



## Members' Newsletter

### From excitation to relaxation and back

The importance of catalysis and its development on the well-being of humankind and our globe was once again recognized in the Nobel Prize award ceremony held in December 2018. The prize in chemistry (1/2) went to Frances Arnold from California Institute of Technology for her work in developing the function of proteins that solve chemical problems. "In 1993, Arnold conducted the first directed evolution of enzymes, which are proteins that catalyze chemical reactions. The uses of her results include more environmentally friendly manufacturing of chemical substances, such as pharmaceuticals, and the production of renewable fuels."

The Society's main event of the year, the Finnish Young Scientist Forum on Catalysis and annual meeting, was held on the 5th of April in Oulu in a very nice place called Voimala 1889. The scientific program was of high standard and the dinner was excellent with live music. I will not go into more detail here, as some of our even younger scientists have written an excellent report on the whole event published later on in this issue. However, I wish to congratulate the colleagues in Oulu including Docent Mika Huuhtanen for the excellent organizing of the event.

The annual meeting of the Society was held after the YSF and besides other important decisions, it brought along some changes to the board. Professor Juha Lehtonen stepped down from the position of chairman after serving a full term. The Society expresses its gratitude for the hard and fruitful work in developing all the activities. Noora Kaisalo

from VTT was elected to the board as a new member, welcome Noora!

The later part of summer and the coming autumn bring along exiting events in the field of catalysis abroad and in Finland. One of the main events in the field, the 14th European Congress on Catalysis, was held in Aachen from 18 – 23 August. We had a rather large delegation attending from Finland, who will report about their experiences in the next issue. Another exiting event, the 5th International Congress on Catalysis for Biorefineries will be organized September 23-27 in Turku / Åbo. Moreover, an interdisciplinary event very relevant also for catalysis, the International Conference on Imaging and Characterization – Future technologies and applications, will be held 8 - 10 January in Oulu. The conference topics cover e.g. recent development in imaging and characterization; atmosphere and environment; materials and processes; and bio and medical sciences. The deadline for abstract submission is 15.9.2019.

Another thing that should get off to a real start in the autumn is the work of our new government. According to the promises made, we should be able to look forward to increasing university and research financing, which should also promote larger company investments. Strong policy emphasis is placed on e.g. climate change mitigation, bio-chemicals and fuels production, processes intensification, and circular economy. Catalysis is in the core of this development!

However, to the question at hand. After a lovely spring, we have enjoyed a delightful summer. Simple extrapolation leads to strong indication of a great autumn. A state of



continuous excitation is not sustainable and relaxation is needed for maintaining stability and for being able to get excited again.

I hope that everyone had an enjoyable summer and I wish you all a pleasant beginning of the autumn!

*Henrik Grénman*

Chairman

## 4<sup>th</sup> Finnish Young Scientist Forum on Catalysis

The 4<sup>th</sup> Young Scientist Forum on Catalysis took place the 5<sup>th</sup> of April. This year in Oulu. A wide variety of young researcher from different academic institutions came to the seminar and exposed their topics under two formats: short oral and Pecha Kucha presentation. There were also two very interesting keynote lectures and a prize lecture.

The seminar was set up with the registration of the participants and a welcoming coffee with plentiful servings. After coffee, the chairman opened the seminar with an introductory speech followed by Dr. h.c. Matti Härkönen's keynote lecture from entitled "From Finnish catalysis research to International environmental business". This lecture presented an industrial perspective on catalysis, which was of high interest for the public, which mainly had an academic background. The seminar continued with a session of short oral presentation and Pecha Kucha with only short breaks in between.



Photo by Satu Ojala

*Dr. h.c. Matti Härkönen giving his presentation.*



The organization of the oral presentation session was on point; all presentations of a same session were part of the same area of research or addressed similar academic and/or industrial issues. This promoted discussions and debates between young researchers, as well as the growth of personal and professional networks. During the coffee breaks, it was common to see post-presentation discussions with additional questions to the presenters. Something, which to some extent was cumbersome for the participants was the timing of the Pecha Kucha presentation, which was an interesting new concept for most.

The invited lecture entitled “Transient methods in catalysis” presented by the Academy Professor Tapio Salmi was a very interesting one. Professor Salmi gave his presentation in a very enthusiastic and energetic way displaying how a deep understating of molecular processes can be crucial for understanding and improving surface based processes.



*Academy professor Tapio Salmi explaining the importance of transient methods.*

Afterwards the forum continued with more Pecha Kuchas, which topics were devoted mainly to the conversion of lactones and the understanding of their reaction pathways

using DFT Calculations. This combination gave an interesting example of how the cooperation of experimental and theoretical studies can work together. The YSF ended with the start of the annual meeting of the Finnish Catalysis Society.

The time between the end of the forum and the dinner was used by our group for exploring the city from many points of interest. The cold weather and the frozen sea provided a nice scenery. After returning to the dinner restaurant, good discussion with people from different universities took place. In stimulating discussions, the topics roamed from science to more casual topics. The group from Oulu was very friendly and fulfilled their role as a host in a spectacular way during and after the excellent dinner.

Wander Perez, Matias Alvear  
and Ole Reinsdorf



*YSF participants at dinner after the seminar.*

## **Please give feedback on organization of the Young Scientist Forum**

The Finnish Catalysis Society is collecting feedback on the FYSFC2019 event, with the goal to develop the event further for next year. All Finnish Catalysis Society members are welcome to give feedback, regardless of whether or not you were present at this year's event. The feedback survey is anonymous; and answering should not take more than 5-



10 min of your time. The survey will be open for answering until September 30, 2019.

Feedback is collected through the Google Forms survey, and it can be found from:

<https://urly.fi/1fGv>



## 5<sup>th</sup> Doctoral Thesis Award to Sakari Tuokko

Dr. Sakari Tuokko was selected as the recipient of the fifth PhD thesis award of Finnish Catalysis Society. Sakari Tuokko defended his PhD thesis in University of Jyväskylä in December 2016.

Prof. Freek Kapteijn from Technical University of Delft, Netherlands selected the winner writing in his evaluation as follows:

*“The work of Dr. Tuokko described in this thesis is of outstanding quality, interdisciplinary of character, covering aspects of heterogeneous, homogeneous and computational catalysis applied to organic chemistry, ranging from experimental to theoretical activities.*

*Dr. Tuokko has succeeded in gaining detailed new insights in and understanding of reaction mechanisms of selective hydrogenation and hydrosilylation over Pt and Pd catalysts, revealing among other the subtle control of chemo- and stereo-selectivity by surface coverage of the reacting species.*

*The research is presented very clearly in a highly readable thesis, in which the candidate shows his knowledgeability and maturity in the fields of organic chemistry, heterogeneous catalysis and theoretical modeling.*

*The thesis presents a major step forward in the combined application of organic chemistry transformations and theoretical simulations to understand the reactivity on surfaces of metal catalysts.”*

The Finnish Catalysis Society warmly congratulates Dr. Sakari Tuokko!



Profs. Juha Lehtonen and Riikka Puurunen presented the award to Dr. Sakari Tuokko.

## Preparations for Nordic Symposium on Catalysis 2020 ongoing

The Nordic Symposium on Catalysis gathers together every second year catalysis researchers from the Nordic countries. The 19<sup>th</sup> Nordic Symposium on Catalysis (NSC2020) will take place in Espoo 24<sup>th</sup> – 26<sup>th</sup> August, 2020, following the 18<sup>th</sup> Nordic Symposium on Catalysis in Copenhagen, Denmark in 2018. This will be the 5<sup>th</sup> time that the symposium is organized in Finland.



The aim of the Symposium is to create a breeding ground for ideas by ensuring meetings between researchers and catalyst developers, from academy as well as from industry. The Symposium will cover catalysis broadly including plenary lectures, Berzelius Prize lecture and parallel sessions with Nordic keynote lectures, oral contributions and poster sessions. In 2020, the scientific themes of the symposium will be (i) Catalysis for the climate change mitigation and (ii) Catalysis in Nordic Countries.

The organizer of NSC2020 is the Finnish Catalysis Society, with Res. Prof. Juha Lehtonen (VTT) as the chairman of the conference; Prof. Riikka Puurunen (Aalto Univ.) chairing the Scientific Committee; and other Organizing Committee members being Prof. Henrik Grenman (Åbo Akademi), Dr. Elina Harlin (Neste), Dr. Salla Likander (Neste), Prof. em. Outi Krause (Aalto Univ.), and Dr. Matti Reinikainen (VTT).

The conference website <http://nsc2020.fi> has been recently opened. The conference has a Twitter account: [@nsc2020](https://twitter.com/nsc2020) and you can also follow it with the hashtag [#NordicSympCat](https://twitter.com/hashtag/NordicSympCat). On the basis of previous conference, we expect about 150-200 participants.

Similarly as in previous years, the goal is to expand some of the conference presentations into scientific articles to be published in a special issue of [Topics in Catalysis](#) journal. The special issue related to the previous conference has just been published: see e.g. the editorial by Riisager et al., *Topics in Catalysis* 62 (2019) 589, <https://doi.org/10.1007/s11244-019-01192-z>.

Juha Lehtonen & Riikka Puurunen

## Catalysis related dissertations

**Dr. Zouhair El Assal** from Environmental and Chemical Engineering Research Unit, Faculty of Technology, University of Oulu defended his thesis on 11<sup>th</sup> of December, 2018. The title of his thesis is

**“Synthesis and characterization of catalysts for the total oxidation of chlorinated volatile organic compounds”**

*Opponent:* Prof. Juan-Ramón González-Velasco, University of the Basque Country, Spain

*Custodian:* Prof. Riitta Keiski, University of Oulu

### Abstract:

The harmful emissions of chlorinated volatile organic compounds (CVOCs) originate only from man-made sources. CVOCs are used in a variety of applications from pharmaceuticals production to decaffeination of coffee. Currently, CVOC emissions are limited by strict legislation. For these reasons, efficient CVOC abatement technologies are required. Catalytic oxidation is very promising option for this purpose, since catalysts can be tailored to each case to maximize the efficiency and minimize the formation of unwanted products, such as dioxins or Cl<sub>2</sub>.

The goal of this thesis was to study the role of the physico-chemical properties of catalysts in dichloromethane (DCM) oxidation. To reach the aim, several catalytic materials were



prepared and characterized, and their performance was tested in total oxidation of DCM. The catalytic materials used were powders of four single metal oxides ( $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, CeO<sub>2</sub>, MgO), three mixed oxides (Al<sub>2</sub>O<sub>3</sub>-xSiO<sub>2</sub>) washcoated on a cordierite monolith and four active phases (Pt, Cu, V, Mn).

At first, support properties were studied. It was found that the DCM conversion and HCl production are dependent on support acidity when the studied single oxides are considered. The best DCM conversions and HCl yields were observed with the support having the highest total acidity ( $\gamma$ -Al<sub>2</sub>O<sub>3</sub>). Further, the quality of the by-products formed was dependent on the type of the acid sites present on the support surface. Secondly, the impregnation of the active compound was observed to improve the selectivity of the material. From the tested active phases, Pt presented the best performance, but also V<sub>2</sub>O<sub>5</sub> and CuO showed almost equal performances. Especially CuO supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, that had less formation of by-products and is less toxic than V-containing oxides, seems to be a promising alternative to Pt. Concerning stability, no deactivation was observed after 55h of testing of Pt/Al<sub>2</sub>O<sub>3</sub>. Furthermore, in the used reaction conditions, the formation of CuCl<sub>2</sub> is not thermodynamically favoured. Finally, the good characteristics of the powder form catalysts were successfully transferred to the monolith. The performance of the Pt/90Al<sub>2</sub>O<sub>3</sub>-10SiO<sub>2</sub> catalyst in DCM oxidation was improved when the channel density was increased due to an increase in geometric surface area and mechanical integrity factor, and a decrease in open fraction area and thermal integrity factor.

**M.Sc. Lidia I. Godina** from Laboratory of Industrial Chemistry and Reaction Engineering, Johan Gadolin Process Chemistry Centre, Faculty of Science and Engineering, Åbo Akademi University defended her thesis on 22<sup>nd</sup> of February, 2019. The title of her thesis is

**“Aqueous-phase reforming of renewable polyols for sustainable hydrogen production”**

*Opponent:* Prof. Sebastien Paul, Ecole Centrale de Lille, Unite de Catalyse et Chimie du Solide Lille, France

*Custodian:* Prof. Dmitry Murzin, Åbo Akademi University

**Abstract:**

Renewable biomass can be utilized for sustainable hydrogen production via aqueous phase reforming (APR), which implies catalytic conversion of aqueous solutions of alcohols and polyols over transition metals at comparably low temperatures with formation of hydrogen, CO<sub>2</sub>, light alkanes, and a number of products in the liquid phase.

The current work is devoted to studies of APR of several alcohols and polyols and their technical mixtures over mono- and bimetallic catalysts [I-IV, VII]. A realistic APR reaction network [I, VII] and a kinetic model [V] were proposed, reactor modelling and process design were performed in [V, VI], and techno-economical analysis of APR was provided in [VI].

Propanol-1, propane-1,2-diol, glycerol, xylitol and sorbitol were studied in APR over different Pt/C catalysts. Influence of feed



chirality was investigated for the first time in APR of sorbitol and galactitol over Pt/Al<sub>2</sub>O<sub>3</sub> catalyst. Conversion of the technical mixture of sorbitol and mannitol was compared to commercial sorbitol in APR over Pt/C. Mono- and bimetallic carbon-supported catalysts were compared in terms of activity and selectivity in xylitol APR.

The reliability of the liquid-phase product analysis was considerably improved. Plausible reaction pathways were proposed according to the product distribution and discussed from a thermodynamic point of view. Different reaction paths of 1,2-propanediol APR were computationally screened on a Pt(111) model surface specifically addressing the competition between C–H, O–H, and C–C bond cleavages.

Experimental data obtained in the xylitol APR was utilized for reaction kinetics modeling, dynamic reactor simulation, and process design development. The process can be considered as a self-sufficient one, since the reactor heat demand is fully covered by the combustion of alkanes produced in APR.

Simulation of in-situ phase equilibrium was based on the results of the sorbitol APR. Process design of a hydrogen production plant with 500 kg/h capacity operating with sorbitol syrup was developed and optimized. A detailed techno-economical analysis was performed for the first time for estimation of hydrogen production price.

**M.Sc.(Tech.) Salla Jaatinen** from Catalysis Research Group, Aalto University defended her thesis on 29<sup>th</sup> of March, 2019. The title of her thesis is

**“Carbon catalysts in biofuel production: from furfural to 2-methylfuran”**

*Opponent:* Prof. Edd Blekkan, Norwegian University of Science and Technology, Norway

*Custodian:* Prof. Riikka Puurunen, Aalto University

**Abstract:**

Production of bio-based chemicals, fuels and energy are essential in the current climate environment. Hydrotreatment of renewable platform chemical furfural yields many valuable products, such as furfuryl alcohol and 2-methylfuran (MF). MF has excellent properties for use as a gasoline octane booster to replace current fossil methyl tert-butyl ether and ethyl tert-butyl ether. The current CuCr-catalyst in furfural hydrotreatment is toxic and new and selective catalysts are required.

In this dissertation, noble metal free and non-toxic catalysts were prepared for production of MF. Metal catalyst options chosen for this work were copper, nickel and iron. High yields (up to 60%) of MF were achieved with the prepared catalysts in liquid phase batch reactor experiments in short reaction time (1 - 2 h). High temperature (230 °C) and high hydrogen partial pressure (40 bar) were optimal for MF production, and the most optimal metal combinations were copper-nickel and copper-iron. Active metals were tested in MF production on various activated



carbon supports and a mesoporous carbon material (CMK-3). Deep characterization was performed to obtain data of beneficial catalyst characteristics for MF production. Production of MF was enhanced by small metal particle size, small pore volume and higher acidity. These enhancements suppressed the production of competitive products and side reactions, and increased the selectivity towards 2-methylfuran.

Solvents may also react in furfural hydrotreatment. The applied 2-propanol can react through catalytic transfer hydrogenation (CTH) offering hydrogen for hydrotreatment reactions and producing acetone. The solvent can also dehydrogenate to acetone and hydrogen. Acetone formation mechanisms were studied with the prepared catalysts. The acetone formation was metal dependent: with nickel and copper acetone formation occurred through CTH while with iron also dehydrogenation took place.

Hydrogen solubility in the reaction media is important for the process and especially in scaling up processes. Hydrogen solubilities in furfural and 2-propanol were measured and observed to increase as a function of temperature (50 - 200 °C) and pressure (50 - 125 bar). Hydrogen solubility in 2-propanol was observed almost three times higher to solubility in furfural. By way of example, at 200 °C and 125 bar hydrogen mole fraction in 2-propanol and furfural was measured to be 0.064 and 0.038 respectively. The solubility data was modelled with PC-SAFT model and the model predicted the hydrogen solubility data well.

This dissertation offers a MF selectivity optimized and fast noble metal free catalyst alternative for the current catalyst, new data of hydrogen solubility in the reaction media and optimized carbon support characteristics for the production of MF.

**M.Sc. Andrea Pérez Nebreda** from Laboratory of Industrial Chemistry and Reaction Engineering, Johan Gadolin Process Chemistry Centre, Faculty of Science and Engineering, Åbo Akademi University defended her thesis on 3<sup>rd</sup> of May, 2019. The title of her thesis is

**“Valuable monomers and oligomers from hemicelluloses”**

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

*Custodian:* Assoc. prof. Henrik Grénman, Åbo Akademi University

**Abstract:**

Current environmental problems such as global warming and climate change related to greenhouse gas emissions have enhanced industrially relevant research aimed towards a more sustainable future. The biorefinery concept plays a key role in the development. Lignocellulosic biomass is the most abundant renewable resource on the earth and it can be potentially converted to different biofuels and biochemicals, which diminishes the current dependence on fossil feedstocks.

Lignocellulosic biomass is composed of three major constituents: cellulose, hemicellulose, and lignin. Hemicelluloses can account for up to 20-40% of the total dry weight of lignocellulosic materials and this fraction is very often underutilized in industry. However, hemicelluloses are heteropolysaccharides which can be cleaved into their monomeric constituents yielding different pentose and hexose sugars, which



can be further be transformed into fuels and chemicals.

Hemicelluloses can be obtained from biomass by different pretreatment methods, in which the biomass is selectively fractionated into its different constituents. Pressurized hot water extraction (PHWE) is a method which can be utilized for extracting hemicelluloses without degrading the extracted sugars. Water is used as a solvent, which makes the process environmentally friendly. The extraction of hemicelluloses by PHWE from stone pine, holm oak and Norway spruce was investigated in the current work. The main experimental parameters were the effect of temperature, raw material, and the solid-to-liquid ratio.

The hydrolysis of two structurally different hemicelluloses was studied in different reactor configurations in the presence of acidic catalysts. Oacetylgalactoglucomanan and inulin were selected as model substrates as they differ significantly from each other; the former being a large, branched and complex molecule while the latter is linear and significantly simpler. The reaction products were mainly sugar monomers.

Hydrolysis of the hemicelluloses using a homogeneous acid catalyst (HCl) was studied in a continuous tubular reactor. The experimental conditions influenced significantly the conversion and product distribution, and the influence of the different parameters on the reactor performance was systematically investigated.

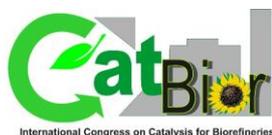
Continuous production of sugar monomers without degradation to low-molecular products was achieved in optimal conditions. The reaction mechanisms and the kinetics of inulin hydrolysis to fructose in the presence of a solid catalyst (cation-exchange resin) were studied in a batch reactor. A detailed

mathematical model was successfully utilized for describing the intrinsic kinetics of the hydrolysis. The kinetic data obtained were subsequently used to design a continuous reactor system of the packed bed type. The continuous reactor developed in this work was equipped with intermediate sampling points between the catalyst beds, which enabled following the progress of the hydrolysis along the reactor. High fructose yields were obtained in the hydrolysis of inulin. Detailed flow characterization was carried out, taking into account mass transfer limitations. An advanced mathematical model comprising kinetics, mass transfer phenomena, and flow characteristics in the reactor was developed and solved numerically. The model was well able to describe the performance of the continuous fixed bed reactor.

Overall, the results obtained in the current work demonstrate the feasibility of the efficient hydrolysis of hemicelluloses in a continuous reactor using a heterogeneous catalyst and they contribute to designing and evaluating the performance of the process.



## Conferences and symposia



### Catbior2019 in Turku!

A top-level international scientific event, the 5<sup>th</sup> International Congress on Catalysis for Biorefineries, Catbior2019, will be held in Turku/Åbo, in the conference and cultural centre Logomo from Monday, September 23 to Friday, September 27, 2019.

The 1<sup>st</sup> Catbior originated in 2011 in Malaga. Since then, the congress alternates worldwide in odd years: the 2<sup>nd</sup> congress was held in Dalian in 2013 followed by congresses in Rio de Janeiro in 2015 and Lyon in 2017.

Catbior2019 covers all aspects of application of catalysis on biorefineries, particularly

- 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

The Scientific programme of CatBior2019 consists of plenary and keynote lectures as well as oral and poster presentations.

The invited plenary lecturers are: Prof. Raghunath V. Chaudhari, The University of Kansas; Dr. Ville Nieminen, Raisio Group; Dr. Catherine Pinel, IRCELYON, Lyon-Villeurbanne; Prof. Keiichi Tomishige, Tohoku University; and Prof. Dionisios G. Vlachos, University of Delaware.

Please, visit the website [www.catbior2019.fi](http://www.catbior2019.fi) and join the conference!

### International Conference on Imaging and Characterization - Future Technologies and Applications

January 8-10, 2020, Oulu, Finland  
[www.oulu.fi/ICFUTURE2020](http://www.oulu.fi/ICFUTURE2020)

NOTE! Abstract submission by September 15, 2019.

### 17<sup>th</sup> International Congress in Catalysis (17ICC) “2020 Vision for Catalysis”

June 14-19, 2020, San Diego, CA, USA  
<https://2020icc.com/>

Abstract submission by October 31, 2019.

### See also e.g.

[www.conference-service.com](http://www.conference-service.com)

[www.iacs-catalysis.org](http://www.iacs-catalysis.org)

### Web pages

<http://www.katalyysiseura.org>

<http://www.kemianseura.fi>

<http://www.efcats.org>

# Katse

1/2019

Suomen katalyysiseura  
Finska katalyysällskapet  
Finnish Catalysis Society



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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.*