Basic research at the Institute of Chemical Process Fundamentals

The tour of the following three laboratories presents examples of our basic research in chemical engineering, physical, and analytical chemistry.

1. Ultrafine atmospheric particles and human health

Dr. Vladimír Ždímal, research scientist and Head of Department of Aerosol and Laser Studies
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Aerosol particles are solid and/or liquid particles suspended in the air, their size varying from several nanometers to up to tens of micrometers. Even though these particles constitute only several parts per billion of the total mass of air, they influence our life on Earth substantially. For example, aerosols are key components of the hydrological cycle serving as cloud condensation nuclei; without them there would be neither rain nor snowfall. Atmospheric aerosols also affect the exchange of energy between the Earth and outer space; both directly, by absorbing and scattering solar radiation, and indirectly, by changing the size distribution of cloud droplets and hence the cloud albedo. As a result, they are an important factor in the global climate change. Aerosols also drastically control atmospheric visibility, because in the absence of aerosol particles in the atmosphere we would be able to observe objects in a distance of more than 300 km!

However, the most important issues connected to the atmospheric aerosol are related to their impact on human health. Over the last decade, many scientific studies confirmed the relationships between concentration of anthropogenic aerosol particles and adverse health effects. Only recently, specific influence of the smallest aerosol particles (the so called ultrafines) on human health is being investigated. To study this issue in detail, it is necessary to monitor concentrations of these ultrafines in the atmosphere over longer periods of time and to correlate them with the numbers of admissions in medical centers of patients with chronic and acute respiratory problems and with other related diagnoses (pollinosis, asthma, *etc.*). The aerosol laboratory of the ICPF is one of the European laboratories performing this research.

More details on this may be found on the website of the UFIREG Project: http://www.ufireg-central.eu/index.php/project-info01 and in folder Aerolab.

2. Ionic liquids: basic research, practical applications

Dr. Magdalena Bendová, research scientist and Deputy Head of E. Hála Laboratory of Thermodynamics
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Ionic liquids (ILs) have been studied for more than two decades by a number of research teams worldwide. Organic salts showing melting points lower than 100°C, they show interesting properties, partly due to the large number of ion combinations that make their properties tunable to the particular application. In spite of extensive basic research on their chemical and physico-chemical properties, and applied research in view of their applications as selective solvents, azeotrope breakers, lubricants or energy storage materials, the characteristics of this ever growing class of compounds still remain unexplored to a large extent. For instance, knowledge of heat capacity is necessary for any heat balance optimization. In mixtures, the extent to which liquids mix may help set the liquid operation range in applications requiring the use of co-solvents. Data on solubility of ionic liquids in water, 1-octanol and the partitioning coefficient octanol-water (K_{ow}) lead us to an estimate of their hydrophobicity and their tendency to bioaccumulation.

For this reason, we address the experimental studies of thermodynamic properties of pure ionic liquids and their mixtures with molecular solvents. At the heart of our research is the investigation of liquid-liquid equilibria in binary and multicomponent mixtures of ionic liquids with molecular solvents by various experimental methods. Using differential scanning calorimetry, we study heat capacity and phase transitions of pure compounds and mixtures. The experimental data are then not only interpreted in view of the practical applications of ionic liquids but we also try to understand the influence of the structure of the constituting ions on the studied properties.

Stanislav Pařez, Ph.D. student at E. Hála Laboratory of Thermodynamics

Phenomena at solid-liquid interfaces play an important role in physics, chemistry, biology, engineering, electrochemistry, geophysics as well as daily life. Among numerous examples, let us mention heterogeneous or photo- catalysis, function of biological membranes, electrochemical cells, corrosion and environment preserving applications. The specific behaviour of liquids, or generally fluids, is caused by the interaction with the solid phase. The introduction of the surface forces gives rise to new phenomena that are quite unexpected on the basis of our knowledge acquired from bulk systems. These include new kinds of phase transitions, *e.g.* capillary condensation, layering, wetting, as well as altering dynamical and transport properties of fluids, *e.g.* space dependence of diffusivity and viscosity. However, properties of fluids at interfaces are very difficult to study from a purely experimental perspective, making molecular simulations an attractive alternative, and in some cases the only feasible, tool.

Dr. Martin Lísal, research scientist and Head of E. Hála Laboratory of Thermodynamics

Applications such as gas storage, gas separation, nanoparticle synthesis and supported ionic liquid phase catalysis depend upon the interaction of different species with the ionic liquid/gas surface. Potential of these applications cannot be fully exploit without molecular-level insight into the surface structure and properties. The key is to develop understanding of the ionic liquid/gas surface structure and the interaction of solutes and gas phase probes with the surface. Generally, physical properties such as density, dielectric constant, solubility or diffusion changes abruptly, yet continuously, in the vicinity of a liquid/gas interface from the value characteristic of one phase to that of the other phase. The molecules located at the interface thus experience a markedly different local environment with respect to the bulk phase. A complementary approach to laboratory experiments can be provided by molecular modelling. The molecular modelling can be used to predict interfacial properties at fluid-fluid interfaces involving ILs; greatly reducing the amount of experimental work and increasing the fundamental understanding of the systems. The art of molecular simulations includes the development of molecular force fields required as input into simulations, and molecular dynamics simulations of particular systems.

More details in folder EHLT-

3. LC-NMR in the Czech Republic

Dr. Jan Sýkora, research scientist and Head of Department of Organic Synthesis and Analytical Chemistry
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The HPLC-NMR experimental technique is extensively used worldwide and finds use in the analysis of *e.g.* natural extracts, pharmaceuticals and their metabolites in bodily fluids. In 2001, an HPLC-NMR hyphenated instrument was installed in our laboratory as well, as the only one of its kind in the Czech Republic.

In the central LC-NMR laboratory, we focus on the analysis of complex reaction mixtures, and on the isolation/identification of the required products. The LC-NMR technique is particularly helpful in separating unstable compounds or compounds that don't absorb in the UV range. The LC-NMR is also useful in cases of insufficient separation and co-elution of some of the studied compounds. In this respect we help analyze the rich plant extracts provided by the supercritical CO_2 extractions. On the other hand the GPC-NMR experiments bring valuable information in various polymer studies. The LC-1H{29Si} NMR enabled us to get a new insight on the analysis of various polysiloxane products and plays also a key role in the analysis of polysilane chains.

More details in folder NMR.

Applied research at the Institute of Chemical Process Fundamentals

The tour of the following three laboratories presents examples of our applied research in chemical engineering.

1. Microreactors – LEGO for chemical engineers

Dr. Jiří Křišťál, research scientist and Deputy Head of Department of Separation Processes
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A microreactor is not a pocket size nuclear plant. On the contrary, microreactors are inherently safe devices for production of even very dangerous substances such as the highly explosive nitroglycerin. In general, microreactors can be described as chemical reactors with a high surface-to-volume ratio and characteristic dimension lower than 1 mm. Thanks to these features microreactors are suitable for complicated reactions that require a highly accurate control of local process conditions, *i.e.* of temperature and pressure. In some cases, microreactors enable us to carry out reactions that are extremely difficult or even impossible to implement in conventional batch systems. Among other assets of microreactors their flexibility, modularity, and easier scale up may be cited. All in all, microreactor technology is a new promising way of decreasing costs and of the environmental impact while increasing the efficiency and sustainability in chemical industry.

In our laboratory, we will show you a modular LEGO-like microreaction system with which you can assemble a small chemical plant on a lab bench.

More details in folder Microreactors_LEGO.

2. Environmental Process Engineering Laboratory

Assoc. Prof. Dr. Karel Svoboda, research scientist, Environmental Process Engineering Laboratory
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Equipment (experimental units)

The laboratory is equipped with two experimental facilities for combustion and gasification processes in fluidized bed and spouted bed. Maximum operational temperature is 1000 °C. One experimental facility has internal diameter 93 mm and height above the gas distributor 105 cm. The other apparatus with spouted fluidized bed has internal diameter in the lower part 51 mm and diameter 99 mm in the upper part. The overall height of the apparatus is 220 cm. Both experimental units are equipped with external electrical heating, inlet gas preheating, cyclone and by optional further filter for removal of dust particles.

Experimental studies

Fluidized bed gasification of coal, biomass, waste and co-gasification of coal with biomass and/or waste.

Material (fuel) for gasification is in the form of solid particles, liquid, or suspension.

Influence of operational conditions (temperature, fluidized bed material, fuel properties and gasification medium) on properties, composition and purity of producer gas is studied. The available analytical devices (IR analyzers, gas chromatography analyses) enable us to carry out detailed analyses of fuel gas including the speciation of sulfur compounds (H_2S, COS, thiophene etc.). Depending on the overall purpose of experimental measurements analyses of HCL, HF and NH_3 contents in fuel gas are also possible. Experimental studies can serve for testing the influence of primary and secondary measures (*e.g.* high temperature gas cleaning) on the fuel gas purity (content of tar compounds, H_2S, NH_3, HCl *etc.*).

Fluidized bed combustion of coal, biomass, waste (including sewage sludge)

Study of emissions of NO_x, N_2O, SO_x, CO, heavy metals and selected POP (*e.g.* PCDD, PAH). Study of operational conditions and presence of additives based on calcium and magnesium compounds on emissions and their interrelations.

Study of modern combustion processes with recirculation of flue gas and oxygen (oxy-fuel combustion). Influence of oxy-fuel combustion conditions and oxygen enrichment on emissions, on SNCR (selective non-catalytic reduction of NO_x) by ammonia, and on desulfurization by limestone addition.

Modeling of processes in fluidized bed combustion, gasification, removal of pollutants *etc.*

More details in folder Envilab.

3. Microwave Technology Research

Dr. Milan Hájek, research scientist, Center of Microwave Technology, Environmental Process engineering laboratory
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Microwave Technology for Recycling of Waste PET Bottles

A new recycling technology has been developed to solve problems related to the accumulation of waste PET bottles. This technology characterized by low energy consumption is based on the use of microwave energy to depolymerize PET material to high purity products, *i.e.* terephthalic acid and monoethylene glycol, in the so called "polymer-grade" quality. It was tested on a pilot plant where 1-10 kg/h of PET bottles may be treated using a microwave reactor of 0.12-1.0 m^3. This unique technology was developed at the Czech Center of Microwave Technology at the Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, v. v. i. and is protected by patent documents both in Czech Republic (CZ299908) and in Germany, Italy, France, UK, and China (PCT/EP/2008/058917).

Microwave Drying and Disinfection of Paper Documents

To rescue flooded books and documents as soon as possible after a flood while maintaining a high quality of drying, a new drying method had to be developed. A novel drying technology using microwave energy was developed at the Czech Center of Microwave Technology at the Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, v. v. i. Compared with conventional drying, this method is fast and safe, the drying process being continuous and providing simultaneous disinfection of the paper if need be. The microwaves interact directly with polar molecules of water. All of the water contained in the document is being excited simultaneously from the inside towards the surface. Consequently the paper document will not be damaged on drying. Moreover, the microwave field is modified to prevent arcing of metallic objects and the creation of „hot spots" that could cause irreversible changes to the document. Further details may be found in our paper Simultaneous Microwave Drying and Disinfection of Flooded Books. *Restaurator* 32(1): 1-12, 2011.

More details in folder Microwave.