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Members' Newsletter

Is dispersion in catalysis a necessity?

"A particular phenomenon associated with the rates of chemical reactions that is of great theoretical and practical interest is catalysis, the acceleration of chemical reactions by substances not consumed in the reactions themselves—substances known as catalysts. The study of catalysis is of interest theoretically because of what it reveals about the fundamental nature of chemical reactions; in practice, the study of catalysis is important because many industrial processes depend upon catalysts for their success. Fundamentally, the peculiar phenomenon of life would hardly be possible without the biological catalysts termed enzymes."

The quotation above is from Encyclopedia Britannica's definition of catalysis. A distinctive feature is that it does not classify and divide catalysis strictly into different subgroups. According to the same logic, introductory courses typically present catalysis broadly, as a phenomenon followed by describing distinct features in the different areas. It is first in the advanced courses that deeper specialization and separation take place.

When a student progresses from the basic and advanced courses towards becoming a researcher in the field, he or she is increasingly classified according to the type of catalysis that is in question and the forums of discussion and interaction diverge. If we look at the catalysis community in Europe, the Nordic countries as well as in Finland, it is typical that an advanced level structure has been adopted. This is of course natural when the aim is to promote deep-going discussions on the details within the selected area. Similarly, practitioners of different subspecialties in internal medicine are as well experts in their specific topics; however, it is a great advantage to remember that the fields are in many ways interconnected.

In the field of catalysis, complex revolution of moving to sustainable carbon-neutral production of commodities requires novel solutions. All our work, be it so-called basic or applied research aims at contributing to industrial production in one way or another. From the industrial (or patients) point of view, it does not really matter who is capable of solving the challenges, but rather that it is done efficiently. In the best case, several issues can be addressed simultaneously, if the communication and collaboration are fluent. The modern biorefinery concept is a prime example of the need for a broad interdisciplinary approach.

Changes in working culture are seldom rapid, thus, it is the common direction that is important. Different fields of catalysis are not competitive, but rather complementary and collaboration is always beneficial, especially in the long run. The common goal is clear – prosper together and avoid the coroner!

Finland is a small country population-wise with top-level expertise in the different areas of catalysis. We can utilize this aspect to our advantage by being more dynamic and coherent than our larger competitors. We need efficient platforms for interaction; novel ideas are often created when different viewpoints are heard and new links are formed. One of the

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basic tasks of the Finnish Catalysis Society is to serve as one of these platforms and everyone interested in catalysis is warmly welcome to take part. This newsletter along with the invitation to our FYSFC has been distributed widely in the Finnish catalysis community and I hope to see many of you (virtually) on the 9th of April!

Henrik Grénman

Chairman

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Update on 19th Nordic Symposium on Catalysis

After cancellation (because of Covid-19) of the event originally planned for August 2020, the 19th Nordic Symposium on Catalysis has been rescheduled to take place on June 6-8, 2022. The event will be organized in Otaniemi, Espoo, Finland.

Please follow the progress of event organization at the website: http://19nsc.fi, and Twitter: @19thNSC, #NordicSympCat.

Juha Lehtonen & Riikka Puurunen

Welcome to the 5th Finnish Young Scientist Forum on Catalysis

The 5th Finnish Young Scientist Forum will be organized as online event on **April 9 2021**, in connection with the Annual meeting of the Finnish Catalysis Society. In the one-day event, doctoral students and companies are invited to present their research in oral talks and online poster presentations. Contributions from all subfields of catalysis are very welcome: homogeneous, heterogeneous, enzymatic, and polymer catalysis; presentations covering aspects from theore-tical chemistry to material science and chemi-cal engineering.

After the Finnish young Scientist Forum event, the annual meeting of Finnish Catalysis Society will take place. Save the date already now in your calendars. More info will be come at the websites of the Finnish Catalysis Society

http://www.katalyysiseura.org

Society members will be also notified with an invitation email and registration form.

Anniversary of the Young European Catalysis Network

Despite the difficult times, YEuCat is growing and already turned 1! A virtual birthday cake was shared at the 1st YEuCats delegate assembly. It was time to meet and look back on all the activities the YEuCat network organized during the first year and communicate all the amazing new activities we are organizing in the year ahead. We were able to meet virtually with our peers, share our opinions and shape the future of the network. New targets were set!

The meeting took place on Zoom platform on the 26th of February 2021. In a buzzing atmosphere, we had a chance to look back on all the past activities that we experienced during our first year of existence, such as virtual Couch Catalysis and Beach Catalyst poster conferences, Catalysis Talks, virtual pub-quiz and others. Through these activities we aimed at giving young researchers an opportunity to present their work and discuss with peers. We also reflected on our collaboration with VS Particle - Material Pioneers and the European Young Chemists' Network (EYCN). Despite the challenges during the year, we had a chance, thanks to the support of our sponsors and colleagues, to take a part in the 2020 EFCATS Summer Scholl in Slovenia having a place on stage.

We disclosed new ways of communication that have become popular and efficient within the younger generations. Strengthened with our new members, we are planning webinars about working paths after graduation and awards for the future generations, which will soon be launched on our web page (www.youngcatalysis.net). Moreover, we are truly happy to welcome all the interested

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young scientist to join our YEuCat Better Together workshop that will take place this summer in Segovia, Spain. There we will actively learn to collaborate while solving a relevant societal problem!

Big thanks to all the young scientists that joined us and made the past year possible! We cordially invite all who missed it to become a part of our network.

On behalf of the YEuCat team,
Nemanja Vucetic

Introduction material to the field of Catalysis

Henna Kleemola (University of Jyväskylä) made an interesting observation during her Master's Thesis work regarding catalysis as a part of high school chemistry syllabus. Her finding was that although catalysis has a significant role in chemistry, the topic is rarely represented in graduate examination (ylioppilaskoe) or high school courses. In order to improve the situation, Henna Kleemola who graduated as chemistry teacher, prepared catalysis introduction presentation material designed for high school students. Although material is mainly targeted to high school students, presentation gives rather interesting summary of topic areas from academia to industry. The material was compiled in collaboration with Prof. Jan Lundell and Prof. Karoliina Honkala from University of Jyväskylä.

Presentation material is available to all members of Finnish Catalysis Society. Inquiries can be sent to Finnish Catalysis Society secretary Niko Heikkinen (e-mail: firstname.lastname at vtt.fi).

Emission catalyst development and production in Dinex Finland

The catalyst technology history and latest news of emission catalyst development and manufacture are here reviewed in Dinex Finland. A long way during the last 38 years has contained many steps and changes as state, investment company (2004-2013) and private (2013- today) owned (Kemira → Kemira Metalkat/1994 → Ecocat/2003 → Dinex Ecocat/2013 → Dinex Finland/2019). Dinex Finland has been since 2013 a part of Danish Dinex Group, which is a private owned company with the main owner of CEO Torben Dinesen.

Early history in emission catalyst business and Open Foil Coating

In 1980s, the state-owned Kemira (CEO Yrjö Pessi) spread in chemical industry to many new countries and fields by company takeovers or own development (emission catalysts, hydrogen peroxide, formic acid, air gases, organic chemicals, etc.). It was looked also for new business to replace the production (ammunitions) in Vihtavuori plant (20 km north from Jyväskylä). The development chemist Pekka Lappi proposed in 1983 a business potential of emission catalysts, which had been already in gasoline car market in USA and Japan since 1970s and emission legislations were planned for Europe and world-wide after next few years [1]. Before that wider concern of emissions, catalysts and particulate filters were applied in certain indoor machine (e.g. oxidation catalysts and filters in mines) applications and locally at least since 1960s. The three-way catalyst (TWC) was an innovative solution in 1970s to remove simultaneously CO, hydrocarbon (HC) and nitrogen oxides (NO_x) in stoichiometric air/fuel conditions (lambda (λ)

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~ 1) of gasoline engines. To reach emission limits, the use of TWCs required also new stoichiometric combustion control, λ sensors and lead-free gasoline. In fact, it has been noted that a key result related to the use of TWCs was the dramatic drop in Pb emissions to nature. TWCs became mandatory for all Western European gasoline passenger cars at the beginning of 1990s, which created a new business field.

Kemira proceeded very quick in development, the first full-time research engineer was hired in 1983 and catalyst development was concentrated since 1984 in Oulu Research Centre, which was the development centre of inorganic chemicals in Kemira. The main commercial catalyst structure had been a ceramic cordierite honeycomb, which was dip coated (→ post-coating) in a wet catalyst slurry and converters were handled as single pieces through the whole process. However, Kemira decided to proceed by developing own metallic substrate, which was formed by spray coating (→ pre-coating) separately flat and corrugated thin foils, which were further rolled to a ready coated catalyst converter (Fig. 1 and 2). After the promising feedback, an investment decision was made in 1987 and the catalyst plant with a capacity of 500.000 converters/year was ready in Vihtavuori already in 1988.

Figure 1. Continuous Open foil coating manufacture process based on thin foils.

Figure 2. A coated product rolled from foils.

Conventionally, the business had been shared by separate companies manufacturing substrates, coating and canning. The use of that continuous pre-coating method and even canning resulted in the product, where the full manufacture process and business was controlled by a company (Fig. 3). That new all-in-same-house strategy gave more space to operate flexible and profitable ways in automotive business of 1990s. Opposite to the existing production, that process was automated with moving foils and large coils in calcination, impregnation and heat treatments. At the very end of manufacture, the foils from the large raw coils were finally rolled to the single products. It was possible with OFC technology to load very high catalyst coating amounts (e.g. 160-250 g/dm^3) as thin layers (~50µm, fast pore diffusion) and reach a low pressure drop on high cell densities up to 600 - 1200 cpsi (cells per in^2, hydraulic diameter < 1 mm, main stream 500 cpsi) without blocking channels. This was an early example about down-sizing catalyst converters (high catalyst amount/volume), where the available space is very limited.

The metallic substrates and the production methods were developed in Vihtavuori and Oulu focused first on the chemistry of TWC coatings, which composed high surface area alumina and metal oxides supports, where

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expensive, active noble metals (Pt, Rh, Pd) were impregnated evenly. The noble metals were not present in spray coating due to losses in process but a separate impregnation was required resulting also in high noble metal dispersions to utilize best every noble metal atom on the catalyst surface.

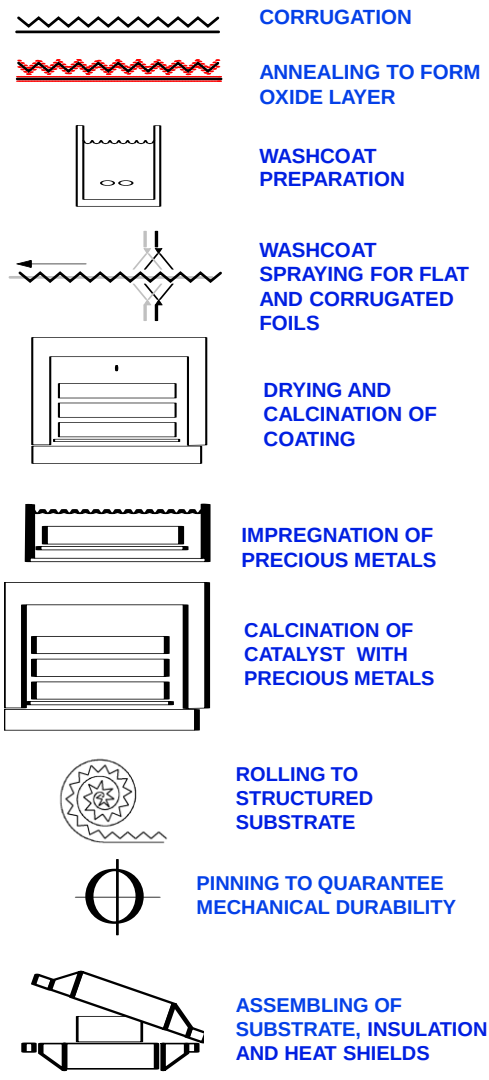

Figure 3. Complete process based on OFC.

OFC mainly as TWCs but as a smaller number of oxidation (diesel, VOC) and natural gas catalysts was the main product type in 1990s. In addition, EPA certificated catalysed components were manufactured for small engines (chain saws, lawn movers). It was also prepared commercially for natural gas applications a differentiated chemistry catalyst with separate compositions on flat and corrugated OFC foils. The main client was the GM group (Opel, Fiat). Millions of complete catalytic converters was exported (>95%) from Vihtavuori plant to European, Asian and US markets in 1990s. In addition to sales offices world-wide, new production units were built based on own or joint-venture companies to be near the customers (localization) in Italy (Genova), India (Faridabad) and USA (Chicago), Romania, Iran, Uzbekistan and China. Even if diesel catalysts were investigated by us and SCR catalysts were already commercial in European power plants since mid-1980s, the lack of demanding regulations for diesel moved the wider commercial activities after year 2000 (Euro 3).

Towards Euro 4/5 limits in 2000-2010

The main business was still based on OFC in 2000 but it was a pressure to move more to the conventional substrates. This was related to development (thinner walls, mechanical durability) with ceramic and other metallic substrates and standardization of catalyst structures. Kemira bough all rights in 2001 and built manufacture lines based on a Swedish-invented metallic substrate technology (Ecocat^{TM}), which had a self-carrying structure without brazing/welding and matched well to diesel applications.

Even if TWCs created the main turnover in 2000-2010, diesel catalysts were developed, new production lines built and commercially supplied for several light- and heavy-duty applications (Diesel Oxidation Catalysts (DOC), Selective Catalytic Reduction (SCR), catalysed Diesel Particulate Filter (DPF)) in Europe. The first commercial EU, EPA and CARB certificated vanadium-SCR catalysts

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were assembly into mobile off-road machines (e.g. tractors) in Europe and USA. Sales of TWC and oxidation catalysts for natural gas applications were also increasing for European and USA mobile and stationary applications, in which niche application we have had a wider market share in 2000-2020 than in any other catalyst business field. When ATSs were becoming more complicated packages, Ecocat focused more to be the catalyst supplier, which products were assembly in daughter or system supplier companies locating near to clients.

Catalysts for Euro 6 applications

After 2010 our company concentrated on diesel applications, particularly when the company became in 2013 a part of Dinex, which was readily a system supplier in diesel field. Euro 6 development for diesel catalysts and systems started about 5-6 years before Euro 6 was launched in 2014 in Europe. When a delay for a launch of Euro 4 was over 10 years between Western Europe and Eastern Europe/Asia (China, India), that delay was only about 5-7 years (2019-2021) in Euro 6 level. In many countries it had taken time to build first the readiness in respect of fuel (low-S diesel), engine and service (urea distribution) quality. On-road Euro 6 and off-road Stage 4 diesel ATSs are complicated including tailored DOCs, catalysed DPFs, SCR catalysts and Ammonia Slip Catalysts (ASC) (Fig. 4). New zeolites had replaced mainly V_2O_5/TiO_2-WO_3 in SCR catalysts. The complete ATS includes also urea tanks/dosing systems and systems/strategies to regenerate DPF or catalysts periodically. The substrates had been changed mainly to ceramics also in our portfolio, because the complicated systems are calibrated for a design and the suppliers require due to the cost and risk management to have flexible changes of suppliers.

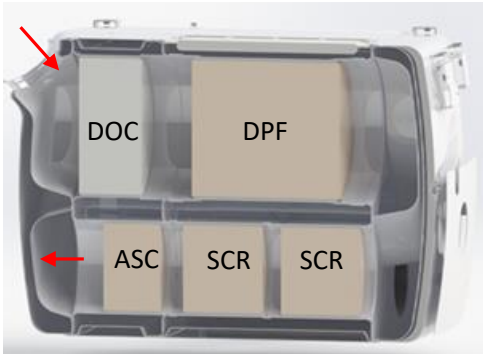

Figure 4. Catalysts in ATS (Euro 6) as integrated into a muffler.

In relation to diesel field, Dinex has had in Finland e.g. SiC-DPF manufacture/coating, Cu-/Fe-/V-SCR catalyst, urea hydrolyser and tailored DOC production after 2014 (Fig. 5). These catalyst components have been installed into complete ATSs in own Dinex factories located in Denmark, Turkey, Russia, Latvia, China, India and USA. R&D was moved in 2016 from old Oulu facilities next to Vihtavuori factory and at the moment Dinex has in Finland Global Catalyst Competence Center (GCCC), where the Group catalyst development has been concentrated including catalyst chemistry, activity testing, surface characterization, pilot/process engineering and engine laboratory facilities. GCCC has also a close co-operation with other Dinex development and engineering teams in Germany and Denmark. In addition to international contacts, Dinex Finland has also co-operated with all Finnish Universities in the field of catalysts during the last 35 years. Even if many new production processes have been first implemented and products manufactured in Finland, the trend is to move an increasing manufacture with wider automation further to foreign Dinex Groups locating near to end clients. That trend will continue in this and next years. In 2020 Dinex Finland will reach preliminarily the highest turn-over ever in the company history.

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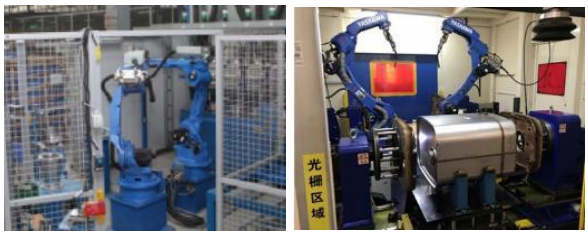

Figure 5. Catalyst and ATS production lines.

Future

Emission control was first developed from noise control (silencers) to pollutant (CO, HC, NO_x, PM) reduction with passive oxidation/three-way catalysts and then up to complicated catalytic systems with active controls. The catalyst durability for biofuels have been investigated already since 2005. Due to DPFs, particle emissions from modern diesel vehicles are as low as from gasoline cars. Even if in the public discussions, the emission reduction means nowadays mainly CO_2 or greenhouse gases (GHG) and a move to electric vehicles, the combustion engines will be still present in most (~80%) of vehicles on European roads in 2030. Hybrid engines requires also catalysts and filters for exhaust gas purification. The combustion engines are more difficult economically to be replaced by electric engines in heavier applications (trucks, ships), where diesel and natural gas engines will be in a wide use at least for the next 20 years. The hybridization level can be different by the applications and hybrids give also good tools to solve many earlier challenges (high power peaks, city driving emissions, electric assisted ATS, intensification). When HC, CO and NO_x emissions (pollutants) are today very low in comparison to 60-70s, the main focus has already turned from the tightening limit values to the control of real-drive pollutant, CO_2 and side product (N_2O, PN, CH_4) emissions over the vehicle life-time.

As seen by our history, the challenges in catalyst development have been followed the requirements by emission regulations and clients. Dinex has the target to remain technically competitive in catalyst development particularly in diesel and gas applications in future.

Reference

1.Lappi, P., Salanne, S. and Maunula, T., Recollection about the emission catalyst production in “Catalysis in Finland – an exciting pathway”, Suomen katalyysiseura, Otava, 2013.

Author: R&D Fellow, Dr Teuvo Maunula has involved to the emission catalyst development since 1985, where since 1987 in Dinex Finland R&D.

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Obituary
Professor Sir John Meurig Thomas

Professor Sir John Meurig Thomas passed away on November 13, 2020 at the age of 87. John Meurig Thomas was born in Wales, UK, as the son of a coalminer on December 15, 1932. He died as one of the most famous scientists, globally recognized for his remarkable achievements on materials and heterogeneous catalysis, even though he never received the Nobel prize.

I first became aware of Professor J.M. Thomas in the autumn of 1972 when I started my licentiate studies in Otaniemi. In those days, licentiate studies also included examinations on certain textbooks. One of the textbooks assigned to me was J.M. Thomas & W.J. Thomas, Introduction to the Principles of Heterogeneous Catalysis, Academic Press, Inc. 1967. I was shocked to see that an "introduction to the principles" would be such a heavy book covering more than 500 pages. At that time, I was much more interested in the practical aspects of catalysis. Later, I realized the immeasurable value of that book which some considered as the "bible" of heterogenous catalysis.

Over the years, I learnt to know Professor John Meurig Thomas personally. In addition to his profound scientific knowledge, I admired his scholarly approach to matters and his elegant and sophisticated style of English, even though during my studies, I did not recognize that. In 1968, an evaluator of the textbook wrote: One of the outstanding features of the text is the excellent writing style. It is a refreshing presentation which is both lucid and interesting. (J. Chem. Educ. 1968, 45, 10, A843, https://doi.org/10.1021/ed045pA843).

Only recently, Professors Richard Catlow and Graham Hutchings wrote an obituary for Professor Sir John Meurig Thomas, published in Nature Materials February 2021. Please, find their writing in https://doi.org/10.1038/s41563-021-00940-5.

Outi Krause
Professor emerita

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Catalysis related dissertations

M.Sc.(Chem.) Tuomo Kainulainen from Research Unit of Sustainable Chemistry, University of Oulu defended his thesis on 27th of November, 2020. The title of his thesis is

"Furfural-based 2,2'-bifurans. Synthesis and applications in polymers"

Opponent: Prof. Heikki Tenhu, University of Helsinki

Custodian: Adjunct Prof. Juha Heiskanen, University of Oulu

Abstract:

Furans are an interesting class of sustainable chemicals derived from biomass. They are prepared from carbohydrate sources and are, therefore, potential platform chemicals and precursors for novel biobased materials. Within the last 20 years, research has elevated 2,5-furandicarboxylic acid (FDCA) into being one of the most important biochemicals, because of its applicability for the preparation of novel polymers. For this reason, its precursor 5-hydroxymethylfurfural has risen to a similar prominence as furfural, despite it not being produced on the same scale currently.

In this work, furfural-based 2,2'-bifuran compounds were studied, with the goal of utilizing them as monomers for novel materials. Novel bifuran-based polyesters were made using dimethyl 2,2'-bifuran-5,5'-dicarboxylate as a monomer, which was prepared using the developed palladium-catalyzed direct coupling method. A traditional melt polycondensation reaction with either ethylene glycol or 1,4-butanediol was used to prepare the bifuran polyesters and FDCA-containing copolyesters. For novel cross-linkable epoxy methacrylates, or so-called vinyl esters, the starting compound was 2,2'-bifuran-5,5'-dicarboxylic acid (BFDCA), and the prepared unsaturated monomers were cross-linked by employing radical polymerization. The materials and monomers were characterized using several techniques (NMR, IR, DSC, TGA, DMA, UV-Vis), which allowed the effects of the bifuran units to be elucidated.

Based on the results obtained, 2,2'-bifuran–based polyesters and copolyesters are a very promising class of materials. Based on measurements, their glass transition temperatures are noticeably higher than those of the corresponding polyesters derived from either terephthalic acid or FDCA. Additionally, their UV and oxygen barrier properties were excellent, and for the latter, close to FDCA-based polyesters, which are considered to be some of the best oxygen-barrier polyesters. Based on tests done on the vinyl esters prepared from FDCA and BFDCA, they are possible replacements for bisphenol A -derived vinyl esters. They can be used to prepare thermosets with high glass transition temperatures.

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M.Sc.(Chem.) Toni Varila from Research Unit of Sustainable Chemistry, University of Oulu defended his thesis on 30th of November, 2020. The title of his thesis is

"New, biobased carbon foams"

Opponent: Prof. Janne Jänis, University of Eastern Finland, Finland

Custodian: Prof. Ulla Lassi, University of Oulu

Abstract:

The use of biomass has grown tremendously among energy-producing factories recently. In addition to burning biomass to produce heat and electricity, new and environment friendly products are being developed in order to utilize biomass more efficiently. Due to the variety of rich carbon sources in biomass, this thesis focuses on the use of such carbon sources in producing activated carbon foams.

The first part of this thesis consists of two sections. First, it notes that carbon foams are produced using sugar as a source of carbon. It further notes that the sugar-based carbon foams that have been produced were too brittle and, therefore, require further adjustment in order to produce mechanically stronger foams. In the second section of the first part, this thesis addresses how hydrolysable tannin, as well as hydrolysable tannin in combination with different lignin types, is used to produce carbon foams and activated carbon foams. This section also studies the physical properties of these foams. The results indicate that changing the catalyst during foaming, or using the right lignin-to-tannin ratio (25 w%) and a four-hour thermal treatment at 1073 K, obtains the highest influence on these foams' mechanical strength. Up to 10 times stronger foams, can be achieved with this method.

The second part of this thesis focuses on studying the properties and performance of activated carbon foams based on hydrolysable tannin, pine bark, and spruce bark extracts as catalyst supports in the conversion of furfural to 2-methylfuran and as adsorbents for the removal of methylene blue. Based on the results, chemically activated carbon foams from spruce bark work better than physically activated carbon foams in removing methylene blue from solutions due to their more developed pore size distribution and higher specific surface area. The performance of activated carbon foam derived from pine bark extracts in the conversion of furfural to 2-methylfuran was similar to commercial reference materials' 58%.

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M.Sc.(Chem.) Yaseen Khan from Aalto University School of Chemical Engineering defended his thesis on 25th of September, 2020. The title of his thesis is

"Structured Microreactors for the Heterogeneously Catalyzed Gas-phase Dehydration and Partial Oxidation of 1-butanol"

Opponent: Prof. Lars Pettersson, KTH Royal institute of Technology, Sweden

Custodian: Prof. Riikka Puurunen, Aalto University

Abstract:

Structured microreactors are considered as a tool to study catalytic activity and intrinsic kinetics because of their characteristic mass and heat transfer advantages. In this thesis, microreactor structures coated with catalysts (γ-Al_2O_3, Au/TiO_2, Pd/TiO_2 and Au-Pd/TiO_2) were applied to study the activity and to investigate the kinetics of the heterogeneously catalyzed gas-phase reactions in dehydration and partial oxidation of 1-butanol. In addition, the morphology and durability of the prepared noble metal catalyst coatings (Au/TiO_2, Pd/TiO_2 and Au-Pd/TiO_2) were studied.

A structured microreactor coated with γ-Al_2O_3 catalyst having a layer thickness of 15-30 µm was used for the heterogeneously catalyzed gas-phase dehydration of 1-butanol. The kinetic parameters were estimated from the produced experimental data. A dynamic 2D plug flow reactor type model with diffusion-reaction in the catalyst layer confirmed insignificant internal mass transfer resistances and prevalence of the kinetic regime. A computational fluid dynamics study using 3D and 2D-axisymmetric models incorporating fluid flow non-idealities, revealed the presence of axial and radial concentration gradients. The insights from the simulations revealed the catalyst layer thickness and the microchannel dimensions as key parameters to improve the performance of microreactors applied for the heterogeneously catalyzed gas-phase reactions.

New heterogeneous catalyst coatings of titania-supported mono- and bimetallic gold and palladium were prepared and tested for the 1-butanol partial oxidation. A sol-immobilization method was used for catalyst preparation and coatings were prepared via a suspension method. A layer thickness of 17±7 µm with an average metal nanoparticle size of 3.6 nm was achieved. The Au/TiO_2 catalyst coatings were most selective towards n-butyraldehyde, whereas Pd/TiO_2 and Au-Pd/TiO2 catalysts were more selective towards propene, CO and CO_2. The kinetic experiments were performed using Au/TiO_2 coated catalyst. Kinetic modeling was performed by applying 1D-pseudo-homogeneous plug flow reactor type model and dynamic 2D model incorporating axial dispersion effects in gas-phase. The model simulations reproduced the experimental data.

In this thesis, preparation of active, selective and durable Au/TiO_2 coated catalysts was demonstrated. The activity of the prepared Au/TiO_2 coated catalyst was reproducible for 57 tested runs that is reported, in the author's knowledge, for the first time for the nanogold catalyst. In addition, kinetic modeling and reactor simulations were performed successfully to describe the system dynamics of both the dehydration and partial oxidation reactions of 1-butanol.

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M.Sc.(Chem.) Irene Coronado from Aalto University School of Chemical Engineering defended his thesis on 5th of February, 2021. The title of his thesis is

"Catalytic Aqueous-Phase Reforming of Biorefinery Water Fractions"

Opponent: Prof. Henrik Grénman, Åbo Akademi University, Finland

Custodian: Prof. Riikka Puurunen, Aalto University

Abstract:

Biorefineries can produce renewable fuels and chemicals through processes such as pyrolysis of lignocellulosic biomass or Fischer-Tropsch (FT) synthesis using syngas derived from biomass gasification. Although commercial-scale plants exist, the production costs of renewable fuels and chemicals are usually higher than the production costs of fossil-based fuels and chemicals. To improve the competitiveness of biorefineries, this thesis proposes processing the water fractions derived from biorefineries to optimise the production of renewable fuels and chemicals.

Biorefinery water fractions include diluted oxygenated hydrocarbons that can be processed using aqueous-phase reforming (APR) technology to produce hydrogen, which is the main desired product, and other gases such as carbon dioxide, carbon monoxide and alkanes. This study tested different Ni-based catalysts, first in the APR of model compounds representative of pyrolysis liquid aqueous fraction (PLAF) and FT waters, and finally, in the APR of a real water fraction derived from FT synthesis.

The APR of model compounds representative of PLAF, i.e. solutions of acetic acid, ethanol, 1-hydroxypropan-2-one and benzene-1,2-diol, resulted in low hydrogen yields and significant deactivation of different Ni-based catalysts. The hydrogen yield was around 10% from ethanol and close to 1% from the other oxygenates. The APR of FT water model compounds, i.e. solutions of C1-C4 alcohols over Ni-based catalysts, yielded relatively high amounts of hydrogen, ranging from 13% to above 100%, and 11% in the APR of real FT water. A copper-doped nickel catalyst supported on ceria-zirconia was selected to conduct the APR of real FT water under different operation conditions. The results were utilised to develop a kinetic model that could be applied through concept development to integrate APR into a FT synthesis process.The hydrogen produced in the APR of FT water could be used in the production of renewable fuels and chemicals to improve their production efficiency. Nickel-copper/ceria-zirconia catalyst is a suitable catalyst to process FT waters. Nonetheless, the catalyst composition should be further optimised to increase the hydrogen yield.

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Conferences and Symposia

The **5th Finnish Young Scientist Forum** will be organized as online event on April 9, 2021.

See also e.g.

www.conference-service.com

www.iacs-catalysis.org

Web pages

http://www.katalyysiseura.org

http://www.kemianseura.fi

http://www.efcats.org

Katse

1/2021

Suomen katalyysiseura
Finska katalyssällskapet
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.