## osvrti

### Historical Development and Current Status of Chemical Engineering at the Institute of Chemical Technology, Prague

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The Czech Republic belongs to those European countries that have a long tradition in chemical production. The need for a good education in chemistry has been increasing with the growing industry. The Institute of Chemical Technology, Prague (Vysoká škola chemicko-technologická – VŠCHT, in Czech) is the largest university specializing in chemistry and chemical technology in the Czech Republic. It was founded in 1952, but its roots date back to 1807 when the first course in chemistry was delivered at the Prague Polytechnic. The reorganization of the Polytechnic in 1920 resulted in the transformation of the chemical department into the School of Chemical Technology, one of the seven sections of the Czech Technical University. Since then, the School has been one of the leading research spots in Central Europe. The ICT Prague has produced a number of outstanding chemists, among them Professor Otto Wichterle, inventor of soft contact lenses in the fifties. Vladimír Prelog, professor at the ETH Zürich and winner of the 1975 Nobel Prize for Chemistry, graduated from the School of Chemical Technology in 1928, and gained his PhD degree there some years later.

The ICT Prague consists of four faculties, Faculty of Chemical Technology, Faculty of Environmental Technology, Faculty of Food and Biochemical Technology, and Faculty of Chemical Engineering. These faculties are accredited to provide three-year Bachelor programmes, two-year Master programmes (ending with the award of the academic title of Engineer), and PhD programmes. The total enrolment is about 2500 Master and Bachelor students and more than 600 PhD students. The ICT Prague cooperates with over 100 universities and institutions mostly in Europe, but also in the USA, Canada, Japan, and other countries. The ICT Prague is the most active of Czech universities in the SOCRATES/ERASMUS student exchange programme. In addition, it collaborates within other programmes, such as the  $5^{\text{th}}$  and  $6^{\text{th}}$ framework programme, COST, EUREKA, Leonardo da Vinci, programmes of overseas grant agencies. Besides the traditional teaching students, the ICT Prague provides postgraduate courses for specialists from industry in the form of life-long education.

After World War II, unlike other developed countries, no technical university in former Czechoslovakia offered courses in chemical engineering. The most significant contribution to the development of this discipline in Czechoslovakia, and to the foundation of the Department of Chemical Engineering was made by Professor George Standart from the California Institute of Technology and Professor Hanuš Steidl. In 1950, a small group led by Prof. Standart began teaching chemical engineering as an optional course under the auspices of the Department of Physical Chemistry at the Faculty of Chemical Technology and Engineering of the Czech Technical University. One year later, this group achieved the status of the Department of Process Engineering with Prof. Steidl as its head. Chemical engineering courses became compulsory for all students of the faculty. After splitting from the Czech Technical University in 1952, the school became the independent Institute of Chemical Technology, Prague, and the department was renamed to the Department of Processes and Apparatuses of Chemical Technology. In 1960, the Faculty of Chemical Production, Automation, and Economics was established, and in 1969 it changed its name to Faculty of Chemical Engineering. Since 1980, the department was again called the Department of Chemical Engineering.

Nowadays, the Department of Chemical Engineering is one of the largest departments at the ICT. The Department provides various courses in chemical engineering subjects for undergraduate students as well as postgraduate students. The main courses, namely "Unit Operations I", "Chemical Engineering Project" and "Laboratories of Chemical Engineering" are provided for all students of ICT Prague. More than 50 other courses are offered for students specialised or interested in chemical engineering; among the most important are "Fluid Mechanics", "Heat and Mass Transfer", "Separation Processes", "Chemical Kinetics and Reactor Design", "Technical Thermodynamics", "Process and System Design", "Process Safety and Reliability", "Mathematical Modelling or Engineering of Biological Processes". Most of the courses are opened also for foreign students coming to Prague within the ERASMUS programme of international student's exchange. The courses "Process Engineering, Informatics and Management" and new "Nano- and Micro-technology in Chemical Engineering" are offered for B.Sc. programmes. The Department collaborates in the organization of the "Chemistry" programme, where graduates are awarded the Euro Bachelor degree. The M.Sc. course is called "Chemical Engineering, Bioengineering and Mathematical Modelling of Processes". On average, about 20 students graduate annually from this M.Sc. programme.

The department's scientific activities range from fundamental research to applied research in close cooperation with industry. Most academic staff members, all PhD students, and some undergraduate students of the Department of Chemical Engineering take part in this important activity. Other activities involve solving industrial problems, also in cooperation with foreign universities, institutes, and companies. International cooperation includes among other the following institutions: University College of Lon-

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don, University of Birmingham, University of Wisconsin, Brandeis University of Waltham, California Institute of Technology, Stanford University, Universita E. Kardelja, Humboldt Universität, Universität Stuttgart, Johannes Kepler Universität, Universität di Bologna, Tenneco Minerals Company and Raschig AG. The staff of the Department of Chemical Engineering participates in various societies, councils, executive committees, commissions and boards, for example in the Czech Society of Chemical Engineering, as well as in the scientific committee of the International Congresses of Chemical and Process Engineering (CHISA), the Council of Universities, the Scientific Councils of Faculties, and in Academic Senates.

The research activity is focused both on fundamental research in traditional unit operations in chemical engineering (including heat and mass transport processes, fluid flow, chemical reactors and bioreactors), and in many cases extends to applications to industrial problems. Together with these traditional disciplines, new multi-branch research activities are being developed, e.g. nano-applications or polymerization reaction engineering. Particular attention is paid also to environmental problems. The research includes both experimental work and mathematical modelling.

The Department of Chemical Engineering consists of several research groups; their scientific interests are described below.

"Biolab" Research Group is focused mainly on development of bioreactors for decolourization and removal of organic dyes from textile industry wastewater, study of micro fluidic systems, development of slug flow microreactors for enzyme transformations and separation of reaction products, development of biological fuel cells, and theoretical investigation of the interactions between transport processes and cellular systems. The lab is well equipped for work with biochemical and biological materials. The scientific team is currently led by two principal investigators, Prof. Pavel Hasal and Ass. Prof. Michal Přibyl.

The "Polymer Reaction Engineering" Research Group is headed by Ass. Prof. Juraj Kosek. The research is conducted in the area of catalytic polymerizations of olefins, but several related problems are also addressed. One could mention the morphogenesis of polymer particles in catalytic polymerization, experimental studies of catalytic polymerization processes (thermodynamics and kinetics of sorption/desorption process in polymers, co-sorption effects), effective-scale models of growing polymer particle, dynamics and stability of polymerization reactors, oligomerization and copolymerization of dicyclopentadiene, mathematical modelling of formation of high-impact polystyrene structure and heat transfer on nano- and micro scale. Modern tools as atomic force microscopy and inverse gas chromatography are exploited. Porous media of various types are used in practical applications involving ionic electrolytes e.g. capillary electrochromatography, nanofiltration, electrodialysis, fuel cells and membrane applications. The group deals with research in the following fields: DNA chips controlled by electric field, electrolyte diodes and transistors in hydrogels, electroosmotic flow in micro-channel devices, ionic permselectivity of ion-exchange membranes, capillary electrophoresis in capillaries packed by porous particles including adsorption effects, production of nanoparticles by electrospraying method. The partners from industry include, e.g., Unipetrol RPA, Synthos and Basell polyolefins.

The "Laboratory of Fluid Mechanics" deals with both basic and applied research in the area of single flow and multi-phase flows. Experimental laboratory tests and flow modelling by means of a computed fluid dynamics method are used for investigation. The range of solutions of problems is rather broad: the flow of liquids in stirred reactors, multi-phase flows (gas–liquid, solid–liquid), flow of exhaust gases on combustion, *etc.* The multi-phase flow is studied also in micro scale region, where interactions between bubbles and particles are explored together with study of wetting and surface properties of solid surfaces. The scientific team is currently led by Ass. Prof. Milan Jahoda and Dr. Pavlína Basařová.

The "Laboratory of Microchemical Engineering" deals with the behaviour of fluids, especially liquids in micro space *i.e.* a space where the characteristic dimensions are within the range 1 -1000 micrometres. To study the fluid confined in microspace, small plastic chips containing microfluidic channel network and arrays of gold microelectrodes are used. The array of gold microelectrodes is a tool both for probing the liquid by measuring electrical quantities and for active control of the liquid flow. The research includes investigation of AC and DC electroosmosis, study of phenomena occurring in selective membrane micro fluidic systems, study of scale-down process in measurement of electrolyte conductivities, characterization and control of a two phase flow, etc. Recently, the lab launched a new project aimed at recycling and separation of noble metals from waste products of semiconductor and photovoltaic industry. The research group is headed by Prof. Dalimil Šnita.

The research in the "Laboratory of nonlinear dynamics of chemical and biochemical systems" group is focused on explaining the mechanistic reasons for complex dynamics, such as oscillations, and on emergent/synergic behaviour of complex systems. The research is carried out both experimentally and theoretically. The experimental part includes interaction of chemical oscillators studied in forced and coupled stirred tank reactors and dynamics of enzyme membrane reaction systems. The theoretical studies deal with mathematical modelling and simulation of the experimentally investigated systems as above and other systems known with temporal oscillations or spatial patterns or both, such as dynamics of mesosphere chemistry, interaction of reaction pathways and transport in catalytic removal of noxious components from exhaust gases on a three-way catalyst, chemical waves in reaction-diffusion-convection media, signal propagation in networks of excitable cellular tissues. Emergent dynamic phenomena are due to interaction of two or more subsystems, which were not hitherto observed if they were considered separately. These phenomena may play an important role in forming functions (biological, such as rhythmic signalling in cells or industrial, and such as interacting pathways for reduction and oxidation of exhaust gases). Conceptually, emergent phenomena are associated with bifurcations due to change in coupling strength among the subsystems. The research group is headed by Prof. Igor Schreiber.

"Mass-transfer Research Group" continues its activities initiated by late Professor Standart. Currently led by Prof. Václav Linek, the research group concentrates on mass-transfer between liquid and vapour phase and its applications in tower mass-exchangers (absorption and distillation columns), agitated aerated tanks (fermentors) and in the ejector columns. The aim of the basic research includes the development of experimental methods and selection of suitable model systems for the measurement of the interfacial area, mass transfer coefficients, pressure loss, energy consumption and other design quantities, as well as the development of methods of their scaling to industrial set-up. Applied research activities are focused on sound design and intensification of the industrial processes involving interfacial mass-transfer. The group participates in data measurement, apparatus build-up and also consultancy with major Czech and international industrial companies and manufacturers, e.g. Lovochemie, Raschig GmbH and GTC Technology.

The "Monolith" Research Group deals with the study of automobile exhaust-gas converters. Mathematical models of catalytic monoliths and predictive simulation software are being developed on the basis of dynamic measurements. Catalyst configurations and operation modes leading to minimum emissions of harmful components are examined both experimentally and with use of simulations. Models of three-way catalysts for gasoline engines, Diesel oxidation catalysts with adsorption of hydrocarbons, and  $NO_x$  storage & reduction catalysts have been developed and successfully applied. Current projects involve also the analysis of complex, non-linear dynamic regimes observed in certain reaction sub-systems, modelling of Diesel particulate filters, selective catalytic reduction of  $NO_x$  by  $NH_3$ , combined exhaustgas after-treatment systems, and development of novel methods for the modelling of porous catalysts in micro/nano-scale (including 3D digital reconstruction from electron microscopy and X-ray microtomography images). The research group is headed by Prof. Miloš Marek. The research partners from automotive industry include, e.g. Daimler, Ecocat and Johnson Matthey.

Finally, the "Chemical Robotics Laboratory" was established in 2008 with the launch of the CHOBOTIX project. This five-year project, funded by the European Research Council, is multidisciplinary and covers many scientific fields, ranging from chemical engineering, materials science, biophysics, and microbiology to applied mathematics and computer simulation. The group is

headed by Prof. František Štěpánek, who is the first recipient of such an ERC research grant in the Czech Republic. The project is focused on the design and synthesis of so-called "chemical robots", which are envisaged as internally structured particulate entities in the 10 micrometres size range that can move in their environment, selectively exchange molecules with their surrounding in response to a local change in temperature or concentration, chemically process those molecules and either accumulate or release the product. Many aspects of the structure and function of chemical robots are inspired by those of single cellular organisms. The fundamental understanding of the behaviour of "chemical robots" and their functional subsystems, will open up new opportunities in diverse areas, including next-generation of chemical processing, the synthesis and delivery of personalised medicines, the recovery of valuable chemicals from dilute resources, and environmental clean-up.

Web site of the Institute: www.vscht.cz/uchi

# Institute of Chemical Process Fundamentals of the ASCR: State of the Art

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### Introduction

The Institute of Chemical Process Fundamentals of the ASCR, v. v. i. (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Academy of Sciences of the Czech Republic (ASCR). In cooperation with several Czech universities, the Institute serves as a centre for fundamental research in the fields of chemical, biochemical, catalytic and environmental engineering, and it acts as a graduate school for PhD studies in the fields of chemical, biochemical, pharmaceutical, environmental engineering and processes, physical chemistry, organic and inorganic chemistry, industrial chemistry including petrochemistry and biotechnology. The multi-disciplinary character of the Institute's activities is great advantage for solving of complex problems and for external cooperation.

The ICPF is the only institute in the field, both in process and chemical reaction engineering, and in the novel instrumentations and technology development. In the Czech Republic, the Institute is leader in fundamental chemical process engineering research. Moreover, there is no doubt that ICPF is the responsible partner in teams of EU Framework Programme projects.

At present, more than 70 different projects are granted every year by different national grant agencies (Czech Science Foundation, Grant Agency of ASCR, Ministry of Industry and Trade CR, Ministry of the Environment CR, Ministry of Education, Youth and Sports CR, etc.) and by industrial companies covering both fundamental and applied research. Research teams of ICPF are largely involved in the Framework Programmes of the EU, NATO Research Programmes and bilateral cooperations based on agreement between ASCR and foreign research institutions, as well as on the basis of other various forms of joint research projects and partnerships. The ICPF research activities are based on a long tradition and cover a wide range of fundamental scientific topics. The acquired know-how enables high-quality research in the fields ranging from pure chemical disciplines, like inorganic, organic, analytic and physical chemistry, applied chemistry in homogeneous and heterogeneous catalysis, chemical reaction engineering, separation and material science, to other related technical and technological areas such as hydrodynamics of multiphase flow systems, environmental biotechnology, aerosol formation and transformation, and chemical processes accelerated by laser beams or microwave field. These aspects are beneficial for the solution of integrated projects.

The Institute is nowadays a well-recognized and respected partner in this field, participating in top class European projects (e.g.  $F^3$  FACTORY, IMPULSE, HUGE, EUSAAR, EUCAARI, MULTI-PRO, etc.). In recent years, the Institute has organized or coorganized many international events, among others the biannual International Congresses of Chemical Engineering (i.e. CHISA meetings, the last one – the 20<sup>th</sup> in this series – held in 2012), the 7<sup>th</sup> Liblice Conference on the Statistical Mechanics of Liquids in Lednice in 2010, the 18<sup>th</sup> International Conference on Nucleation and Atmospheric Aerosols held in Prague in 2009. The Institute benefits from its international recognition based on the long-term scientific contacts, intensive publication activities, high rate of success in acquiring grant and project funding, as well as from the close links to companies involved in chemical industry business of the Czech Republic.

### Scientific Departments and their facilities

Department of Separation Processes (Dr. Vladimír Jiřičný, Head)

Mathematical modelling of complex multiphase systems based on sophisticated experiments is a useful tool in the design and/or optimization of modern chemical processes. Research of super-

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