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Institute of Chemical Process Fundamentals of the ASCR: Expectation

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Introduction

The Institute of Chemical Process Fundamentals of the ASCR, v. v. i. (ICPF) covers a wide variety of topics of fundamental and applied research in the field of chemical, catalytic, combustion, biochemical and environmental engineering. This specific role places the Institute among workplaces, which deal with basic research in chemical engineering as well as with design of chemical equipment, not only due to the available system of pilot plants laboratories. These facilities enable the transfer from laboratory investigation to large-scale applications. Consequently, such a background determines the position of ICPF both in the process and chemical reaction engineering research and in the development of novel instrumentation and technology. The basic aim in the forthcoming period is to strengthen and further develop this position.

Historically, the ICPF was established in 1960 by fusion of the Laboratory of Chemical Engineering of the Czechoslovak Academy of Sciences, and the Department of Technology of the Institute of Organic Chemistry of the Academy. Thus, the Institute consists of departments, which reflect chemical engineering unit operations or deal with catalysis and organic synthesis. With a certain simplification, the chemical engineering part of the Institute consists of *Department of Separation Processes*, *E. Hála Laboratory of Thermodynamics* and *Department of Multiphase Reactors*, while the *Department of Catalysis and Reaction Engineering* together with the *Department of Organic Synthesis and Analytical Chemistry* belongs to the "more chemically oriented" laboratories of the Institute. The list is completed by the *Department of Aerosols and Laser Studies*, which has grown due to the development of new specializations in chemical engineering science and organic synthesis. Last but not least, the *Environmental Process Engineering Laboratory* unifies a great deal of applied research for the protection of the environment and the development of new, environmentally friendly technologies. An important aspect is to use experimental facilities in pilot plant labs, which will be exploited for solution of projects leading to industrial applications.

In this historic manner, a somewhat wide range of research topics has emerged, which gradually distinguished themselves into the five following main areas forming simultaneously the frame of our scientific interests for the near future:

1. Physico-chemical processes in multiphase systems,
2. Up-to-date catalytic processes applicable also to environmental protection,
3. Development of processes for synthesis of chemical specialties and their modelling,
4. Investigation of new processes under unconventional conditions,
5. Chemical-engineering aspects applicable in biotechnology.

These general directions of investigation are connected with the research plan of individual departments and/or are realized with their mutual cooperation.

Concept of further development of ICPF

The above-described structure of departments is optimal for fulfilment of our current tasks and I can state that ICPF is a stabilized institution with a well-established system of research. However, this virtual stability might result in a certain preservation of such "steady state" with following consequences:

– Unsatisfactory personnel situation – lack of new acquisitions, low alteration on the leading positions,

– Keeping of traditional directions of research.

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The intention of the new management of the Institute is to create conditions for more flexible structure of control, which would help to reach the top level of research. The following measures are planned for achievement of this ambitious aim: regular open competition for position of department heads; to strengthen the position of young scientific workers by introduction of junior research teams, and last but not least to stress a reliable process for evaluation of quality of scientists.

Further development depends on the manner of research funding in the Czech Republic. If we consider the lack of institutional funds, it would be necessary to take part in different projects of applied research without the possibility of choosing perspective problems. Our Institute is relatively well prepared for collaboration with industry, but we need cooperative partners ready for funding of ambitious research and development, e.g. research toward utilization of carbo- and heterohelicenes as chiral selectors for applications in chiral HPLC and membrane processes. For example, one natural partner of the Institute in this research is an innovative company owned by our former colleague. One of our priorities for the future seems to be a search for such strategic partners.

A significant success in this effort represents the status of the recipient of "Competence Centre – BIORAF", which the Institute has obtained recently. The Competence Centres program is focused on support of creation and operation of research, development and innovation for progressive fields with strong application potential and a prospective for important contributions to the growth of the competitiveness of the Czech Republic. The BIORAF Centre is concentrated on complex utilization of biomass by the methods of "green chemistry".

Website: www.icpf.cas.cz;
YouTube presentation:
http://www.youtube.com/watch?v=EmN4ts_oiKY.

Chemical Engineering Application of Transport Characteristics

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Introduction

The industrial application of porous solids is quite widespread. Porous heterogeneous catalysts, adsorbents and membranes are used in the chemical industry and biotechnology, porous materials are common in building engineering, porous catalysts form the basis of mufflers in cars, *etc.* The rates of processes taking place in the pore structure of these materials are affected or determined by the transport resistance of the pore structure. Inclusion of transport processes into the description of the whole process is essential when reliable simulations/predictions have to be made. Trends, in modern chemical/biochemical reaction engineering, point to utilization of more sophisticated and therefore more reliable models of processes. The basic idea is that the better the description of individual steps of the whole process the better its description and, perhaps, even extrapolation. Dependable process description forms the basis of process control and process optimization. For example, optimum pore structure of adsorbents, membranes, enzyme/cell supports or heterogeneous catalysts can be suggested which will guarantee best activity or selectivity. Similarly, optimum operating conditions can be found when the process description is based on as full as possible knowledge of the process steps.

Because of the unique nature of pore structure of various materials, the pore structure characteristics relevant to transport in pores have to be determined experimentally. One of the possibilities is the evaluation of simple transport processes taking place in the porous solid in question. The relevance of evaluation of transport parameters from simple transport processes which take place in the porous solid in question stems from the possibility to use the same pore-structure model both for evaluation of transport parameters and for description of the process in question. It is a good idea to use a mass transfer process, which is similar to the gas transport process under consideration. It is of advantage to choose for determination of transport parameters a (simple) process that can be followed easily at near-laboratory conditions and does not require sophisticated instrumentation.

Various choices can be made:

– pure counter-current diffusion of gas mixtures under steady-state conditions;
– binary diffusion under dynamic conditions;
– dynamic or steady-state permeation of individual gases;
– combined diffusion and permeation gas transport.

At the same time it is a good choice to use inert (*i.e.* nonadsorbable) gases; this eliminates transport of adsorbed gas along the surface of pores (surface diffusion) the nature of which is not very well understood.

The best way for experimental evaluation of transport parameters (material constants that are independent on pressure, temperature as well as the composition of used gases) are the mentioned simple transport processes. Thus, at least four combinations of transport processes can be used.[1]

The practical utilization of described methods and their wide practical impact are presented as examples from different areas of chemical engineering.

Determination of effective diffusion coefficients of exhaust gases in automotive catalyst

Structured catalyst supports are widely used in automotive exhaust-gas converters.[2] Small sized channels are contained in monoliths to provide large surface area of the car catalytic convertors. Typically, both metal and ceramic monoliths are used.[3,4] Ceramic monoliths made from cordierite with square cross-section channels are employed quite extensively because of relatively low production costs.[5,6] The active catalyst is supported

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