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Members' Newsletter

From disruption to development

The world encountered a disruptive shock in the spring of 2020, in the form of an unknown virus. Humankind has not suffered from similar hardship during the last decades, in the era of very active global traveling and highly interconnected multi-stage and -site production of chemicals and drugs. We have never been as interdependent globally and the COVID-19 crisis has become a timely reminder that Europe needs its own versatile industrial capacity.

We all have been strongly influenced by the restrictions and lockdowns, as catalysis related experimental sciences cannot be performed at home and all the conferences and meetings in the field have been canceled or postponed. The 19th Nordic Symposium on Catalysis will be organized in 2022 in Espoo instead of 24-26.8.2020 and our traditional Young Scientist Forum on Catalysis will take place next time in spring 2021 in Åbo.

Despite the challenges, the scientific community has shown to be flexible and innovative in shifting to distance work and doing what is possible. Meetings, discussions, teaching, doctoral defenses, and even coffee breaks have been successfully carried out online. The internet is an excellent tool and our work would have halted without it, however, it cannot replace face-to-face human interaction. We have hopefully passed the most critical stage of the pandemic and, even though taking two steps forward and one step back, are headed in the right direction.

In many fields of science related to human behavior e.g. social sciences and economy, researchers encountered an unprecedented change in their subject of research and in some cases a severe outdating of research data before publication. This is luckily not the case with catalysis; the laws of nature are still intact.

Disruptive shocks can also enable advancement and even disruptive innovation. We have an unprecedented temporary flood of funds being allocated by governments and the EU to support the economy. Old business models, which were barely hanging on before the crisis, should be allowed to be replaced by more sustainable ones. A part of the resources is being allocated to develop and take into use innovations and support sustainable development. The EU Recovery Plan can transform this crisis into an opportunity to build a more resilient European economy whilst delivering on the European Green Deal objectives. As a solution provider for a climate-neutral and circular economy, the chemical industry will play a critical role in this transition.

Catalysis is, perhaps, the most important interdisciplinary technology in the chemical industry, and certainly one of the areas with the largest societal impact. Catalysis and catalytic processes overall account for about 25% of global GDP and they are in key roles in Europe. We must actively take our share of the possibilities and responsibilities in shaping a more sustainable future.

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I wish you all a successful continuation of the autumn and hope to see you soon, in person!

Henrik Grénman

Chairman

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Nordic Symposium on Catalysis 2020 update

Due to COVID-19 situation, the 19th Nordic Symposium on Catalysis (NSC2020) was postponed to year 2022. Schedule of the postponed event is currently under evaluation and specific date will be decided during autumn 2020. The original date for the event was set to 24th - 26th August 2020.

The organizing committee has started to prepare postponed event and will inform participants as soon as possible.

Follow the updates from Symposium website: http://nsc2020.fi, Twitter account: @nsc2020, #NordicSympCat.

Best regards,

Henrik Grénman

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International Congress on Catalysis for Biorefineries

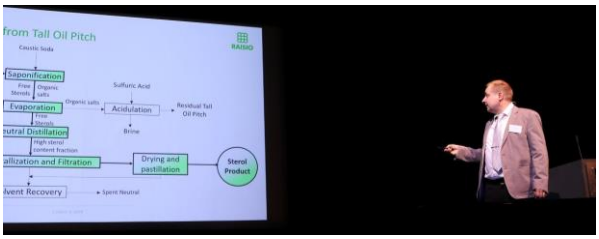
www.catbior2019.fi 23-27.9, 2019

The chairman of the scientific committee Professor Dmitry Murzin giving a talk.

We had the pleasure to host the 5th International Congress on Catalysis for Biorefineries in Turku/Åbo. The 1st CatBior was organized in 2011 in Malaga. Since then, the congress has alternated worldwide. High scientific quality, global visibility and strong cross-disciplinary approach have always been the prominent features of the CatBior conferences.

The 5th CatBior congress covered all aspects of application of catalysis to biorefineries, in particular,

- Fundamental and applied catalysis in biorefinery
- Molecular insights in processing of biomass
- Utilization of lignocellulosic, algal biomass, vegetable oils and other biomass
- Industrial demonstrations
- Catalysis in its variety – homogeneous, enzymatic and heterogeneous catalysis



Dr. Ville Nieminen from Raisio Group delivering a plenary talk.

It was a big challenge to organize the final conference programme, but the result became very exciting and inspiring. Five plenary lecturers and five keynote speakers were invited and the organizers were very y happy that they agreed to come and contributed to the programme. The event was full of great visions: new raw materials, new catalysts and new processes.

Participants enjoying the gala dinner in the Turku Castle.

A characteristic feature of the conference was a very strong interaction: the lecturers got a lot of questions and the poster sessions were really crowded. We are very grateful that leading scientists all over the world came to conference and cultural centre Logomo in Turku/Åbo and shared their experience. After few years, the next CatBior conference will take place in P.R. China: *Ni hao*, what is the activity and selectivity of your catalyst?

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Young Scientist Forum

Unfortunately the 3rd of April 2020 Young Scientist Forum and annual meeting of the Finnish Catalyst Society at Kakola Prison, Turku was cancelled.

Next event is currently planned to be held during spring 2021 along with Catalysis Society annual meeting. Further information will be delivered to the members of the society as soon as possible.

Catalysis related dissertations

M.Sc.(Tech.) Erfan Behravesh from Laboratory of Industrial Chemistry and Reaction Engineering, Åbo Academy University defended her thesis on 6th of March, 2020. The title of his thesis is

"Development of microreactor technology for partial oxidation of ethanol on gold catalyst"

Opponent: Prof. Lars Pettersson, Kunglika Tekniska Högskolan (KTH), Sweden

Custodian: Acad. Prof. Tapio Salmi, Åbo Academy University

Abstract:

Oxidation of alcohols from biological origin is of significant industrial relevance for the production of fine and specialty chemicals. Aldehydes from polyols are important intermediates in pharmaceutical and alimentary industries. Gold nanoparticles dispersed on porous materials are effective catalysts in the oxidation of hydroxyl (-OH) to carbonyl groups (C=O) in the presence of environmentally friendly oxidizers such as molecular oxygen. Microreactors are suitable tools for especially oxidation reactions because of having excellent heat and mass transfer properties due to a high surface-to-volume ratio.

A range of gold catalysts supported on zeolites and oxides were synthesized via a deposition-precipitation method. The effects of the surface charge as well as the pH of the solution on the gold particle size and loading were investigated. The effect of gold deposition on the support acidity was revealed. Both a conventional fixed bed and a microreactor were used for the partial oxidation of ethanol at atmospheric pressure and temperature range of 100–250°C. Catalyst screening was conducted using neat and gold-supported catalysts in the fixed bed reactor. The activities and the selectivities of the catalysts were discussed taken into account the effect of gold particle size and the support acidity. Two catalytic coating methods of microreactor elements were developed using an Au/Al2O3 catalyst selected from the screening step as one of the most promising catalysts in terms of the activity and selectivity to the desired products. The first coating method was based on the use of a catalyst slurry. The second method was inkjet printing. In this method, the alumina suspension was first printed into the microchannels followed by gold deposition via a deposition-precipitating step. Inkjet printing has the advantage of a higher precision but a more complicated chemistry since additives are needed.

A model was generated to explain the experimentally observed fixed bed and microreactor behaviors in the ethanol oxidation on gold nanoparticles. The model for this heterogeneously catalyzed gas-phase multireaction system consisted of dynamic mass and energy balances as well as expressions for the reaction kinetics. The gas fluid flow was described with convection and dispersion terms. The axial and radial

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concentration and temperature profiles inside the reactor and the concentration profiles within the catalyst particles were predicted by the model. Numerical simulations were performed to illustrate the influence of the feed temperature and the catalyst loading as well as the effect of the flow pattern, i.e. the Péclet number on the obtained results.

Molecular modelling computations at the DFT level were conducted to elucidate the reaction mechanism of the oxidative dehydrogenation of ethanol. Using the mechanism inspired by the computational studies, an improved kinetic model was developed by revisiting the previous data obtained with the microreactor to explain the measured rates of acetaldehyde formation. Moreover, the concentration profiles in the catalyst particles and layers were calculated numerically to evaluate the role of internal diffusion in the catalyst pores. The simulation results indicated the absence of internal mass transfer limitations for catalyst layer thicknesses less than 200 µm.

M.Sc. Soudabeh Saeid from Laboratory of Industrial Chemistry and Reaction Engineering, Åbo Academy University defended his thesis on 16th of March, 2020. The title of her thesis is

"Destruction of selected pharmaceuticals by ozonation and heterogeneous catalysis"

Opponent: Professor, Dr-Ing. habil. Rüdiger Lange, Technische Universität Dresden, Germany

Custodian: Acad. Prof. Tapio Salmi, Åbo Academy University

The defence was the first of a kind – with the defender in one room, the opponent in another, and the audience in a third, due to the distance rules of state of emergency.

Ms Soudabeh Saeid defends the thesis in front of an almost empty auditorium with the Custos (Salmi), the evaluation committee, and the opponent (Lange) on the screen.

Abstract:

The availability and quality of clean and safe water supplies is directly connected to the modality of wastewater treatment. Municipal wastewater treatment processes are designed to purify and degrade polluting components from water, most of these technologies are not capable to eliminate organic micro-pollutants entirely but might even increase the toxicity of the treated water compared to untreated water by transforming these contaminants to more toxic components. Among these organic pollutants, the frequently occurrence of pharmaceuticals in surface waters has attracted a significant concern due to their non-biodegradability, chemical resistance, and toxicity impact on the aquatic life. These contaminants and the by-products of their degradation continuously discharge to surface waters and maintain their chemical structure, and therapeutic efficiency for a long period of time.

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The degradation of four frequently detected pharmaceutical molecules in the Baltic Sea region, ibuprofen, carbamazepine, diclofenac and sulfadiazine by catalytic and non-catalytic ozonation was studied in this work. The purpose of the research was to synthesize active and durable heterogeneous catalysts that, combined with an ozonation process could eliminate these contaminants without toxic by-products.

All these components were pharmaceutical destroyed within one hour by ozonation in a laboratory scale semi-batch reactor, however, the ozonation process produced several long-lasting degradation by-products. The kinetics of the pharmaceuticals degradation and formation of by-products were investigated in detail. Twenty-four heterogeneous catalysts were screened in the presence of ozone to optimize the destruction process. For a better mass transfer between the phases and easier separation of catalysts, the catalysts were immobilized inside the SpinchemTM Stirrer. The catalytic ozonation technology allowed the enhancement of the degradation rate of pharmaceuticals and the suppression the formation of by-products. The catalytic and non-catalytic ozonation screening revealed the reaction kinetics of the pharmaceuticals and their transformed intermediates during the ozonation experiments. Later on, based these results, a kinetic model for the ibuprofen ozonation was derived. The model exhibited a good correspondence with experimental data.

The heterogeneous catalysts were synthesized by several methods and screened in the ozonation process to reveal the impact of various catalyst preparation techniques, type of metals, loading of metals on the catalysts, amounts of Lewis and Brønsted acid sites, type of supports, on the elimination of pharmaceuticals as well as the transformation and degradation of by-products. All-important characterization devices were employed to understand the performance of the catalysts (X-ray powder diffraction, transmission electron microscopy, nitrogen physisorption, scanning electron microscopy, energy dispersive X-ray micro-analyses, pyridine adsorption-desorption with FTIR spectroscopy, X-ray photoelectron spectroscopy). Evaluation of the catalytic activity showed that some of the employed catalysts have the higher influence on the elimination of the pharmaceuticals such as Fe-H-Beta-25-EIM catalysts. Higher specific area, metal concentration and Brønsted acidity are some of the characteristics which made these catalysts valuable for the ozonation process.

The audience is listening in the auditorium of Hotel Scandic Julia, 500 meters away. Kuvat: Pasi Tolvanen

Obituary

Professor Bernard Delmon

Professor emeritus Bernard Delmon, of the Faculty of Bioengineers of Université Catholique de Louvain-la-Neuve, Belgium, passed away on April 7, 2020 at the age of 87.

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I remember Professor Bernard Delmon as a man who was very eagerly involved in almost “all” activities related to catalysis. He initiated several series of international congresses still running today, among which the Symposium on Homogeneous and Heterogenous Catalysis started in 1974 in Brussels and the Symposium on the Scientific Bases for the Preparation of Heterogenous Catalysts jointly organized every four years with the Katholieke Universiteit Leuven. His name could be found in organizing and scientific committees of numerous conferences and symposia globally. In addition, Professor Delmon was the founder of the journals "Applied Catalysis" and "Catalysis Today" and the series "Studies in Surface Science and Catalysis".

Professor Delmon started his career at the Institut Français du Pétrole (IFP) from 1959 to 1970. Later, he moved to UCLouvain. He founded the research group on heterogeneous catalysis still active in UCLouvain. His research interests widely covered many aspects of catalysts and catalytic reactions, mainly related to heterogeneous catalysis. Especially, his activities on hydrotreating and conversion of biomass became familiar to our group as they were closely related to our research at TKK (presently Aalto University). During his active career, Professor Delmon was an author of more than 600 research papers and 18 patents. In addition, he co-edited 18 books and several special issues of journals.

Honouring Professor Bernard Delmon, Applied Catalysis published a special issue on his 80th birthday in 2014 (Appl. Catal. A, Gen. 474 (2014) 1–280).

Outi Krause
Professor emerita

Web pages

http://www.katalyysiseura.org

http://www.kemianseura.fi

http://www.efcats.org

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The Board of the Finnish Catalysis Society wish to get feedback about the Katse newsletter from the members of the society.

In addition, please send news and information of activities e.g. doctoral dissertations, national and international events, prizes, and courses to be published in the Katse. The feedback and news can be sent to the Board members.

Thank you.