th Liquid Matter Conference, Poster Abstracts p. 34 (P2.34), Wien, Austria, 06-10 September 2011.

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[37] Linek J., Morávková L., Wagner Z., Sedláková Z.: Volumetric Properties of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from 298.15 K to 328.15 K. Thermodynamics 2011, Book of Abstracts, pp. 205-206, Athens, Greece, 31 August - 03 September 2011.

[38] Linek J., Morávková L., Wagner Z., Sedláková Z.: Volumetric Properties of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from 298.15 K to 328.15 K. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 221 (pp.1159 -1170 full text on CD-ROM), Tatranské Matliare, Slovakia, 23-27 May 2011.

[39] Machanová K., Sedláková Z., Boisset A., Bendová M., Jacquemin J., Aim K.: Thermophysical Properties of Alkylammonium-Based Ionic Liquids. 19th European Conference on Thermophysical Properties, Book of Abstracts, p. 230, Thessaloniki, Greece, 28 August - 01 September 2011.

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[41] Morávková L., Wagner Z., Linek J.: Volumetric Properties of Pyridine, 2-Picoline, 3-Picoline, and 4-Picoline at Temperatures Up to 328.15 K and at Pressures Up to 40 MPa. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 63 (pp. 301-307 full text on CD-ROM), Tatranské Matliare, Slovakia, 23-27 May 2011.

[42] Morávková L., Wagner Z., Sedláková Z., Aim K.: Measurement of Excess Volumes of Ternary Systems. 36th International Invention Show (silver medal awarded), Katalog, p. 132, Zagreb, Croatia, 09-12 November 2011.

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[44] Nezbeda I.: Generalized excluded volume: Its origin and effects. 36th Conference of the Middle European Cooperation in Statistical Physics MECO 36, Lviv, Ukraine, 05-07 April 2011.

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[48] Sedláková Z., Rotrekl J., Bendová M., Vrbka P., Aim K.: Measurement of Solid–Liquid and Liquid–Liquid Equilibria in Organic System Containing Ionic Liquid [emim][NTf_2]. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 387-388, Saint Petersburg, Russia, 24-27 June 2011.

[49] Sedláková Z., Wagner Z., Aim K.: High-Pressure Phase Equilibria in Systems Containing CO_2 and Ionic Liquids. 36th International Invention Show (bronze medal awarded), Katalog, 10, p. 131, Zagreb, Croatia, 09-12 November 2011.

[50] Setničková K., Wagner Z., Noble R.D., Uchytil P.: Model transportu toluenu polyethylenovou membránou založený na datech aparatury nového typu. (Czech) Semi-Empirical Model of Toluene Transport in Polyethylene Membrane Based on the Data of New Type of Apparatus for Gas Permeability,

Diffusivity and Solubility. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 39 (A2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[51] Smith W.R., Moučka F., Lísal M.: A Molecular Based Osmotic Ensemble Monte Carlo Simulation Method for Free Energy Solvation Curves and the Direct Calculation of Aqueous Electrolyte Solubility. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, p. 27, Saint Petersburg, Russia, 24-27 June 2011.

[52] Trejos V.M., Lísal M., Nezbeda I., Smith W.R., Figueroa-Gerstenmaier S.: Thermodynamic Properties at Fixed Enthalpy for Alternative Refrigerants by Molecular Simulations. Thermodynamics 2011, Book of Abstracts, pp. 480-482, Athens, Greece, 31 August - 03 September 2011.

[53] Wagner Z., Fridrich M., Schwarz J., Ždímal V., Váňa M.: Measurement and Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol. 36th International Invention Show (gold medal awarded), Katalog, p. 130, Zagreb, Croatia, 09-12 November 2011.

[54] Wagner Z., Fridrich M., Schwarz J., Ždímal V.: Zpracování hromadných dat distribuce velikosti aerosolových částic v reálném čase a jejich prezentace v evropských i celosvětových databázích. (Czech) Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol and Their Presentation in International Databases. TeXperience 2011 (4.ročník) a Stakan 2011 (6.ročník), Kniha abstraktů dvoukonference, pp. 33-34, Železná Ruda, Czech Republic, 20 September - 02 October 2011.