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## Chemreactor on the Danube

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The XIX International Conference on Chemical Reactors (Chemreactor-19) was held on September 5–9, 2010, in Vienna, Austria. The conference was one part of events scheduled by the European Federation of Chemical Engineering. The Boriskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, has traditionally been the main organizer of the conference. Coorganizers were the Russian Center of Science and Culture in Vienna; the federal agency Rossotrudnichestvo; the RF Ministry of Science and Education; the Scientific Council on the Theoretical Foundations of Chemical Technology, Russian Academy of Sciences; and the Scientific Council on Catalysis, Russian Academy of Sciences.

The Chemreactor conference has deep traditions that can be traced back to the All-Union meetings on the modeling of chemical reactors in the 1960s. It is held every two years in major scientific, industrial, and cultural centers around the world. The choice of venue for the XIX International Conference on Chemical Reactors went to Vienna.

Contemporary knowledge of catalytic processes and reactors is basic in the chemical and petrochemical sectors of industry. It forms the basis of environmentally safe technologies and encourages the development of chemical methods for the efficient use of renewable natural raw materials. The Chemreactor-19 conference assembled more than 200 recognized experts, half of whom were representatives of Russian science and industry while the other half was made up of participants from 37 countries around the world. The conference's scientific program included six plenary and seven keynote lectures, 70 oral reports, and 100 poster events.

It was resolved at the Chemreactor-18 conference to introduce a scientific lecture in honor of Prof. M.G. Slin'ko, the founder of the conference, its permanent head until 2003, and its honored chairman until 2008. The right to deliver this lecture is granted to well-known scientists who have achieved considerable results in the mathematical modeling of chemical pro-

cesses and reactors. Prof. Yu. Matros (Matros Technologies, United States), one of M.G. Slin'ko's students, opened the conference with the first Slin'ko Memorial Lecture, on the ever-popular theme of how to design an optimal catalytic reactor, showing once again the wealth of Slin'ko's creative heritage and the role of his scientific school. After covering Slin'ko's scientific biography, the lecturer reflected the state of the art in studies developing Slin'ko's ideas in the mathematical modeling of catalytic processes and problems of the nonlinear dynamics of catalytic processes; described the comprehensive, multilevel, and multidisciplinary nature of designing optimal reactors; and analyzed the main achievements and failures on this path.

Plenary lectures were of a survey nature and reflected the key directions in the range of scientific problems considered at the conference. A lecture by Prof. L. Giorno (Institute of Membrane Technologies, Italy) described the state of the art in the development of membrane reactors and the prospects for their use in the separation of gases, the purification of wastewater, and in the food industry and medicine. Membrane bioreactors and the biotechnologies based on them are especially attractive from the environmental standpoint. Moreover, the use of membrane reactors fits well into the general ideology of the concept of sustainable development.

Multifunctional contactors are of special interest in creating prospective new chemical reactors, and were the question to which the lecture of Prof. J. Schouten (Eindhoven University of Technology, the Netherlands) was devoted. He began with a brief excursion into the history of creating multifunctional microreactors and showed the relation between microreactors and contactors with multiple spinning discs. High heat- and mass-exchange coefficients are attained in such contactors due to the intense stirring of a gaseous mixture, thus allowing a sharp increase in the productivity and selectivity of a catalyst, relative to conventional reactors.

Dr. H. Stitt (Johnson Matthey Company, Great Britain) proposed some interesting ideas for performing multiphase catalytic processes in reactors structured on the scale of 0.5–5.0 mm. Microchannel and monolithic systems of this type enable us to improve stirring and intensify the transfer of heat and mass,

<sup>1</sup> V.A. Chumachenko, S.I. Reshetnikov, A.P. Kagyrmanova, E.I. Smirnov, V.A. Yakovlev, and T.V. Zamulina took part in the preparation of this material.



Photo 1.

thus preventing a decrease in the productivity of agitated reactors as a result of their scaling. Dr. Stitt focused on the problems of searching for new fields of application in which the unique properties of structured multiphase reactors could best be employed.

V. Likholobov, Director of the Institute of Hydrocarbon Processing and Corresponding Member, Siberian Branch, Russian Academy of Sciences (Omsk) showed that different forms of nanostructural carbon materials such as fullerenes, bulbous structures, nanotubes, nanowires, graphenes, etc., could provide the basis for a nanomaterial industry. In his plenary lecture, Likholobov explained the technological foundations for the production of special-purpose nanocarbon materials from gaseous and liquid hydrocarbons through the formation of nanoglobules, demonstrated the prospects for their practical application, and talked about new directions in the high-temperature synthesis of nanostructural carbon composites.

The plenary lecture of Dr. V. Yakovlev (Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences) was devoted to the main trends in the development of bioenergetics, with emphasis on the production of motor biofuels. The most attention was given to works devoted to the development of catalysts and processes based on them for the production of biodiesel and green diesel fuel with high cetane numbers. The conjugated processes of transesterification and mild hydrocracking allow the complex processing of vegetable oils and other vegetable raw materials into biofuel. The lecturer showed the possibility of synthesizing biofuels from another renewable raw material: products of wood pyrolysis.

The conference participants noted the high scientific level of the plenary session, at which authors presented the latest results on the main directions in the development of chemical technologies. An important

role in shaping the scientific discussion of the conference's main trends was played by the key reports, which dealt generally with the formulation of problems and set the tone for the section's oral reports.

In keeping with tradition, the Chemreactor-19 conference's scientific program comprised reports in the three sections and included works devoted to kinetic research, the physicochemical and mathematical foundations of processes in reactors, and the study of heat and mass transfer and hydrodynamics in chemical reactors.

Section I was devoted to achievements in the field of kinetic research and developing the scientific foundations for the design of chemical reactors.

In the field of fundamental aspects, considerable attention was given to the development of prospective types of chemical reactors. The plenary lecture of Prof. J. Schouten was devoted to multifunctional microreactors, which was of special interest to those working in this field. The oral reports of R.G. Jordi (Sasol Technology, South Africa) and E. Rebrov (Eindhoven University of Technology, the Netherlands) were devoted to heat and mass transfer and the modeling of gaseous mixture flow aerodynamics in similar reactors.

The development of kinetic studies on synthesizing hydrocarbons directly from methane (i.e., the so-called oxidative coupling of methane) over the last 30 years was analyzed in the keynote lecture of M. Sinev (Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow). The stages in the development of kinetic models, from phenomenological approaches to detailed studies of the reaction mechanism based on current physicochemical methods, were noted. The results from modeling this process in a fluidized bed catalytic reactor were presented in the oral report of S. Jaso (Berlin Institute of Technology, Germany). The history of the develop-



Photo 2.

ment of reverse-flow reactors that combine chemical reactions with the generation of heat in a fixed catalyst bed was considered in the keynote lecture of G. Bunimovich (Matros Technologies, United States). The greatest attention was given to the results from their technological application in different industrial processes.

Application of the methods of computer-aided CFD-modeling in studying the behavior of reacting media in different chemical reactors was covered in the reports “Synthesis of Liquid Fuels by the ‘Gas-to-Liquid’ Method” of S. Antal (Interphase Dynamics, United States), “Gas-Liquid Flows in Narrow Capillary Channels” of E. Erkoç (Dresden University of Technology, Germany), and “Hydrodynamics of Three-Phase Reactors with a Suspended Catalyst” of O. Klenov (Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences).

Altogether, 26 reports concerning different catalytic reactions, from the reforming of methane on perovskite catalysts (V. Sadykov, Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences) and the oxidation of cyclohexane (O. Temkin, Moscow State Academy of Fine Chemical Technology) and *o*-xylene (F. Lopez-Isunza, University of Mexico) to, e.g., the synthesis of camphene (used in the production of fragrances and synthetic camphor) from  $\alpha$ -pinene (I. Simakova, Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences), were read within this section.

Section II reflected the development of new reactors, the modeling of physicochemical processes in reactors, and the optimization of their operational modes to improve their performance characteristics. Within this section 24 oral reports were read, seven of

which were devoted to using structured reactors (including the traditionally popular microreactors) to increase the selectivity and productivity of catalytic processes and ensure their safety. The strongly exothermal processes of the production of hydrogen by the partial oxidation of hydrocarbons, the selective oxidation of CO in the presence of hydrogen, and the processes of hydrogenation were considered in particular.

Great interest was aroused by the report of Prof. D. Luss (University of Houston, United States) on regeneration of the particulate filters of shell-type diesel engines. Experimental results on the optimum filter regeneration conditions that ensure a high rate and completeness of chemical reactions in the combustion of soot particles and prevent filter microchannels from clogging, were presented.

The results from investigating the selective oxidation of carbon monoxide in the presence of hydrogen on a copper–cerium catalyst, and the methanation of carbon monoxide on a nickel–cerium catalyst, were covered in the reports of P. Snytnikov and M. Zyryanova (Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, Novosibirsk). Three reports were devoted to using membrane technologies to increase the efficiency of chemical processes by shifting the chemical equilibrium toward the formation of useful products. In particular, A. Kucherov (Zelinskii Institute of Organic Chemistry, Russian Academy of Sciences, Moscow) demonstrated a high-performance and safe method for the synthesis of ethylene by the oxidative dehydrogenation of ethane in a membrane reactor.

Several works were devoted to studying the possibilities of applying hydrodynamic effects (jets, vortices) to the intensification of heat and mass transfer in chemical

apparatuses. Two reports concerned the advantages of using microwave radiation as an energy source for such endothermic catalytic processes as the production of hydrogen via the steam conversion of methanol and the catalytic pyrolysis of heavy hydrocarbons.

The mathematical modeling of physicochemical processes in different reactors, including multiphase, fixed- and fluidized-bed, structured, membrane, and multifunctional reactors, was the basic tool of research in nine reports. Ways of increasing the efficiency of distillation processes by optimizing reactor structure were discussed in the report of S. Thotla (Max Planck Institute, Germany). The advantages of the new progressive acetal synthesis technology based on reactive distillation (combining the catalysis and separation of reaction products and initial reagents) were described in the report of I. Agirre (Bilbao University, Spain).

Several reports told of the successful application of mathematical modeling methods for optimizing the industrial catalytic processes for the synthesis of ethylene oxide (X.-G. Zhou, East China University, Shanghai), the partial oxidation of *o*-xylene (C. Castillo-Araiza, Izatapalapa University, Mexico), and the synthesis of nicotinic acid (E. Ovchinnikova, Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Science, Novosibirsk).

Section III reflected the subject area associated with questions of the production and use of alternative fuels. The processing of biomass into fuel and chemical products was represented by 18 oral reports and 15 poster sessions in Subsection A. Prof. V. Kafarov (Colombian Petroleum Institute) presented his interesting results on the production of third-generation biofuels from microalgae with a high content of lipids (one of the most popular fields of bioenergetics) in his keynote lecture. The keynote lecture of Prof. K. van Geem (Ghent University, Belgium) was devoted to the synthesis of olefins by catalytic cracking of the heavy fractions of biomass pyrolysis products. We should also note the works of the collaborators from Åbo Akademi University (Turku, Finland), where studies on the processing of vegetable raw materials with the production of important chemical compounds are being conducted under the supervision of Prof. D.Yu. Murzin. Prof. E. Heeres (Groningen University, the Netherlands) reported on a state-of-the-art approach to the fractionation of biopetroleum (a product of the fast pyrolysis of biomass) to isolate important water-soluble chemical compounds (e.g., carboxylic acids, aldehydes, phenols, furanes, and levoglucosan). Such a complex approach ensures more complete use of biomass pyrolysis products, thus allowing us to increase the competitiveness of pyrolysis technologies. The importance of using cutting-edge approaches in catalysis and engineering for the processing of renewable vegetable biomass and designing catalytic processes for the synthesis of biofuels was emphasized once again in the reports.

Subsection B of Section III included reports devoted to environmental protection technologies in

the processing of solid wastes (two reports), the production of hydrogen and pollution-free fuels (five reports), the processing of natural gas and petroleum (three reports), and the processing of bioethanol into important products (two reports). In particular, the thermal processing of tyres by their liquefaction with coal was considered in the report of M. Sigano (Nihon University, Japan). The production of hydrogen from biomass was discussed in the reports of Professor J. Hanika (Institute of Chemical Process Fundamentals, Prague) and S. Hernandez (Italian Institute of Technology, Torino). Technology for the synthesis of motor fuels with low contents of aromatic compounds from bioethanol was described in the report of Yu. Makarfi (Moscow State Academy of Fine Chemical Technology), while test results on a process for the synthesis of ethylene from bioethanol were represented in the report of A. Kagyrmanova (Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, Novosibirsk). The experimental results and modeling of the pollution-free catalytic combustion of natural gas in gas turbine power plants were presented in the report of Prof. Z. Ismagilov (Boreskov Institute of Catalysis, Siberian Branch, Russian Academy of Sciences, Novosibirsk).

The conference has traditionally included an exhibition of chemical equipment and presentations by different firms. Great interest was aroused by the exposition of the UOP Company (United States), a leader in high technology for the oil refining, gas processing, and petrochemical industries. The Peter Huber Company (Germany) presented the results from its practical application of thermostats. LAAKS (Russia), OOO Rostbiokhim (Russia), and the Autoclave Engineers Division of Snap-Tite Inc. (United States) displayed laboratory equipment for catalytic research at high pressures, particularly a reactor for the Fisher–Tropsch and other high-temperature processes. Attention was also drawn by the exhibits of the Tirit Company (Switzerland), one of the world's largest suppliers of high-pressure reactor systems. Paul Peters (United States), head of the European Office of the international Chemical Abstracts Service Company took part in the exhibition. The company's advertising and informational materials aroused great interest among the delegates to the conference. Discussion of the presented exhibits was continued at round table meetings organized by the different companies' representatives.

On the whole, we can say the Chemreactor-19 conference reflected the progress achieved in world science and industrial practice in the field of developing and studying chemical reactionary processes lasting recent years. It allowed the participants to exchange valuable scientific information, to establish contacts for future collaboration, and to grasp the most important trends in future developments and research. The combination of profoundly fundamental works and



Photo 3.

reports of great practical importance was a distinctive feature of the scientific forum.

Great support in holding the conference was rendered by the Embassy of the Russian Federation in the Repub-

lic of Austria and the Russian Centre for Science and Culture (RCSC) in Vienna. Their active participation ensured the rapid solution of many questions during preparations and promoted efficient organization of this



Photo 4.



**Photo 5.**

international event. S.Yu. Nechaev, RF Ambassador Extraordinary and Plenipotentiary to the Republic of Austria, congratulated the conference upon its opening, and O.Yu. Ksenofontov, the Director of the RCSC, took part in the opening ceremonies. During the conference, Ambassador Nechaev met with a delegation of conference participants in the Embassy of the Russian Federation. Leading Russian scientists, business representatives, and foreign nationals were present at the meeting. The parties noted a high level of the conference's organization and confirmed their mutual interest in and readiness for further expansion

of their cooperation in scientific and technical works. Ambassador Nechaev offered to make Vienna a regular conference site with the participation of Austrian and Russian scientists, and a venue for European and international congresses on the development of innovative technologies in science-intensive, high-technology fields.

No sooner had the Chemreactor-19 conference come to an end in Vienna than the initiative group began organizational work to prepare for the next conference, Chemreactor-20, planned to be held in 2012.