Laboratory of Aerosols Chemistry and Physics

HEAD
VLADIMÍR ŽDÍMAL

DEPUTY
MARTIN LÍSAL

SCIENTISTS
DAVID BRUS, JAN JIRSÁK, VALERI V. LEVDANSKI, PAVEL MORAVEC, IVO NEZBEDA, JAKUB ONDRÁČEK, JAROSLAV SCHWARZ, MICHAEL ROUHA, JIŘÍ SMOLÍK, ALEXANDR MALIJEVSKÝ

POSTDOCS
MICHAEL CUSACK, LUCIE ONDRÁČKOVÁ, STANISLAV PAŘEZ, ZBYŠEK POSEL

RESEARCH ASSISTANTS
IRENA BENEŠOVÁ ŠEVČÍKOVÁ, JOSEF KUGLER, MARTIN SVOBODA

PHD STUDENTS
JANA KOZÁKOVÁ, LUCIE KUBELOVÁ, OTAKAR MAKEŠ, LUDMILA MAŠKOVÁ, JAN PUŠMAN, LENKA ŠKRABALOVÁ, NICHOLAS TALBOT, PETR VODIČKA, NADĚŽDA ZÍKOVÁ

Fields of research

- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Heat and mass transfer in aerosol systems
- Interaction of aerosols with electromagnetic radiation
- Emissions sampling
- Engineered nanoparticles and health
- Aerosol technology
- Density functional study of interfacial phase transitions and nanodrops
- Dynamic properties of simple and complex fluids on a molecular scale
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Development of equations of state based on molecular theory
- Molecular simulations of solid–liquid interfaces
- Mesoscale simulations of polymeric and energetic systems
- Density functional study of interfacial phase transitions and critical phenomena at non-planar surfaces
- Dynamic non-equilibrium properties of complex fluids and their mixtures

Research projects

Molecular-level simulations aqueous electrolytes

(I. Nezbeda, ivonez@icpf.cas.cz; joint project with the University of Ontario, Institute of Technology, Oshawa, ON, Canada and UJEP; supported by UJEP)

This series of papers deals with common non-polarizable models of electrolytes with the goals to (i) assess their appropriateness, (ii) find ranges of their applicability, and (iii) examine the possibility of their improvement by a reparametrization. Consistency tests of available literature data for the chemical potential were also performed. All simulations used the recently developed MPM-MC method demonstrating thereby its efficiency. [Ref. 3]

Tailored self-assembly of polyelectrolyte copolymers with surfactants in aqueous solutions

(Z. Posel, M. Lísal, posel@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-02938S)

Multidisciplinary study of the tailored self-assembly of branched polyelectrolyte copolymers with surfactants in aqueous solutions aimed at deeper understanding of the relationship between the chain architecture and the structure, stability, thermodynamic behavior and properties of nanostructures formed under different conditions (pH, ionic strength, temperature) was carried out. A combination of dissipative particle dynamics and newly developed hybrid Monte Carlo method with experiments was used. [Refs. 20-22]

A controlling of diffusion processes in pores with varying permeability

(A. Malijevský, M. Lísal, malijevsky@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-09914S)

Interfacial phase transitions at non-planar surfaces have been studied in the framework of a density functional theory and effective Hamiltonian theory. New hidden connections (covariances) between adsorption phenomena at different substrate geometries have been found and explained. While most of the results obtained by the two theories give mutually consistent conclusions, the molecular-based density functional theory whose implementation was newly extended for the geometries possessing nontrivial symmetries, provides a more microscopic insight into the understanding of the interfacial phenomena and revealed some new and surprising predictions. These results are not only interesting by their own rights but also serve as a pre-requisite for a further study of dynamical properties of fluids (such as diffusive processes) at modified surfaces and between patterned walls. [Refs. 14-16]

Mesoscopic modeling of protein - surface interactions

(A. Malijevský, Z. Posel, and M. Lísal, malijevsky@icpf.cas.cz, posel@icpf.cas.cz, and lisal@icpf.cas.cz; supported by Grant Programme of the MEYS, project No. LH12020)

Mesoscopic modeling using dissipative particle dynamics was employed to systematically study the effect of shape, size and hydrophobicity / hydrophilicity of proteins on their adsorption kinetics. Mesoscale models of proteins and surfaces were obtained from atomistic simulations of individual proteins in water and individual proteins close to walls using mapping from the atomistic to mesoscopic level. [Refs. 5, 12]

Mesoscale Modeling of Dynamic Response of Reactive Materials

(M. Lísal, lisal@icpf.cas.cz; supported by Cooperative Agreement W911NF-10-2-0039)

The Dissipative Particle Dynamics method was extended to simulate chemical reactivity (DPD-RX) of multi-step decomposition reactions, and was applied to a thermally-initiated RDX decomposition reaction model. For the DPD-RX methodology extended to multi-step reactions, a coarse-grain particle equation-of-state (CG-EOS) was further developed based on the internal partition function, which accounts for the standard-state contributions in a thermodynamically-consistent manner. Finally, the gas expansion that follows RDX decomposition was captured via composition-dependent particle interactions based upon a one-fluid approximation. [Refs. 2, 7, 8]

Human EXposure to Aerosol COntaminants in Modern Microenvironments

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, Marie Curie Actions - Initial Training Networks, project No. 315760, FP7-PEOPLE-2012-ITN, HEXACOMM, project partner)

The main research goal of HEXACOMM is to apply scientifically-based modelling and experimental methods to relate concentrations of particulate matter in the indoor domestic environment to its sources and human exposure implications. The second research objective is to determine the human exposure arising from such exposure at both individual and collective (population) scales at modern microenvironments.

Contributions from outdoor air will be taken into account. Central idea of HEXACOMM is that a combination of tools and methods will enable us to relate indoor air quality to aerosol contaminants in urban homes, offices, vehicles with human exposure in a quantitative manner. To achieve our goal and objectives we propose to undertake, in parallel, a carefully designed validation programme at the European scale combining specifically targeted indoor air quality measurements, source apportionment studies, micro-environmental modelling, dosimetry modelling and exposure studies. Ultimately, our vision is that such enhanced understanding of the underpinning science will lead to improved indoor air quality in European domestic environments, while facilitating development of strategies to mitigate the impacts of aerosols on human exposure. [Ref. 4]

Aerosols, Clouds, and Trace gases Research Infra Structure Network

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, project No. INFRA-2010-1.1.16 ACTRIS, as “initial associated partner”)

ACTRIS (Aerosols, Clouds, and Trace gases Research Infra Structure Network) is an European Project aiming at integrating European ground-based stations equipped with advanced atmospheric probing instrumentation for aerosols, clouds, and short-lived gas-phase species. ACTRIS will have the essential role to support building of new knowledge as well as policy issues on climate change, air quality, and long-range transport of pollutants.

ACTRIS is building the next generation of the ground-based component of the EU observing system by integrating three existing research infrastructures: EUSAAR, EARLINET, CLOUDNET, and a new trace gas network component into a single coordinated framework. ACTRIS is funded within the EC FP7 under "Research Infrastructures for Atmospheric Research". [Refs. 1, 17]

Centre for studies on toxicity of nanoparticles

(P. Moravec, moravec@icpf.cas.cz; supported by GACR, project No. P503/12/G147)

The rapid expansion of nanomaterials production and their use in many products create a need for understanding the mechanisms of nanomaterial interactions with living systems. This need is above all given by unique properties of nanoparticles related to their dimensions and by their ability to penetrate into various tissues and cells in organism. Nanoparticles are also formed unintentionally as a result of the anthropogenic activities (industry, local heating). The proposed interdisciplinary centre of basic research will integrate laboratories capable to perform complex studies on mechanism of the toxicity of important and widely used engineered nanoparticles, as well as anthropogenic nanoparticles in the environment with a special attention paid to heavily polluted areas of the Czech Republic. The studies will be performed on thoroughly characterized nanoparticles to obtain valid and comparable results on biological action and toxicity of nanoparticles.

Advanced study of physical and chemical properties of atmospheric aerosols in high time resolution

(V. Ždímal, zdimal@icpf.cas.cz; supported by GACR, project No. 209/11/1342)

Advanced physical and chemical properties of Central European atmospheric aerosol at rural background and urban background sites will be studied in high time and size resolution. Parallel measurement of aerosol volatility will be carried out using a C-ToF-AMS equipped with a thermodenuder inlet, aerosol hygroscopicity using a Hygroscopic Tandem Differential Mobility Analyser (HTDMA), and particle number size distribution using a Scanning Mobility Particle Sizer (SMPS). The information about aerosol particle density will be extracted from the SMPS and AMS. Hygroscopicity closure will be obtained from the combined HTDMA and AMS chemical composition data allowing to study the influence of organic aerosol on particles' hygroscopicity. The content of primary and secondary organic aerosol and the extent of aerosol ageing will be determined using AMS data at each site. In addition, at least a year-long time evolution of number size distributions obtained using the SMPS and OC/EC concentrations from the OC/EC analyzer will be delivered to the EBAS database, to be available for global atmospheric modeling groups. [Refs. 26-29]

Thermophysical properties of water in unexplored, technologically significant regions

(V. Ždímal, zdimal@icpf.cas.cz; joint project with Institute of Thermomechanics of the CAS, CTU, and University of West Bohemia, Plzeň; supported by GA ASCR, project No. IAA4200760905)

This project focuses primarily on liquid water and solutions of selected salts below the freezing point (supercooled water), and water in nano-droplets. Existing hypotheses include the possibility of phase separation of supercooled water into two liquid phases below the second critical point. Density of supercooled water is only known at 0.1 MPa. Suggested measurements up to 100 MPa will provide first data. A new method and apparatus will be developed. The surface tension of supercooled water and a salt solution will be measured. The surface tension of nano-droplets will be estimated from nucleation experiments. A range of theoretical approaches including phenomenological methods, simplified microscopic models, and molecular simulations, will be used with experimental data to obtain fundamental findings and engineering models. [Ref. 23]

Development and application of new experimental methods to measure heterogeneous particles in superheated steam

(V. Ždímal, zdimal@icpf.cas.cz; joint project with CTU and Institute of Thermomechanics of the CAS; supported by GACR, project No. 101/09/1633)

The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), will be used to measure heterogeneous particles at selected power stations. To enable measurements of particles down to about 1 nm, a fast expansion chamber will be developed, enabling resolution of particle size by variable supersaturation. Collected data will serve as a basis for understanding the transport and the state of agglomeration of chemicals present in the steam circuit, for quantifying their effect on condensation, and, consequently, on the efficiency and reliability of steam turbines. [Ref. 6]

Black and elemental carbon at two European urban sites – site specific similarities and differences in method intercomparability

(J. Schwarz, schwarz@icpf.cas.cz; supported by MEYS, program MOBILITY, project No. 7AMB12AT021)

The method intercomparison studies will be conducted both under summer and winter conditions at both sites lasting 2 weeks each. By pooling the instruments and expertise of the two partners, BC will be measured on-line with the MAAP and the aethalometer techniques and from filter samples with the integrating sphere technique; EC will be investigated both from bulk samples with a Sunset Analyzer set both in reflection and transmission modes with three thermal protocols (NIOSH, DRI, EUSAAR2) and quasi on-line with two Sunset Field Analyzers set to two different temperature protocols. BrC will be analyzed with the modified integrating sphere technique. Background information on the aerosol will be obtained in parallel. [Ref. 28]

Methodology of evaluation of air quality effect on library and archival collections

(J. Smolík, smolik@icpf.cas.cz; supported by the Ministry of Culture of the CR, project No. DF11P01OVV020)

The aims of the project are: a) development of evaluation methods for indoor air quality in libraries and archives, targeted at reduction of damages on library and archival collections caused by adverse effects of environment and b) gaining detailed knowledge of direct dependences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Ref. 13]

International co-operations

Imperial College London, London, UK: Confined fluids
Penn State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behavior of model proteins on surface
University of Loughborough, Loughborough, UK: Dynamic density functional theory
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
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, Switzerland
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behavior
Technical University of Crete, Chania, Greece: Aerosols in the indoor environment
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
University of Vienna, Faculty of Physics, Dept. of Aerosol physics and Environmental Physics, Vienna, Austria: Black and elemental carbon analysis, aerosol optical properties

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
M. Lísal: The University of Alabama, Tuscaloosa, AL, USA (1 month)
A. Malijevský: Imperial College London, London, UK (3 months)

Visitors

Coray M. Colina, Department of Materials Science, Penn State University, State College, USA

Teaching

V. Ždímal: Faculty of Mathematics and Physics, Charles University in Prague, undergraduate course: “Aerosol Engineering”

V. Ždímal: UCT, Faculty of Chemical Engineering, graduate course “Aerosol Engineering”

J. Jirsák: UJEP, Faculty of Science, courses "Introduction to Chemistry", "Physical Chemistry", "Physical Chemistry Seminar" and "Free Software in Natural Sciences"

M. Lísal: UJEP, Faculty of Science, courses “Parallel Programming”, “Numerical Mathematics”, “Molecular Simulations” and “Mesoscale Simulations”

A. Malijevský: UCT, Faculty of Chemical Engineering, courses “Physical Chemistry I”, “Physical Chemistry of the Micro-World", "Introduction to a Modern Theory of Phase Transitions", "Mathematics for Physical Chemistry" and "Statistical Thermodynamics", Molecular Simulations and Modelling

Publications

Original papers

[1] Beddows D.C.S., Dall’Osto M., Harrison R.M., Kulmala M., Asmi A., Wiedensohler A., Laj P., Fjaeraa A.M., Sellegri K., Birmili W., Ždímal V., Zíková N.: Variations in Tropospheric Submicron Particle Size Distributions Across the European Continent 2008-2009. *Atmos. Chem. Phys.* 14(8), 4327-4348 (2014).

[2] Brennan J.K., Lísal M., Moore J.D., Izvekov S., Schweigert I.V., Larentzos J.P.: Coarse-Grain model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials. *J. Phys. Chem. Lett.* 5(12), 2144-2149 (2014).

[3] Figueroa-Gerstenmaier S., Lísal M., Nezbeda I., Smith W.R., Trejos V.M.: Prediction of Isoenthalps, Joule–Thomson Coefficients and Joule–Thomson Inversion Curves of Refrigerants by Molecular Simulation. *Fluid Phase Equilib.* 375, 143-151 (2014).

[4] Glytsos T., Ondráček J., Džumbová L., Eleftheriadis K., Lazaridis M.: Fine and Coarse Particle Mass Concentrations and Emission Rates in the Workplace of a Detergent Industry. *Indoor Built Environ.* 23(6), 881-889 (2014).

[5] Hart K., Abbott L., Lísal M., Colina C.M.: Morphology and Molecular Bridging in Comb- and Star-Shaped Diblock Copolymers. *J. Chem. Phys.* 141(20), 204902 (2014).

[6] Kolovratník M., Hrubý J., Ždímal V., Bartoš O., Jiříček I., Moravec P., Zíková N.: Nanoparticles Found in Superheated Steam: a Quantitative Analysis of Possible Heterogeneous Condensation Nuclei. *Proc. Inst. Mech. Eng. Part A-J. Power Energy* 228(2), 186-193 (2014).

[7] Kuba P., Lorinčík J.K., Lísal M., Urbassek H.: Molecular Dynamics Simulations of Ar Gas Ejection from a Ruptured Subsurface Bubble in Cu(100) Induced by Impact of 200 eV Ar Atoms. *Mol. Phys.* 112(15), 2040-2045 (2014).

[8] Larentzos j.P., Brennan J.K., Moore J.D., Lísal M., Mattson W.D.: Parallel Implementation of Isothermal and Isoenergetic Dissipative Particle Dynamics using Shardlow-like Splitting Algorithms. *Comput. Phys. Commun.* 185(7), 1987-1998 (2014).

[9] Levdansky V.V., Roldugin V.I., Žďanov V.M., Ždímal V.: Free-Molecular Gas Flow in Narrow (Nanoscale) Channel. *J. Eng. Phys. Thermophys.* 87(4), 802-814, 2014 [*Inzh.-Fyz. Zh.* 87(4), 778-790, 2014].

[10] Levdansky V.V., Smolík J., Ždímal V.: Influence of Size Effects on the Formation of Aerosol Nanoparticles in Supersaturated Vapor Condensation. *J. Eng. Phys. Thermophys.* 87(5), 1249-1254 (2014) [*Inzh.-Fyz. Zh.* 87(5), 1199-1204, 2014].

[11] Levdansky V.V., Smolík J., Ždímal V.: Size Effect in Evaporation of Atoms (Molecules) from Aerosol Nanoparticles. *J. Eng. Phys. Thermophys.* 87(2), 469-473 (2014) [*Inzh.-Fyz. Zh.* 87(2), 454-458, 2014].

[12] Lísal M., Chval Z., Storch J., Izák P.: Towards Molecular Dynamics Simulations of Chiral Room-Temperature Ionic Liquids. *J. Mol. Liq.* 189(SI), 85-94 (2014).

[13] Mølgaard B., Ondráček J., Šťávová P., Džumbová L., Barták M., Hussein T., Smolík J.: Migration of Aerosol Particles inside a Two-Zone Apartment with Natural Ventilation: A Multi-Zone Validation of the Multi-Compartment and Size-Resolved Indoor Aerosol Model. *Indoor Built Environ.* 23(5), 742-756 (2014).

[14] Malijevský A.: Does Surface Roughness Amplify Wetting? *J. Chem. Phys.* 141(18), 184703 (2014).

[15] Malijevský A.: Complete Wetting Near an Edge of a Rectangular-Shaped Substrate. *J. Phys. Condens. Matter* 26(31), 315002 (2014).

[16] Malijevský A., Parry A.O.: Condensation and Evaporation Transitions in Deep Capillary Grooves. *J. Phys.-Condes. Matter* 26(35), 355003 (2014).

[17] Mann G.W., Carslaw K.S., Reddington C.L., Pringle K.J., Schulz M., Asmi A., Spracklen D.V., Ridley D.A., Woodhouse M.T., Lee L.A., Zhang K., Ždímal V.: Intercomparison and Evaluation of Aerosol Microphysical Properties among AeroCom Global Models of a Range of Complexity. *Atmos. Chem. Phys.* 14(9), 4679–4713 (2014).

[18] Parry A.O., Malijevský A., Rascón C.: Capillary Contact Angle in a Completely Wet Groove. *Phys. Rev. Lett.* 113(14), 146101 (2014).

[19] Pařez S., Předota M., Machesky M.: Dielectric Properties of Water at Rutile and Graphite Surfaces: Effect of Molecular Structure. *J. Phys. Chem. C* 118(9), 4818-4834 (2014).

[20] Posel Z., Limpouchová Z., Šindelka K., Lísal M., Procházka K.: Dissipative Particle Dynamics Study of the pH-Dependent Behavior of Poly(2-vinylpyridine)-block-poly(ethylene oxide) Diblock Copolymer in Aqueous Buffers. *Macromolecules* 47(7), 2503-2514 (2014).

[21] Posel Z., Rousseau B., Lísal M.: Scaling Behaviour of Different Polymer Models in Dissipative Particle Dynamics of Unentangled Melts. *Mol. Simul.* 40(15), 1274-1289 (2014).

[22] Šindelka K., Limpouchová Z., Lísal M., Procházka K.: Dissipative Particle Dynamics Study of Electrostatic Self-Assembly in Aqueous Mixtures of Copolymers Containing One Neutral Water-Soluble Block and One Either Positively or Negatively Charged Polyelectrolyte Block. *Macromolecules* 47(17), 6121-6134 (2014).

[23] Škrabalová L., Brus D., Antilla T., Ždímal V., Lihavainen H.: Growth of Sulphuric Acid Nanoparticles Under Wet and Dry Conditions. *Atmos. Chem. Phys.* 14(12), 6461-6475 (2014).

Chapters in books

[24] Dvorská A., Hanuš V., Váňa M., Zíková N., Janata V., Pavelka M.: 6.1 Design, Scientific Goals and Challenges of the Atmospheric Station Křešín u Pacova. In: *Košetice Observatory - 25 Years*. (Holubová Šmejkalová, A., Ed.), pp. 36-43, Czech Hydrometeorological Institute, Prague 2014.

[25] Levdansky V.V., Pavlyukevich N.V., Ždímal V.: Svobodnomolekulyarnoe techenie gaza v kanale pri adsorbtsii molekul postoronnikh gazov na ego vnutrennei poverkhnosti. (Russ) . In: *Teplo- i Massoperenos - 2013*. (Carkova, V.I. - Michaleva, T.G., Ed.), pp. 76-80, Institut teplo- i massoobmena imeni, Minsk 2014.

[26] Ondráček J., Vodička P., Schwarz J., Smolík J., Ždímal V.: 6.4 Long Term Measurement of Aerosol Hygroscopicity at Rural Backround Station Košetice, Czech Republic. In: *Košetice Observatory - 25 Years.* (Holubová Šmejkalová, A., Ed.), pp. 55-58, Czech Hydrometeorological Institute, Prague 2014.

[27] Schwarz J., Chalupníčková E., Pokorný R., Novák J., Smolík J., Ždímal V.: 6.5 Water Soluble Ions OC/EC in MP10 at Košetice. In: *Košetice Observatory - 25 Years.* (Holubová Šmejkalová, A., Ed.), pp. 59-63, Czech Hydrometeorological Institute, Prague 2014.

[28] Vodička P., Schwarz J., Ždímal V.: 6.6 Comparison of EC and OC Aerosols in PM2.5 at the Košetice Observatory and at the Prague-Suchdol Backround Sites with Two-Hour Time Resolution. In: *Košetice Observatory - 25 Years*. (Holubová Šmejkalová, A., Ed.), pp. 64-68, Czech Hydrometeorological Institute, Prague 2014.

[29] Zíková N., Ondráček J., Schwarz J., Ždímal V.: 6.7 Continuous Aerosol Number Size Distributions Measurement at Košetice Observatory. In: *Košetice Observatory - 25 Years*. (Holubová Šmejkalová, A., Ed.), pp. 69-73, Czech Hydrometeorological Institute, Prague 2014.