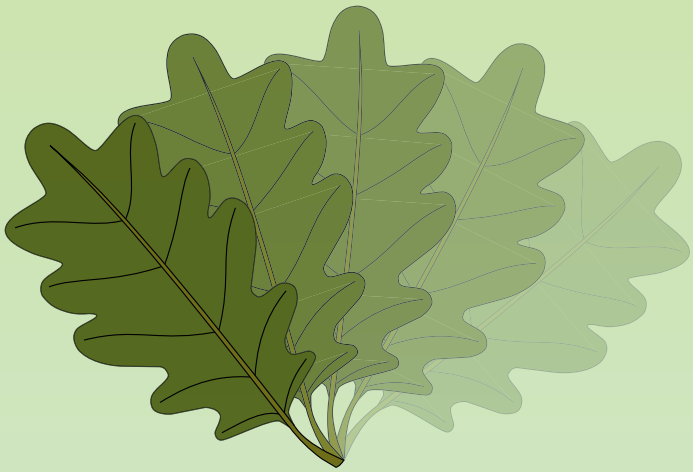
Åbo Akademi University
Science and Engineering

Annual Report 2018–2019



Johan Gadolin

Process Chemistry Centre

Johan Gadolin Process Chemistry Centre

at

Åbo Akademi University

Annual Report 2018–2019

Edited by

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*Picture from the **PCC** annual meeting in November 2019*
Photo: Maria Grönroos (Studio Liikkuva)

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2020

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1. Overview of PCC activities in 2018–2019

Background and news

The Johan Gadolin Process Chemistry Centre (***PCC***) began its journey in 1998 as a centre with common objectives and research strategy. The original **mission of *PCC*** to "*aim at detailed understanding of physico-chemical processes in environments of industrial importance, in order to meet the needs of tomorrow's process and product development*", which we call "***Molecular Process Technology***" is still highly relevant, and so are our **fundamental values** once declared in our strategy:

- Deep knowledge and high quality in science
- Curiosity and creativity
- Respect for individuality
- Openness and transparency
- Sustainable development

PCC has a unique combination of knowledge in chemistry and chemical engineering that gives us a solid platform to address global challenges that the World is facing today. We have the tools to promote renewable and clean energy, sustainable industrial production, health and well-being. One can say that ***PCC*** continues a long and successful tradition of chemistry and chemical engineering in Åbo/Turku. Already in 1764, Pehr Adrian Gadd, who was the first professor of chemistry at the former Royal Academy in Åbo/Turku, emphasized the importance of applied chemistry for the benefit and welfare of society. As we all know, Gadd's successor Johan Gadolin received wide international recognition in the field of chemistry. At Åbo Akademi University, chemical engineering is celebrating its 100th anniversary this year (2020).

PCC is active in two profiling areas at Åbo Akademi University, *i.e. Molecular Process and Material Technology (MPMT)* and *Drug Development and Diagnostics (DDD).* Associate Professor Henrik Grénman from ***PCC*** is a tenure track professor in Molecular Process and Material Technology at the Faculty of Science and Engineering, supported by the MPMT profiling area.

Our *Forum for Society* enables our interactions with society and industry, while our *Johan Gadolin Scholarship Programme* helps us to maintain and expand our international scientific collaboration network. The cooperation between ***PCC*** and the Johan Gadolin Scholarship fellows has so far produced more than 200 scientific articles in total.

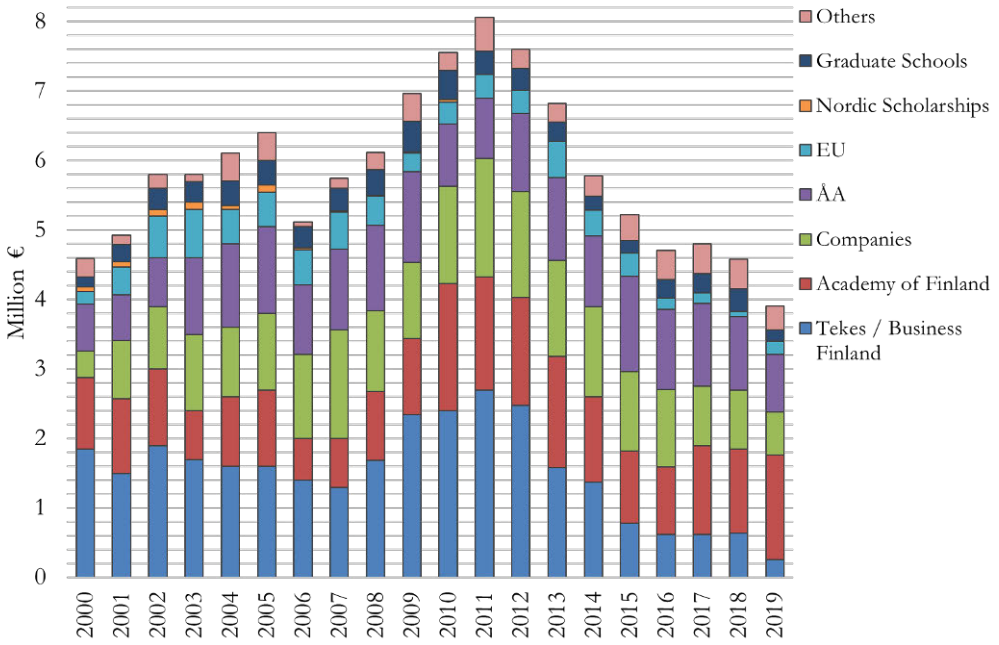
Our cooperation with the Turku Centre for Biotechnology (CBT), Biocity Turku, and the newly established Health Campus Turku has been very successful. Biocity Turku has seven research programmes, where ***PCC*** and its members are active in four and have cooperation with also some of the others. The main programme where ***PCC*** is active is the Advanced Bioresources and Smart Bioproducts – Towards Sustainable Bioeconomy, "Smartbio" (director: Academy Professor Eva-Mari Aro, vice-director: Professor Stefan Willför). Our groups are also members or associated members of the Biomaterial and Medical Device Research Programme (director: Professor Pekka Vallittu, vice-director: Professor Leena Hupa) and Diagnostic Technologies and Applications (directors: Professors Tero Soukka and Jessica Rosenholm, vice-directors: Professors Johan Bobacka and Pekka Hänninen).

The core of our research plan 2015-2018, "*Future Refining of Forest Biomass – the Molecular Process Technology Approach*" was built on our strengths in experimental and modelling capabilities to explore chemical details in novel processes and products that use biomass-based raw materials. The focus was on refining and modification of biomass towards high-value applications such as structural biocomposites, 3D biomaterials in biomedical applications, immunostimulatory glycoclusters, and various fine and specialty chemicals. Our status as Centre of Excellence at Åbo Akademi University ended in 2018. Therefore, 2019 was a kind of transition state for ***PCC***, where we partly followed our previous core research strategy and partly looked towards new research openings. As always, ***PCC*** and its members have been very active in applying for funding on both national and international level. In this Annual Report we highlight some of our achievements during the years 2018 and 2019. A special highlight is Academy Professor Tapio Salmi's five-year research project (2019-2023) funded by the Academy of Finland.

The years 2018–2019 in numbers

In 2018–2019, more than 100 senior researchers and full-time PhD candidates worked in the research projects of the Centre. In addition, a number of shorter-term visitors, Master's students, and support personnel participated in our activities.

The figure below shows the funding of the Centre since the year 2000. The key external funding sources in 2018-2019 were the Academy of Finland, Åbo Akademi University, Companies and Business Finland.



The funding of the Johan Gadolin Process Chemistry Centre 2000-2019

The decrease in funding since the top-year 2011 has raised the demand level of the Centre to maintain its high-level productivity of research. The decline in funding for our Centre since 2011 is mainly due to a drop in funding from Tekes/Business Finland from 2.7 million € in 2011 to 0.3

million € in 2019. It is noteworthy that although the funding is even below the level we had when ***PCC*** first started, our production is still excellent and thus the production per invested euro is better than ever.

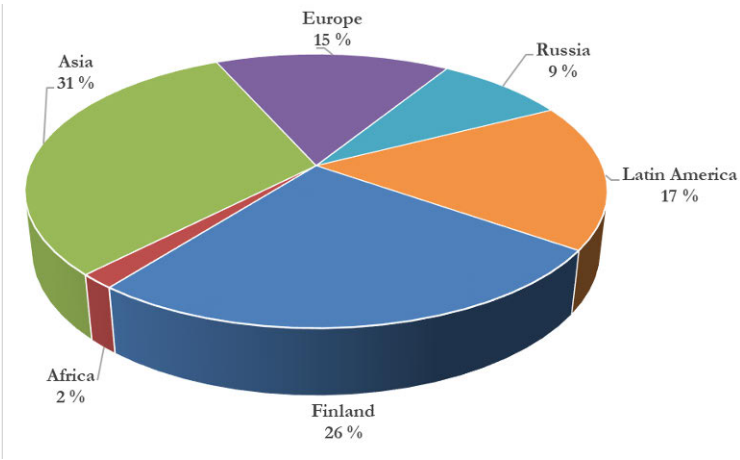
From the academic point of view, the years 2018–2019 were productive. The table below gives some key numbers of our academic activities 2000–2019. Once again, the Centre kept a very high production rate and published 138 (131) papers in scientific publication series with the full referee system in 2018 (2019). The number of theses show some fluctuations but remain at a fully satisfying level.

	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009
Doctoral Theses	5	7	8	2	11	8	8	8	9	7
Master's Theses	21	23	27	26	17	15	20	23	19	17
Journal Articles	60	71	94	77	106	109	113	116	101	118
	2010	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**2017**	**2018**	**2019**
Doctoral Theses	6	10	10	15	16	12	6	6	4	6
Master's Theses	15	11	14	12	16	25	10	18	15	17
Journal Articles	138	126	130	139	136	152	146	122	139	131

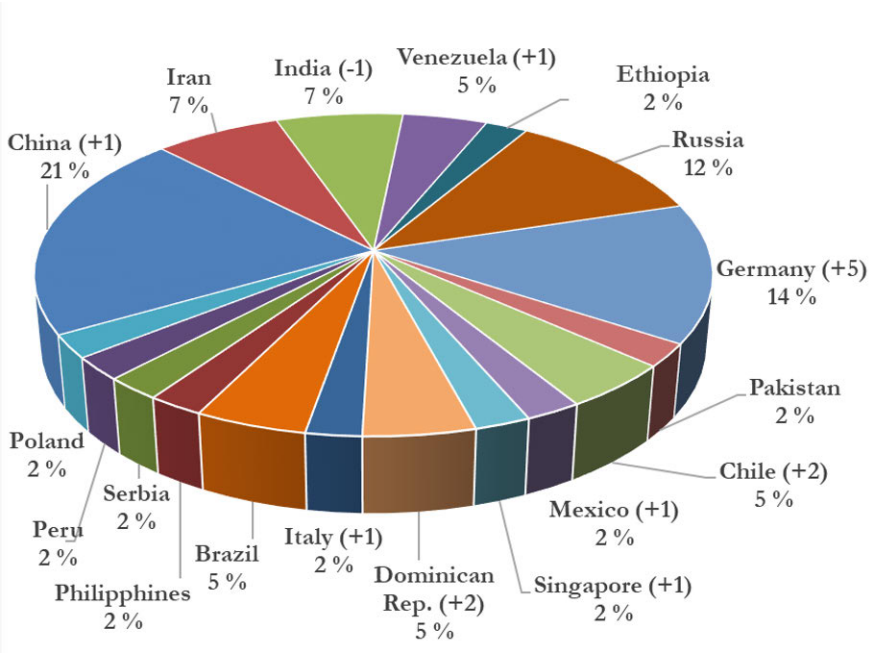
Theses and peer reviewed journal articles by the Johan Gadolin Process Chemistry Centre.

Doctoral students

A central part of our research activities is done as doctoral theses works. Altogether 58 PhD thesis projects are actively underway at the Centre. Our doctoral students are very international, as 74 % originate from countries other than Finland (see the graph below). Among our foreign doctoral students in 2018–2019, the top-3 nationalities were China (21 %), Germany (14 %) and Russia (12 %). ***PCC*** is certainly one of the most international units at our university.



Origin of PhD students at Johan Gadolin Process Chemistry Centre



Nationality of foreign PhD students at Johan Gadolin Process Chemistry Centre

In addition to projects, CoE funding, and grants, the Åbo Akademi doctoral network programme and therein the Graduate School in Chemical Engineering (GSCE) and Doctoral Network of Materials Research (DNMR) are important sources of funding for the PhD students in ***PCC***.

Johan Gadolin Scholarship Programme

Our Johan Gadolin Scholarship Programme started in 2007. It was funded by the Åbo Akademi Foundation during the years 2007–2011 and continued for 2012–2013 on other sources of funding, after which the Åbo Akademi Foundation decided to continue funding for the Johan Gadolin Scholarships Programme for the period 2014–2019.

In the Johan Gadolin Scholarship Programme we have been able to invite PhD students and post doctoral researchers to join ***PCC*** for a period between 3 to 9 months. So far, 98 fellows from 33 different countries and 81 different universities worldwide have participated in the programme. Also, 11 fellows joined the JGS with their own funding. The visitors have participated in on-going research projects at the Centre. The cooperation between ***PCC*** and the Johan Gadolin fellows has so far produced more than 200 scientific articles.

Boards and task forces

PCC is led by an *executive board* consisting of Prof. Johan Bobacka (chairman), Prof. Henrik Grenman (vice chairman), Prof. Leena Hupa, Prof. Reko Leino, Acad. Prof. Tapio Salmi and Dr. Chunlin Xu. Furthermore, Dr. Markus Engblom takes care of the coordination of ***PCC*** and functions as secretary of the executive board, while Ms. Ekaterina Korotkova coordinates our Johan Gadolin Scholarship programme.

The ***PCC*** executive board is supported by a *Scientific Advisory Board* and a *Forum for Society*. 2018-2019 our Scientific Advisory Board consisted of the *Prof. Jiri Janata* from the Georgia Institute of Science and Technology in Atlanta, USA, *Prof. Raimo Alén* from the University of Jyväskylä, Finland, *Prof. Lars Pettersson* from the Royal Institute of Technology in Stockholm, Sweden, *Prof. Andreas Seidel-Morgenstern* from Max Planck Institute, Germany and *Prof. Jan-Erling Bäckvall* from Stockholm University, Sweden. Our Forum for Society, led by *Dr. Lars Gädda*, consists of representatives of key industrial companies, as well as members of the society, who are collaborating with ***PCC***.

Spinoffs

In this annual report, we present four start-up companies where PCC has played a key role. *GlucoModicum Oy* develops a wearable device for non-invasive monitoring of glucose and other analytes in interstitial fluid. *CutoSense Oy* develops a device for treatment of chronic wounds and assessment of the wound status. *CH-Bioforce Oy* has developed a breakthrough fractionation technology for wood and other biomasses. *Eco-Oil* has managed to develop a fuel based entirely on biomass with the same properties as fossil fuels. More about these innovative start-ups can be found in Chapter 2.2.

Acknowledgements

This report is published this year (2020) to honor the 100th Anniversary of Chemical Engineering at Åbo Akademi University. We are grateful to be part of the Faculty of Science and Engineering that has its roots in the historical KTF.

We want to thank all our collaborating partners in Finland and all over the world for another two years of interesting and inspiring work together.

On behalf of the Board of the Johan Gadolin Process Chemistry Centre,

Johan Bobacka
Chairman

2. Highlights from *PCC*

2.1 Experiences of the Johan Gadolin Scholarship researchers

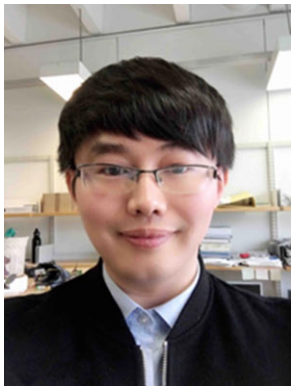
Mouad Hachhach

I am Mouad Hachhach, and I studied Mathematics, Physics and Engineering at the Prepratory classes. In 2016, I completed my Master's degree in Process, Energy and Environment Engineering at National School of Applied Sciences of Agadir, Morocco (ENSA Agadir). Currently, I am doing my PhD in the Chemical Engineering at FST, Tangier. My research focuses on the Process Design, Modeling and Scale-up, Techno-Economic Analysis, Life Cycle Assessment of novel processes. I was awarded a Johan Gadolin Scholarship for a period of five months under the supervision of Academy Professor Tapio Salmi, which provided me with a unique learning and research experience both in the personal and professional fields.

In Åbo, I had the opportunity to address my research from different scientific and technological perspectives owing to the diverse expertise and backgrounds of the cooperative team at the Industrial Chemistry and Chemical Reaction Engineering lab. We had a lot of fun producing good results and I am sure that I will publish the results obtained in my hemicellulose valorization project. On the other hand, there were a number of extra factors such as getting to know really great people from various backgrounds, to live inside the awesome Finnish culture, and especially the amazing landscapes in Finland which made my stay a unique and life-changing experience.

In summary, for me, Åbo Akademi University is the best place and choice to understand that personal practical work experience abroad is invaluable. I highly recommend applying for Johan Gadolin Scholarship in Åbo Akademi, this place has left only joyful moments in my heart.

Long Li



My name is Long li and I am from China. I obtained a PhD degree in environmental science from Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, University of Chinese Academy of Sciences. After that, I worked as a lecturer in College of Environment and Safety Engineering, Qingdao University of Science & Technology. I have received a scholarship at the Johan Gadolin Process Chemistry Center (***PCC***) for a period of 6 months, under the supervision of Johan Bobacka. At ***PCC***, my research interest is conducting MOF based solid-contact ion-selective electrodes (SC ISEs) with coulometric readout strategy. Two kinds of hierarchical MOFs (Ni-HHTP-MOF and Co-HHTP-MOF) templated by ordered PS nanospheres (with a diameter of 500 nm) were synthesized and used as transducing layer for SC ISEs. I have learned how to use new instruments and I met many other people from different cultures. Moreover, I love Turku so much. I appreciate for the opportunity to join the ***PCC***. If you have a chance to join ***PCC***, do not hesitate to apply.

René Herrera Díaz

I am René Herrera Díaz from the University of the Basque Country in San Sebastian, Spain. I have been working in the chemical and environmental Engineering department as a postdoc in the field of the valorisation of wood and wood products during the last years. I was joining to the Wood and Paper Chemistry at ***PCC*** during 3 months from March to May, working in extraction, analysis and separation of low molecular weight compounds from wood and from agroforestry waste. The instruments and infrastructure used for extraction and chromatography analyses were totally adequate for my research topic, and the most important thing was the support and advice that I received from the scientists working there, which are very friendly and helpful. After my stay there, I could say that I have learned several characterization techniques used in biomass materials, also how to manage sample preparation and how to use correctly instruments. It is a place where you can work in your own pace and own schedule, what motivates you to be more confident and independent. I highly recommend researchers to apply to the Johan Gadolin Scholarship programme because it is an unforgettable academic and personal experience. Åbo in Finland is a comfortable place to live, and the ***PCC*** is located in downtown close to everything. The student village is located within walking distance, where you can find apartments with fair prices and a nice environment.

Abrar Ahmed

My name is Abrar Ahmed and I am working at University College of Pharmacy, University of the Punjab, Lahore Pakistan. I am interested in identification of chemical leads from tropical flora for medicinal efficacy, which in future, may lead to the development of new drug candidates against complex and challenging drug targets. During 2020, I have earned Johan Gadolin Fellowship to pursue post-doctoral programme at Abo Akademi University, Turku Finland. In Finland, the spruce and pine forest is an enormous source of stilbenoids with great potential for therapeutic effects. Johan Gadolin Post-doctoral Fellowship gave me an opportunity to work for the development of novel anti-inflammatory and analgesic agents derived from natural stilbenoids. During this time, we optimized the challenging isolation procedures making the extraction and purification of stilbenoids more efficient and simple. Furthermore we explored the role of transient receptor potential vanilloid 1 (TRPV1) channels to get the deeper insight into the analgesic and anti-inflammatory attributes of stilbenoids by utilizing molecular modeling and simulation strategies. Johan Gadolin Post-doctoral Fellowship has provided me opportunity to learn from international scientific environment, mastering the experimental skills and extending my expertise to computer aided drug design (CADD). Working at state of the art Laboratory of Organic Chemistry (LOK) in center of excellence has so far remained an extremely delighted experience for me. Additionally, this research visit has strengthened the scientific collaboration with University of The Punjab Lahore, Pakistan. This was the time when COVID-19 pandemic hit the globe hard but at LOK we remained together encouraged and supportive during this time. While living in Turku taking the long stroll across the Finnish forests and lakes is always heart touching. I am thankful to Patrik Eklund, Outi Salo-Ahen and rest of all my colleagues for their selfless support during this time. I only have beautiful memories in Finland.

2.2 Spinoffs

GlucoModicum Oy

Johan Bobacka, Zhanna Boeva

GlucoModicum Oy was founded in March 2018 by a group of entrepreneurs and scientists from the University of Helsinki and Åbo Akademi University. Among these were Professor Johan Bobacka and Dr. Zhanna Boeva from ***PCC***.

GlucoModicum Oy develops a novel needle-free solution for monitoring of glucose and other analytes in interstitial fluid. The concept builds on proprietary technology for non-invasive extraction of interstitial fluid developed since 2015 at the University of Helsinki. The unique way of sampling interstitial fluid is combined with novel chemical sensor technology for needle-free determination of glucose. The core technology is protected world-wide by a patent portfolio owned by GlucoModicum Oy.

In the world today, there are over 400 million people suffering from diabetes. Traditionally glucose is measured from a blood sample obtained from the finger tip by a needle puncture. The blood sample is transferred to a disposable biosensor strip connected to a glucometer that measures and displays the glucose concentration. Due to discrete blood sampling, this traditional method does not allow continuous monitoring of the glucose level. Additionally, pricking the fingers several times per day is unpleasant and painful. For these reasons, there is a tremendous need and a huge market opportunity for non-invasive glucose monitoring.

Today, GlucoModicum Oy comprises a committed team of more than 15 people, including senior professors, several PhDs (physics, bio-electronics, biosensors, medicine) combined with expertise of global technology, sales and distribution. Our vision is to create a needle-free biomarker and health monitoring solution in order to improve health and wellbeing for millions of people. A prototype glucose monitor, which is the size of a smartwatch, has already been developed and built by GlucoModicum Oy.

The founders of GlucoModicum Oy. Back row (from left to right): Jokke Mäki (managing director), Edward Haggström (scientific advisor, chairman of the board), Alejandro Garcia (chief technology officer), Zhanna Boeva (sensor lead), Johan Bobacka (scientific advisor, member of the board). Front row (from left to right): Teemu Nurminen (R&D scientist), Risto Vänskä (R&D scientist)

CutoSense Oy, from the TUTLi-project MC-Patch

Main funding: Tekes

Mikael Bergelin, Jan-Erik Eriksson, Max Johansson, Atte Kekonen, Sami Kielosto, Jari Viik, Heimo Ylänen, Annikki Vaalasti

The aim of the MC-Patch project was to develop a wound assessment and stimulation device, capable of administering LIDC (low intensity direct current) treatment to a chronic wound while in stimulation mode and assess the wound status via means of bio-impedance measurements. By combining electronics knowledge from Aalto University with knowledge of biotechnology from Tampere University of Technology and electrochemical measurement knowledge of Åbo Akademi University (coordinator of the project), this project came to an excellent start. The first aim was chosen as LIDC stimulation is known to have a beneficial effect on the rate and outcome of wound healing, in particular regarding to hard-to-heal chronic wounds with a vascular insufficiency-related background. The second aim was chosen as the state-of-the-art treatment process still typically involves the dismantling of the compression dressings and exposure of the wound to inspect the treatment response with a 3-day interval visually. Treatment of a chronic wound is costly as it is a very time-consuming process, the specialized dressings are expensive. They need unnecessarily to be changed frequently, and the resulting mechanical stress to the newly formed tissue delays full re-epithelization. By bio-impedance measurements, it is possible to create a wound status map as shown below, thereby avoiding the need for 2 out of 3 visual inspections while still maintain a good treatment response follow-up.

In the MC-patch project, a wound foil/electrode dressing was designed with electrode layouts optimized to allow for accurate impedance measurements, as well as efficient and even distribution of current across the wound while used in treatment mode. The malleability and durability of the dressing were paramount, as it needed to allow for wound contact for extended periods without chafing or stressing the tissue. A device for measurement and stimulation was constructed. The measurement parameters were optimized to allow for sufficient resolution and reliable response. At the end of the project, a seven patient clinical trial was conducted with the full system to verify the functionality. As seen in figure 1, the results from this study were very encouraging, and consequently, a decision was made to establish the enterprise CutoSense Oy in late 2015. The IPR was bought from Åbo Akademi University and Tampere University of Technology, two patents have been granted, and two more are still in the application stage.

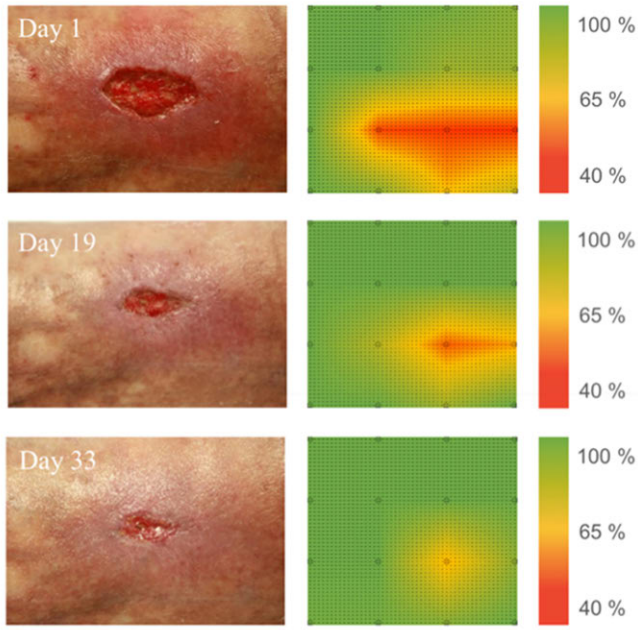


Figure 1. *correlation between visual inspection and measured wound status during healing of a lower limb chronic wound*

With time, we were able to secure a sufficient volume of outside funding. This funding allowed CutoSense Oy to develop the initial dressing design to improve wound healing status resolution even further. Additionally, the design and manufacture of a combined electronics device with both stimulation and measurement capabilities, as well as assessment software running on Android-based phones or tablets were developed.

During the device development phase, the system evolved from an "academically-oriented lab-made design" via a sequence of development stages, as illustrated in figure 2.

Figure 2. *Upper row; the patch, the full system and the measurement device as available during clinical trial 1. Lower row; the close to final patch design, pre-production electronics and user interface. The design of the final system is not shown as market entry is expected during Q1 2021.*

This device development process - including a substantial amount of regulatory work, setting up quality systems, finding subcontractors, passing audits, EMC- and bio-compatibility tests - has now led us to a point where we can apply for the CE-mark. The CE-mark application will be submitted as soon as our second clinical trial results are available and the last documentation for the notified body is compiled and finalized.

For more information, please visit our web-site www.cutosense.fi

CH Bioforce Oy

Chunlin Xu, Lari Vähäsalo, Sebastian von Schoultz

CH-Bioforce Oy (CHB) has developed a breakthrough fractionation technology for wood and other biomasses. Biomass fractionation is done through pressurized hot water extraction (PHWE), which makes the process practically chemical-free, and can be scaled up to industrial scale in an in economically sound way. CH-Bioforce´s technology produces pure dissolving pulp, polymeric hemicellulose and sulphur-free lignin, which enables the mass production of totally new high value end products. CH-Bioforce technology provides chemical industry a new bio-based feedstock, and will eventually replace the fossil-based raw materials in numerous applications, as a new, non-food alternative.

The first trials with the technology were made in 2011 by wood chemistry experts Mr. Sebastian von Schoultz, Dr. Lari Vähäsalo, and Mr. Nicholas Lax. Mr. Sebastian von Schoultz, Dr. Lari Vähäsalo are alumni of PCC. CH-Bioforce Oy was established in 2016 together with Chemec Oy. Since 2011, several trials, prototypes and a pilot plant have been built, and the produced materials have been widely tested in, e.g., Åbo Akademi, and VTT (Finnish Technical Research Centre) and together with industrial partners. CH-Bioforce has received significant public funding from Business Finland (Finnish Funding Agency for Innovation) and H2020 SME Instrument to develop and commercialize the technology. In latest closed financial period, CH-Bioforce gained revenue of close to €1 million. Below are a few **highlights of CH-Bioforce's Innovation**.

Natural polymers to stabilise technical emulsions

CH-Bioforce recently participated in the "BITE" research project (novel biomass-based solutions for technical emulsions) led by PCC at Åbo Akademi with the University of Helsinki, Tikkurila and CH-Polymers as partners. The project was funded by Tekes – the Finnish funding agency for innovation, which now operates as Business Finland – together with partners from industry. The BITE project set out in part to study the functionality of hemicelluloses in stabilising alkyd paints, which are examples of high-volume technical emulsions that could benefit from the properties of wood hemicelluloses. Åbo Akademi and CH-Bioforce produced various wood-derived hemicellulose samples. The University of Helsinki built paint prototypes using each material sample and evaluated the samples for their capacity to emulsify and stabilise alkyd resins in water.

As a result, non-toxic, bio-based and biodegradable natural polymers proved to be an attractive option for stabilising technical emulsions. Wood hemicelluloses have the advantage of being economic, as they are currently viewed as low-value side products. Furthermore, the functionalisation of wood hemicellulose does not require chemical derivatisation but can instead be done by adjusting the isolation method to produce hemicellulose with optimised properties. It is expected that the emulsion-stabilising properties of wood hemicelluloses will be able to be exploited in a number of other value-added industrial processes and may help encourage a shift in industry towards a circular bioeconomy.

Lignin as a renewable alternative to chemical industry

Today, lignin is mostly produced as part of chemical pulping processes, namely Kraft and sulphite pulping. While cellulose/pulp is the main product, lignin is actually a by-product. 98 per cent of lignin is burnt for energy. Globally, this equates to approximately 50 million tons every year. The extraordinary material properties of lignin therefore mainly go unutilised. On the other hand, technical lignin derived from commercial pulping processes is extensively altered in terms of its chemical makeup compared to native lignin. The most abundant aryl alkyl (β-O-4) ether linkages

are readily fragmented and the structures further condensed due to the harsh pulping conditions. Lignin gained from kraft pulping, the pulping process most commonly used around the globe, also contains sulphur, which destroys the reactivity and material properties of commercially available lignins.

CH-Bioforce has solved the problem in a fundamentally different way. A method was developed to gently extract all of the main components of biomass in one process. The resulting biomaterials – dissolving pulp, polymeric hemicellulose and sulphur-free lignin – are extremely pure and close to their natural form. Furthermore, the process can produce these high-quality biomaterials also from agricultural residue streams such as straw. The structure and properties of the extracted lignin depend on the feedstock (softwood, hardwood, straw, etc.), type of fractionation process, and also the process parameters. Therefore, it is extremely important that lignins are properly characterised with an eye to specific process parameters in order to optimise their use in different applications. Together with PCC and industry partners, several studies were conducted to understand how the fractionation process and its parameters impact on the chemical structure of the resulting lignin and thus how they affect the material properties of the final product.

Helping world's biggest brewing company turn brewing waste into textiles

CH-Bioforce has been chosen for AB InBev´s global start-up accelerator programme, 100+Accelerator. The world's biggest brewing company, AB InBev, manufacturer of brands like Budweiser, Beck's and Corona, generates millions of tons of co-product every year. The multinational company is now looking for new, sustainable solutions to put the waste streams into use. CH-Bioforce is one of the 17 international start-ups that have been chosen to be part of the second cohort of the 100+Accelerator.

Brewing waste like barley straw or brewer's spent grain can be repurposed into other types of consumer products for food products or even as ingredients in cosmetics or pharmaceuticals. Packaging solutions are another option. CH-Bioforce has been able to develop a breakthrough biomass fractionation technology which can use almost any kind of lignocellulosic biomass as feedstock. In 100+Accelerator, CH-Bioforce fractionates the barley straw delivered by AB InBev and works with chosen partners to make high-quality textiles. The end product could be a T-shirt, towel or a shopping bag. The technology is already in place and fully functional. The brewing process produces also other biomass waste streams in addition to straw, such as brewer's spent grain. These can be used to produce high-quality biopolymers, which can then be used in the production of plastics, cosmetics or even food additives.

Mr. Nicholas Lax, Mr. Sebastian von Schoultz, and Dr. Lari Vähäsalo (CH Bioforce Oy)

Eco-Oil, a shortcut to the future

Jyri-Pekka Mikkola, Kent van Klint

Chemistry professor Jyri-Pekka Mikkola at Turku's Åbo Akademi and Sweden's Umeå University has managed to develop a fuel based entirely on biomass with the same properties as fossil fuels. He says the new fuel is a made by combining water and ethanol with a catalyst. The resulting concoction is a fuel with a higher octane than petrol or diesel.

The discovery resulted, after experiments, which were performed hidden in a forest for ten years, into a Spinoff company called Eco-Oil. The company was initiated in 2007 and coupled to the Umeå University in the Bio4Energy project in 2008, aiming to produce 100% renewable and CO_2-neutral gasoline, diesel and jet fuel.

The secret of the process lies in the catalysts used. The green fuel can be made from energy crops, forest waste, food residues, household waste, agricultural waste or even old newspapers. Just like normal gasoline, this green fuel releases CO_2, in a same way as the equivalents of the fossil derived petrol, diesel and jet fuel.

"But this carbon dioxide is green carbon dioxide, it's not pumped from the earth in the form of oil, but instead it is from vegetation and it is re-absorbed by vegetation," says Jyri-Pekka Mikkola, Research Director at Eco-Oil.

The fuel is green because it is renewable. The process, where input material, with the help of catalysts, is transformed into renewable diesel or gasoline as well as by-products in the form of a smaller amount of pure gas and pure deionized water, is green too.

The characteristics of the catalyst, which consist of solid, highly porous particles, is that it has a very high surface area, where the active metal particles can meet the reactants and convert them to the products.

> **A single catalyst grain can have a surface area equal to two football pitches, which is approximately 2,000–3,000 square metres per gram**

The process begins with hydrolysis, which involves adding sulphuric acid and letting the lignocellulose in the biomass to disintegrate, a step that is unnecessary when the raw material is sugar beets or sugar ca-ne. Then, the sugar is fermented to form alcohol - primarily ethanol - but all types of alcohol will do.

The ethanol and water mixture is then run into the reactor system, which consists of two 1.5 metre long pipes that contain extremely complex catalysts. A catalyst increases the rate of chemical reactions without being consumed itself.

Toward a world free from fossil fuels

Interest in the new invention has been huge since the patent was published. Mikkola's email is subjected almost daily to intrusion attempts by hackers and his phone is ringing constantly. People want to know how the invention works and how they can invest in it.

For the time being, there is no clear idea as to what type of financing approach will be used. One thing is sure: enormous investments will be necessary to restructure the way fuel is currently produced.

"We now have a functional technology, but the problem is that we need an enormous amount of metal to produce and store the fuel. In order to put together all the pipes, reactors and storage tanks needed to satisfy the demand for fuel, we would need so much metal that it will cost astronomical sums of money."

One possible solution that Mikkola is now working on is to keep fuel production local in smaller quantities, in small reactors inside containers.

"Containers can be transported anywhere in the world. Then we'll have smaller facilities that can be run by another operator and, bit by bit, we'll reach our goal," says Mikkola.

"It's an appealing alternative. When you have a local village council or a hauling firm that buys a container, or an outfit running a pulp mill with excess heat that can be used to start the process, or a sawmill with plenty of sawdust at its disposal, it becomes possible to set up a fermentation plant to produce ethanol and run the plant according to the same integration of various processes."

Mikkolas father´s old Saab went like a rocket when he tested his own renewable fuel (photo by Nicklas Hägen)

www.catbior2019.fi
September 23–27, 2019 Turku/Åbo

2.3 Leading scientists gathered in Turku/Åbo

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: the 2nd congress was held in Dalian in 2013 followed by congresses in Rio de Janeiro in 2015 and Lyon in 2017. 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,

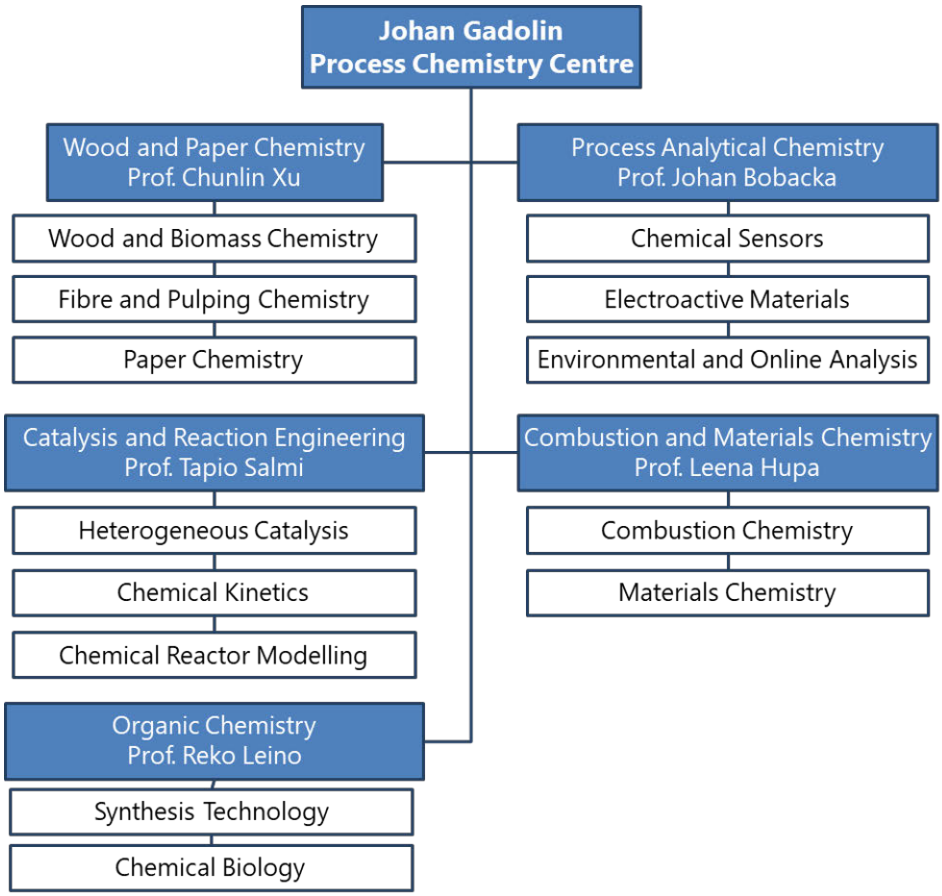
- Fundamental and applied catalysis in biorefinery
- Molecular insights in processing of biomass
- Utilization of lignocellulosic, algal biomass, vegetable oils and other biomass
- Industrial demonstrations
- Catalysis in its variety – homogeneous, enzymatic and heterogeneous catalysis

More than 200 abstracts were submitted to the conference. Based on the evaluation of the contributions by the members of the scientific committee and some other experts in the field of catalysis and biorefinery, 66 oral and 144 poster presentations were selected. 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.

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?

3. Our organization and who we are

3.1 Organization of *PCC*



Executive Board

- Professor Johan Bobacka (chairman)
- Associate Professor Henrik Grénman (vice chairman)
- Professor Leena Hupa
- Professor Reko Leino
- Academy Professor Tapio Salmi
- Professor Chunlin Xu

Coordinator

- Dr. Markus Engblom

Scientific Advisory Board (SAB)

- Prof. Raimo Alén, University of Jyväskylä
- Prof. Jan-Erling Bäckvall, Stockholm University
- Prof. Jiri Janata, Georgia Institute of Technology
- Prof. Lars J Pettersson, KTH Royal Institute of Technology
- Prof. Andreas Seidel-Morgenstern, Max Planck Institute Magdeburg

Forum for Society (FS)

- Lars Gädda, FS Chairperson
- Örjan Andersson, Novia
- Ilmo Aronen, Raisio
- Stig-Erik Bruun, Chemigate
- Kenneth Ekman, Crisolteq
- Jonas Konn, Kemira
- Linda Fröberg-Niemi, Turku Science Park
- Christine Hagström-Näsi, CLIC Innovation
- Patrik Holm, Orion Pharma
- Bertel Karlstedt, Valmet
- Kari Kovasin, Metsä Fibre
- Björn Lax, Chemec
- Timo Leppä, Chemical Industry Federation of Finland
- Lars Peter Lindfors, Neste
- Pia Nilsson, UPM-Kymmene
- Karri Mikkonen, Turku Future Technologies
- Leena Paavilainen, Luke
- Jarkko Partinen, Outotec
- Leena Sarvaranta, VTT
- Mathias Snåre, Nordkalk
- Kenneth Sundberg, Brinkhalls Sparkling
- Kari Toivonen, Elomatic
- Petri Vasara, Pöyry
- Stefan Wallin, Member of Parliament

3.2 Wood and Paper Chemistry

The mission of our research group is to *promote sustainable and multipurpose use of wood for high-value biomaterials and biochemicals and for fibre products*. We strive towards creating and publishing novel and significant scientific findings and to educate students and scientists with excellent skills and creative problem-solving ability for the needs of industry and the society.

Our research is directed towards promoting sustainable, resource efficient, and multipurpose use of wood and other renewable raw materials in products including pulp, paper, fibre, and wood products, but also for novel biomaterials, biocomposites, biochemicals, and bioenergy. Advanced analytical techniques are our tools to obtain knowledge at the molecular level on the various components of different natural raw materials and their reactions, interactions, and functions in different processes and products. Our biorefining approach aims at utilizing forest or other renewable resources as wide-ranging as possible, thus minimizing the amount of waste in the end. For example, selective extraction and recovery of hemicelluloses, cellulose, lignin, or polyphenols from wood, bark, or process waters is followed by functionalization and utilization in different value-added end-uses. A strong research approach is the utilization of nanocellulose, modified hemicelluloses, and lignin for hydrogels and materials in biomedical applications, especially through 3D bioprinting. Nanocomposites based on both lignin and nanocellulose have been developed to remove the heavy metal ions and organic contaminants in waste waters, respectively. We also work on understanding the fibre-fibre joint structure and molecular level interactions between fibre surfaces to obtain high extensibility of the fibre networks for novel mouldable packaging. Furthermore, we provide analytical services and support in process problem solving to the industry in the forest and bioeconomy sectors.

External research support 2018-2019 was obtained mainly from Academy of Finland and the industry, from Royal Swedish Academy of Agriculture and Forestry in the research programme Tandem Forest Values, and from the China Scholarship Council in form of grants for PhD students. We also have close cooperation with e.g. KTH in Sweden, University of Wollongong in Australia, and BOKU in Austria with researcher exchange and joint research and teaching. Other active partners are University of Helsinki, Tampere University, LUKE, and groups affiliated to the Turku Centre for Biotechnology in Finland.

A list of key projects is shortly described below.

- *'Design of biobased extracellular matrix-mimicking scaffolds with tunable rigidity for 3D cell culture and potential tissue engineering (3D Bioscaff)' funded by Academy of Finland, 1.9.2016–31.8.2020.* Wood-based polysaccharides, especially cellulose, which is the most abundant biorenewable material with its promising properties such as excellent mechanical strength and flexibility, biocompatibility, and environmentally friendly nature has found its potential applications in medical treatments, e.g. cell culture and tissue engineering. The ultimate goal of this multidisciplinary research project is to tailor wood biopolymers to scaffolds with different rigidity for in vitro cell culture and tissue engineering. Both wood nanocellulose and hemicelluloses are applied. The outcomes of the project will be the foundation of a new knowledge platform, which will open up new possibilities of utilizing wood biopolymers in such novel biomedical applications as cell culture and tissue engineering.

- *'Revolutionizing Biomedicine with Biopolymers: Engineering nanocellulose hydrogel scaffolds for the delivery of bioactive cues in soft tissue engineering (BioforBio)' funded by Tandem Forest Values – KSLA, 01.01.2019-31.12.2020.* Tissue engineering (TE) scaffold is a promising strategy for treating chronic wounds. Cellulosic nanomaterials are emerging alternative natural polymers well suited for fabricating hydrogel scaffolds for TE strategies. The matrices of engineered scaffolds should provide both physical protection and spatiotemporally controlled bioactive cues for the seeded cells aiming to establish a bidirectional crosstalk between the microenvironments in scaffold and the resident cells. With this truly multidisciplinary research proposal, we aim to specially tailor cellulose nanofibril (CNF) networks to be used in TE strategy and to modify CNF with a focus on tuning the mechanical stiffness of CNF hydrogel and to optimize the CNF bioink formulation for successful 3D printing of hydrogel scaffolds via direct ink writing (DIW). The main outcome is an extracellular matrices (ECM)-mimicking hydrogel scaffold made of a CNF matrix constructed via 3D bioprinting, which carries multiple therapeutic functionalities.

- *'Healing the wounds with Finnish woods: Conductive hydrogel scaffolds of cellulosic nanomaterials and polysaccharide biopolymers for delivery of bioactive cues in soft tissue engineering' funded by Jane and Aatos Erkkos Foundation, 01.09.2019-31.08.2022.* To meet the demands in the mega trend of being more increased regenerative and customized for tissue repair therapy, tissue engineering (TE) approach has become a promising strategy, which deals with in vitro engineering human tissues by stimulating the body's own repair mechanism to heal the irreparable tissues. Nanocelluloses present an emerging catalogue of nanomaterials for versatile applications in constructing advanced functional materials in TE. The ultimate goal of this multidisciplinary research project is to extend the biofunctionalities of 3D printed nanocellulose-based hydrogel scaffolds with integration of a variety of bioactive cues in the hydrogel matrices. The project is anticipated to provide the basis for a new generation of biomaterials, which will open up new possibilities of utilizing woody cellulosic nanomaterials and biopolymers in high-value biomedical applications.

Personnel December 2019

Professors

Chunlin Xu (Research Leader)
Stefan Willför (Vice Rector of Åbo Akademi 2019-2024)
Bjarne Holmbom (Emeritus)

Docents

Andrey Pranovich
Annika Smeds
Anna Sundberg (University Lecturer)

Researchers

Jarl Hemming
Ekaterina Korotkova
Xiaoju Wang
Liping Tan (Johan Gadolin Scholar)
Xiaodeng Yang

Early-stage researchers

Maryam El Hajam
Liqiu Hu
Sara Kesäläinen
Rui Liu
Luyao Wang
Qingbo Wang
Hichem Zergane
Yongchao Zhang
Weihua Zhang

Secretary Karita Åberg

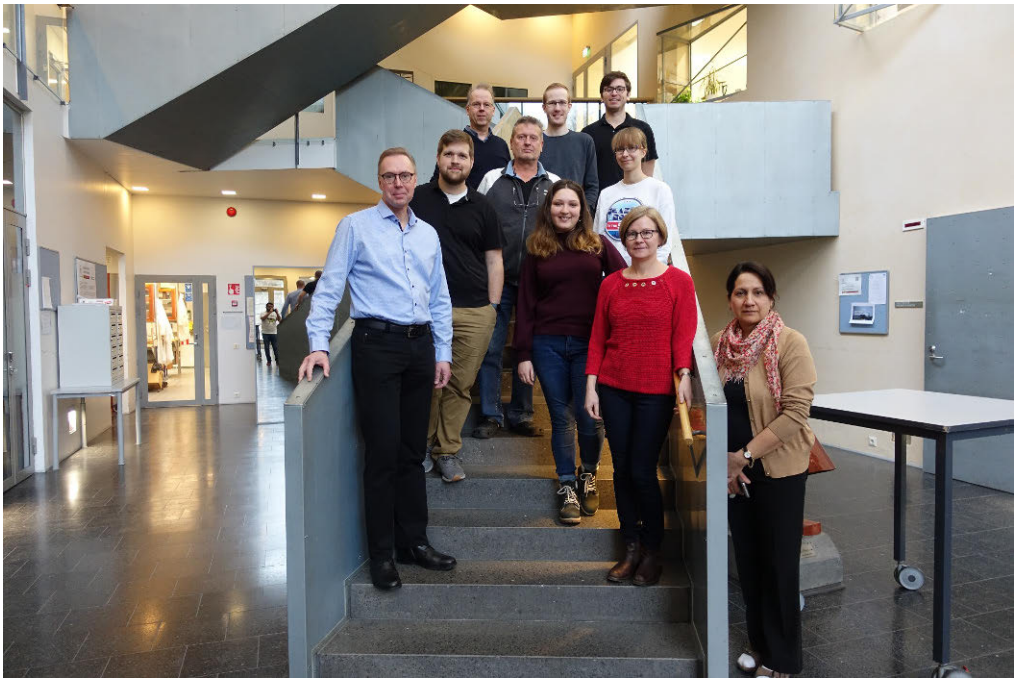
https://www.abo.fi/en/wood-and-paper-chemistry-research-and-researchers/

3.3 Process Analytical Chemistry

Our main expertise in Analytical Chemistry is in the areas of chemical sensors, electroactive materials and electrochemistry. Our research is focusing on the development of novel electrochemical sensors based on advanced functional materials, new receptor molecules and new signal transduction methods. This involves basic research and characterization of new materials as well as design and engineering of novel electrochemical sensors for various applications.

Continuous (on-line, in-line, non-invasive) chemical analysis is well established in the process industry and is becoming more common also in environmental monitoring and personal health diagnostics. Wearable chemical sensors is a hot research topic at the moment. All these analytical applications would benefit greatly from calibration-free and maintenance-free chemical sensors. This is a major driving force for our research. Our solid-contact ion-selective electrodes and solid-state reference electrode represent two important steps towards maintenance-free ion sensors. Our on-going work aims at eliminating the need for calibration of these sensors.

Our electrochemical studies of conducting polymers has recently resulted in a new method to amplify the analytical signal of ion sensors. Our development of anion sensors based on new receptor molecules is in progress. Some unique features of conducting polymers are utilized for the development of electrochemical sensors for detection of DNA hybridization. Furthermore, our research on carbon nanomaterials, such as graphene, will strongly support the development of new chemical sensors. Other project activities include dynamic extraction of heavy metals from soil and electrocatalytic reduction of CO_2. In a wider perspective, our knowledge in electroactive materials and electrochemistry is relevant also for further development of rechargeable batteries and supercapacitors that support the transition towards utilization of solar energy and electrical vehicles.



Process Analytical Chemistry personnel in 2019 (missing from the photo: Zhanna Boeva, Ulriika Mattinen, Tingting Han, Sara Lund, Narender Joon, Jay Pee Oña)

External research funding during 2018-2019 was obtained from the Academy of Finland, Business Finland, industrial partners and foundations. We perform our research in close collaboration with national and international partners from academia and industry. Our participation in the *Erasmus Mundus* joint master degree programme *Excellence in Analytical Chemistry* (EACH), supported by EU, has dramatically increased the number of MSc theses in analytical chemistry from our group.

Personnel

Professors
Johan Bobacka
Tom Lindfors (associate professor)
Ari Ivaska (Emeritus)
Andrzej Lewenstam (Emeritus)

Docents
Adriana Ferancova
Carita Kvarnström
Tom Lindfors
Li Niu
Di Wei
Leo Harju
Rose-Marie Latonen
Zekra Mousavi
Tomasz Sokalski
Anna Österholm

Senior researchers
Zhanna Boeva
Grzegorz Lisak
Kim Granholm
Ulriika Mattinen

Doctoral students and researchers
Ashiq Ahamed
Tingting Han
Sara Lund
Ville Yrjänä
Jesus Arroyo
Narender Joon
Jay Pee Oña

Laboratory Engineer
Tor Laurén

Secretary
Mia Mäkinen

Economy secretary

Britt-Marie Haahti (-8/2019)
Anna Lyubavina (10/2019-)

Technician
Sten Lindholm (-10/2019)

https://www.abo.fi/en/analytical-chemistry-research-and-researchers/

3.4 Industrial Chemistry and Reaction Engineering

The core competence of Industrial Chemistry and Reaction Engineering is in catalysis, kinetics, chemical reactor technology as well as exploring new reaction environments and development of green process technology. Process intensification is a vital part of our research effort. The approach is strongly methodological, but the main application area is the valorization of molecules originating from biomass to fine and specialty chemicals. Heterogeneous catalysis combined to very detailed kinetic studies and avant-garde reactor technologies are the keys for success in the 'great transformation to sustainable chemical processes and products. Our know-how is continuously developed on catalyst technology as well as new approaches to chemical kinetics and reactors. From green chemistry to green process technology is our long-term strategy.

Green process technology progresses in many fields, particularly in the development of new continuous processes for sophisticated chemicals, such as bio-degradable surfactants, platform chemicals, bio-lubricants and chemical intermediates. This is in many cases done in micro- and milliscale reactors, which provide a real technology jump; we use them for catalyst development, kinetic screening and continuous production of chemicals in gas and liquid phases. By utilizing these technologies, a considerable process intensification is obtained, because the mass and heat transfer resistances can be suppressed, and the equipment size is minimized. All the experimental efforts are coupled to advanced mathematical modelling of chemical and physical phenomena in batch, semibatch and continuous systems. Several processes based on molecules originating from biomass are under investigation, for example epoxidation of fatty acids fatty acid esters and alkenes, catalytic transformation of furfural, oxidation of sugars originating from hemicelluloses, aqueous-phase reforming to produce bio-hydrogen as well as catalytic oxidation of ethanol. Microwave and ultrasound technologies are used to enhance the epoxidation fatty acids and carbonation of fatty acid epoxides. Molecular oxygen and hydrogen peroxide are used as environmentally friendly oxidation agents. A fruitful and cross-disciplinary research project devoted to catalytic destruction of pharmaceuticals in wastewaters by using ozone as the oxidation agent is in progress. This extensive research effort is materialized in close collaboration with the researchers in Organic Chemistry/PCC. Novel catalyst structures, such as solid foams are under investigation in order to shift from traditional trickle bed technology to intensified reactor systems. National and international collaboration is flourishing with several universities and research centers. The main

Personnel of the Laboratory of Industrial Chemistry and Reaction Engineering in 2020. (Photo by Atte Aho)

financers of our research are Academy of Finland, Business Finland, as well as several domestic foundations and industrial enterprises. We have been very successful in obtaining project financing from Academy of Finland: totally five projects are in progress. In the beginning of 2019 Academy Professor T. Salmi started a five- year intensive research period devoted to deep understanding of the mechanisms of three-phase oxidation and epoxidation processes on solid surfaces. In autumn 2019 we had the pleasure to host the 5th International conference in Catalysis for Biorefineries (www.catbior2019.fi) – the very successful event gathered around 200 participants all over the world. A luxury conference banquet took place in the medieval castle of Turku/Åbo.

Personnel

Professors

Tapio Salmi (Academy professor 1.1.2019-31.12.2023)
Dmitry Murzin
Johan Wärnå
Jyri-Pekka Mikkola (joint professor with Umeå University)
Päivi Mäki-Arvela, associate professor
Henrik Grénman (tenure track), associate professor
Heather Trajano (visiting professor 2019-2020, University of British Columbia, Vancouver)

Docents

Atte Aho
Narendra Kumar
Matti Reinikainen
Fredrik Sandelin
Pasi Virtanen
Ikenna Anugwom
Sébastien Leveneur
Vincenzo Russo
Pasi Tolvanen

Laboratory manager

Kari Eränen

Senior researchers

Adriana Freites Aguilera
Sigmund Fugleberg
Javier Ibanez Abad
Jussi Rissanen
Nataliya Shcherban
Erfan Behravesh
Teuvo Kilpiö
Marisa Navas
Soudabeh Saied
Zuzana Vajglová

Doctoral students and researchers

Shekoufeh Adhami
José Delgado Liriano
Ramakrishna Jogi
Mark Martinez Klimov
Jay Pee Oña
Christoph Schmidt
Anna Barone
Sebastian Franz
Rossana Suerz
Matias Alvear
Mouad Hachhach
Ekaterina Kholkina
Ananias Medina
Wander Perez-Sena
Tyko Viertiö
Simon Engblom
Cristina Pizzolitto
Francesco Taddeo
Leolincoln Correia da Silva
Maria Herrero Manzano
Xiaojia Lu
Ali Najarnezhadmashhadi
Ole Reinsdorf
Nemanja Vucetic
Michele Fortunato
Carmen Rossano
Cogliano Tommaso

https://www.abo.fi/en/industrial-chemistry-and-reaction-engineering-research-and-researchers/

3.5 Organic Chemistry

Organic Chemistry at Åbo Akademi University strives for excellence in research and education, training students and researchers on all levels for successful careers in industry and academia. The research groups operate in two of the main research profiling areas of Åbo Akademi University: Molecular Process and Materials Technology, and Drug Development and Diagnostics. Within these areas, the main efforts are focused on 1) Development of sustainable chemical synthesis technologies using both homogeneous and heterogeneous transition metal catalysts with special emphasis on understanding of reaction mechanisms and kinetics; 2) Synthetic carbohydrate chemistry and glycobiology; 3) Novel carbohydrate derived functional materials; 4) Natural product chemistry, with particular focus on wood extractives such as lignans and hemicelluloses and lignin. All these key research areas rely heavily on utilization and understanding of advanced NMR spectroscopic techniques.

Other research activities range from energy research to environmental organic chemistry including studies on the environmental fate of pharmaceuticals, antibiotics and endocrine disruptors.
We also closely collaborate with several national and international partners and actively participate in research networks.

Personnel of the Laboratory of Organic Chemistry in September 2018

Personnel

Professors

Reko Leino
Jorma Mattinen (Emeritus)

Docents

Patrik Eklund
Tiina Saloranta-Simell
Leif Kronberg
Annika Smeds
Filip Ekholm (University of Helsinki)
Ari Rosling (Arctic Biomaterials)

Experienced Researchers

Jan-Erik Lönnqvist
Risto Savela
Carolina Méndez-Gálvez
Jani Rahkila (Instrument Centre)

Early stage researchers

Sofia Galasheva (10/2018-9/2019, SPCPU, St. Petersburg)
Matilda Kråkström
Lucas Lagerquist
Robert Lassfolk
Ida Mattsson
Sabine Rendon
Patrik Runeberg
Atefeh Saadabadi

Laboratory engineer

Teija Tirri

Secretary

Mia Mäkinen

Economy secretary

Britt-Marie Haahti (-8/2019)
Anna Lyubavina (10/2019-)

https://www.abo.fi/en/organic-chemistry-research-and-researchers/

3.6 Combustion and materials chemistry

Our research strategy is to provide expertise on the detailed knowledge of chemistry in high-temperature processes and properties of high-temperature-made materials. Our main research endeavours are foremost in bioenergy and biomedicine, with a wider outreach to clean-tech and circular economy. Management of material streams and emissions, treatment and recycling of different waste streams that contain inorganic materials in energy efficient and environmentally friendly manner are essential topics in our research.

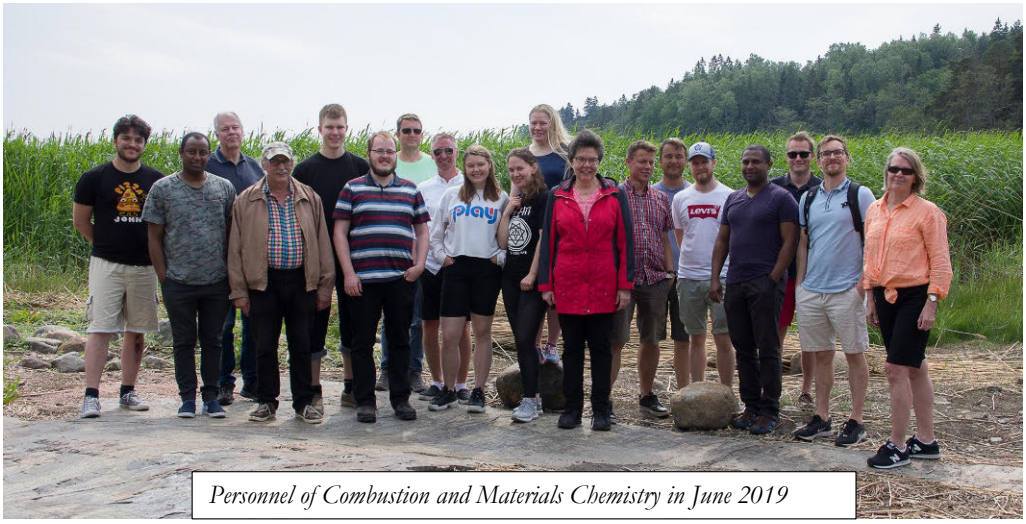
Within the bioenergy field, our research includes characterising the composition and behaviour of different biomasses and waste-derived fuels, modelling of combustion processes, measurement of emissions to the atmosphere, and development of a generic understanding of the interactions between the materials in the combustion devices, the fuels and their ashes.

Within the biomedical field, development of composites containing bioactive glasses for wound healing and tissue engineering scaffolds are our main research focuses. Over the years, our strategy has been to understand thoroughly the influence of the oxide composition of the bioactive glasses on various cellular responses. One key goal is to develop detailed knowledge of the reaction and dissolution kinetics of the bioactive glasses when they are used in various biomimetic devices in hard and soft tissue regeneration applications.

We utilise thermodynamic equilibrium calculations to describe high-temperature processes, especially in various ash, slag and glass forming systems. For this, we develop thermodynamic databases of the high-temperature systems through thermal analysis in ambient and pressurised atmospheres containing different gases.

We use several experimental tools (single-particle reactor, thermogravimetric analyser/differential scanning calorimeter, lab-scale fluidised bed, heat microscope, scanning electron microscope and x-ray diffraction) to study the high-temperature chemistry of different fuels, ashes and materials.

We also develop sub-models to describe the chemistry in high-temperature processes, such as NOx-formation reactions in various fuels to be adapted to the modelling of combustion-related processes with computational fluid dynamics. One distinctive attribute of our research is the development of cleaner and more efficient combustion technologies using fuels that are "difficult".



Personnel of Combustion and Materials Chemistry in June 2019

The research is not only in laboratory scale but also includes measurements and sampling campaigns in full-scale combustion processes. Some of our core competence areas are exploring the high-temperature corrosion and erosion mechanisms of steam tubes and ceramic refractories induced by bed materials and various ashes that contain alkalis, chlorides, bromides, fluorides, etc. Recently, we have developed new techniques to accurately measure and understand the corrosion and reaction mechanisms of the materials in their target environments.

Our research is in collaboration with groups and people from many different universities, companies and research centres. It is financed by Åbo Akademi, Tekes, Academy of Finland, the EU, NordForsk, industry and small to medium-sized enterprises. In addition to novel generic knowledge and competence, our research gives the industry partners new strategic scientific information and tools for innovations, new products and business concepts for the global market.

Personnel

Professors
Leena Hupa
Mikko Hupa (Rector of Åbo Akademi 2015-2019)

Docents
Anders Brink
Niko DeMartini
Bengt-Johan Skrifvars
Sonja Enestam
Daniel Lindberg

Laboratory manager
Tor Laurén

Senior researchers
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Oskar Karlström
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Emil Vainio
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Roland Balint
Nina Bruun
Meheretu Dirbeba
Jan-Erik Eriksson
Stefan Heberlein
Elisa Hupa
Arturo Keim
Thomas Kronberg
Paulo Santochi
Daniel Schmid
Christoffer Sevonius
Minna Siekkinen
Polina Sinitsyna
Adrian Stiller
Raju Viswamoorthy

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Luis Bezerra
Jaana Paananen
Linus Silvander

Secretary
Maria Lastuniemi
Mia Mäkinen

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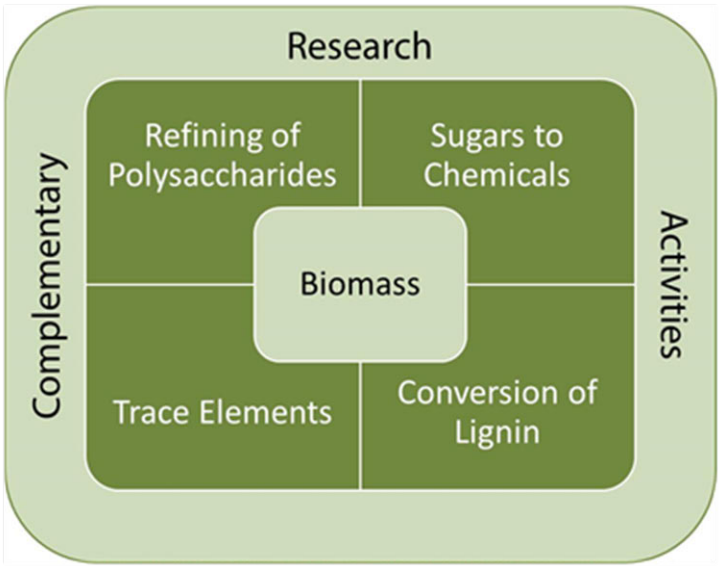
4. Actual Research

Our major research plan "***PCC*** – Future Refining of Forest Biomass" is in the core of the Finnish Bioeconomy, Circular Economy, and Cleantech areas. Finland can become one of the pioneers in a global perspective in the evolutionary development of forest biomass, because 70% of our territory consists of forest, which is rich in lignocellulosic biomass. Finland actually has the largest amount of forest per capita in the whole of Europe and this biomass has a yearly growth that is larger than what we utilize. Forest biomass is potentially a very rich source of molecules, which can be further refined to new materials, chemicals and fuel components. The challenge is big, because the molecules appearing in biomass deviate substantially from those in fossil sources. Molecules from biomass have a high degree of functionality and high oxygen content compared to the molecules appearing in fossil sources. This implies that many of the current technology solutions cannot be applied directly to molecules originating from biomass and therefore new chemical technology is needed.

The development of new technologies should be based on a very deep-going understanding of the underlying chemical and physical processes, which we call Molecular Process Technology. ***PCC*** merges chemistry and chemical engineering to provide industrially relevant solutions for the future. The goal is to develop new, sustainable technologies for making selected platform chemicals, fine and specialty chemicals, as well as health promoting materials and chemicals. The research is mainly focused on two important types of molecules appearing in forest biomass, namely polysaccharides (hemicelluloses and cellulose) and lignin. Additionally, our research includes multiple complementary research activities. Our research areas are illustrated below, and specific research projects are highlighted further in the rest of this Chapter.



PCC *research areas.*

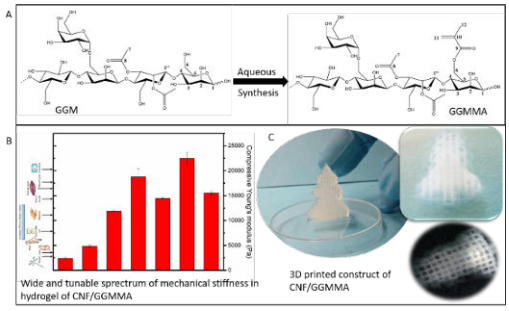
All-wood biomimetic inks based on nanocellulose and UV cross-linkable wood biopolymer for 3D printing

Main funding: Johan Gadolin Process Chemistry Centre (PCC), Academy of Finland

Wenyang Xu, Xiaoju Wang, Stefan Willför, Chunlin Xu

Biomedical hydrogels are one intriguing profiling area for nanocelluloses. For developing hydrogel scaffolds that mimic the three-dimensional (3D) architecture of tissues and recapitulate biological functions, 3D bioprinting outstands to enable creating individually tailor-made tissue engineering scaffolds to provide desired architecture, and furthermore, integrating with biological cues to direct cell response in a controlled manner. A bioink refers to a multicomponent biomaterial system used in 3D bioprinting where a biocompatible matrix provides appropriate surface and adequate spaces to accommodate the cells and other bioactive substances as well to foster and direct the crucial cellular activities in three dimensions. Recently, nanocelluloses have also emerged as renewable constituents in formulating bioinks, which are extrudable thanks to their shear-thinning rheological properties. One of the challenges to apply the nanocellulose-based bioink in 3D bioprinting is to keep ink fidelity after the extrusion and further to achieve mechanical integrity of the prints during and after printing. UV crosslinking is a facile and easily applicably strategy to integrate in 3D bioprinting to address this perspective.

In highlight of the intrinsic affinity of hemicellulose anchoring onto cellulose surface, the biomimetic combination of cellulose nanofibrils (CNFs) of different kinds with hemicellulose derivatives in formulating bioink present a state-of-the-art approach. We have successfully developed the bioink formulation based on TEMPO-oxidized CNFs and UV cross-linkable galactoglucomannan methacrylates (GGMMA), where the GGMMA aids the ink fidelity by UV-crosslinking and further reinforces the hydrogel network of CNFs. By tuning the degree of substitution of the GGMMA and compositional ratio between CNF and GGMMA, the compressive Young's moduli of the formulated inks after cross-linking presented a tunable wide spectrum from 2.5 kPa to 22.5 kPa. Rapid gelation of the CNFs/GGMMA upon UV irradiation also defines the competitiveness of this bioink on fabricating large objects with complex geometry, but also with high resolutions. Used as the seeding matrices in the cultures of human dermal fibroblasts and pancreatic tumor cells, the scaffolds printed with the GGMMA/CNF inks showed great cytocompatiblity as well as supported the matrix adhesion and proliferative behaviour of the studied cell lines. We envisage the biomimetic ink formulations of CNF/GGMMA amend sustainable and high-performance alternatives to the bioink catalogue, which potentially meets the requirements for a variety of in vitro cell-matrix and cell-cell interaction studies in the context of tissue engineering, cancer cell research, and high-throughput drug screening, etc.



***A**) UV-crosslinkable wood heteropolysaccharide polymer GGMMA; **B**) Mechanical stiffness achieved for the hydrogel scaffolds printed with CNF/GGMMA ink suitable for multiple cell lines in TE context; **C**) 3D printed construct of CNF / GGMMA in complex geometry as well in high resolution.*

Cooperation: Docent Fang Cheng in Department of Cell Biology of ÅAU and Prof. Monika Österberg from Aalto University

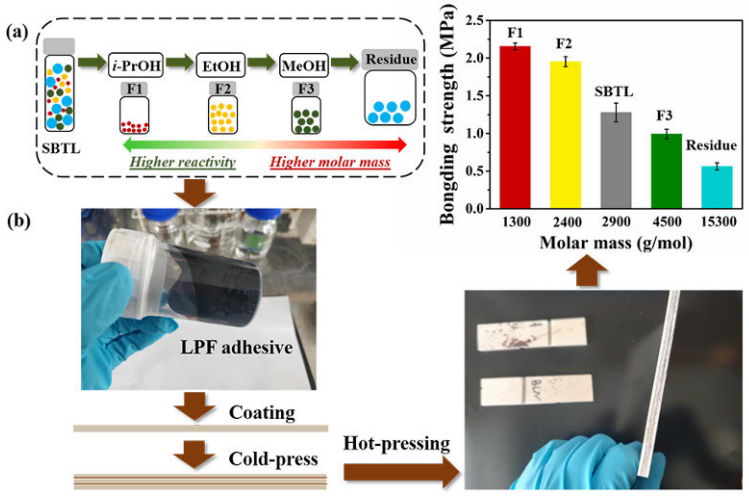
Lignin Fractionation and Its Valorization in Thermosetting Wood Adhesive

Main funding: China Scholarship Council, Fortum Foundation

Luyao Wang, Lucas Lagerquist, Yongchao Zhang, Andrey Pranovich, Thomas Rosenau, Patrik Eklund, Stefan Willför, Chunlin Xu and Xiaoju Wang

Technical lignin generated from pulping industry or upon cellulosic ethanol production is by far the most abundant and available aromatic bioresource. Because of the structural similarity, technical lignin represents a natural, promising sustainable alternative to the petroleum-based phenol in phenol-formaldehyde (PF) wood adhesive. However, a given sample of technical lignin possesses significant variability concerning impurities, as well as extremely heterogeneous chemical features in terms of the molar mass variation, molar mass dispersity ($Đ_M$), functionalities, and constituent inter-unit bonding patterns. These aspects have substantially constrained the industrial valorization of technical lignin. To tackle the issues associated with the inherent heterogeneity of technical lignin, fractionation technology has been utilized to produce relatively homogeneous lignin fractions with well-defined characteristics, such as defined range of molar mass and enriched functional groups that are desired in the respective applications.

The present work aims to elucidate the correlations of molar mass, functionality, and chemical structures of lignin with the bonding strength performance of the lignin-containing PF (LPF) wood adhesives. In practice, soda birch technical lignin (SBTL) was subjected to a sequential solvent extraction (*i*-PrOH, EtOH, and MeOH), in order to derive lignin fractions for the use in manufacturing LPF adhesives (Fig. a). The molar mass-dependent profiles of the reactive sites for LPF synthesis and contents of carbohydrate and stiff inter-unit linkage (β-β') were revealed in this study. The covalent integration of lignin structure into the PF adhesive was successfully achieved through effective phenolation. The wet bonding strength of the LPF adhesive, tested by gluing wood pieces (Fig. b), increased with decreasing molar mass and $Đ_M$ of the integrated lignin fraction, as attributed to the high chemical accessibility and low steric hindrance. This study demonstrates a clear structure-property-application relationship of SBTL in the LPF wood adhesive field, which might pave the way for a more effective bulk valorization.



(a) Schematic description of the sequential lignin fractionation process. (b) The preparation process of the plywood and the wet bonding strength of the plywood as a function of the lignin molar mass

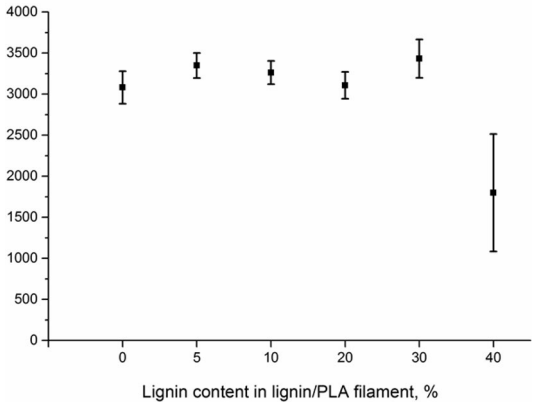
Cooperation: Institute of Chemistry of Renewable Resource in BOKU University, Vienna, Austria

Lignin/polylactic acid (PLA) composites as 3D printer feedstock materials: adapt lignin modification with fatty acid to improve the miscibility with PLA

Main funding: PCC, Fortum Foundation

Xiaoju, Wang, Lucas Lagerquist, Yongchao Zhang, Wenyang Xu, Andrey Pranovich, Patrik Eklund, Chunlin Xu, Stefan Willför

Additive manufacture (AM), also known as three-dimensional (3D) printing, offers rapid prototyping capability and precise control over the complex geometry and fine feature resolution for the fabricated objects with the aid of computer-aided design (CAD) model and computer-controlled software. In the AM technology family, fused deposition modeling (FDM) has shown greatest versatility by nozzle-deposition-based extrusion with the utilization of a variety of biodegradable polymers. PLA is one of the main desktop 3D printer feedstock materials, owing to its favorable mechanical properties and thermoplastic processability, as well as the green feature of its synthesis routes from renewable resources. More recently, as one of the wood biorefinery side and waste-stream products, lignin has showed great potential in preparing composites to be used as 3D printing feedstock materials, which shows money can be made from lignin. In our project, we have investigated whether the fatty acid (FA)-modified lignin can have improved miscibility with PLA in formation of the composite, as that was the problem accounting for the brittleness in PLA when we previously blended unmodified lignin with PLA with a solution casting method to obtain filaments of lignin/PLA via hot melt extrusion (HME). Result of flexural modulus of composite filaments shows upto 30% lignin can be blended with PLA without comprising their mechanical strength (figure).



Flexural modulus of different Lignin/PLA filaments´ composition.

The esterification of the refined lignin, fractionated from a pine resource, with a series of FAs with varied aliphatic chain length was carried out. The influence of the aliphatic chain length in fatty acid on the thermal properties of the FA-modified lignins is under investigation. Also, the miscibility of FA-modified lignins with PLA in the composite preparation and the consequent impact on the mechanical properties of obtained composites with PLA are also the main focuses of the ongoing project. The obtained composites of FA-modified lignin/PLA composite are extrudable and FDM 3D printing has successfully employed the extruded filament to print objects such as screw species.

Nanostructured biocomposites for wastewater treatment

Main funding: China Scholarship Council (CSC), Graduate School in Chemical Engineering (GSCE), Fortum Foundation

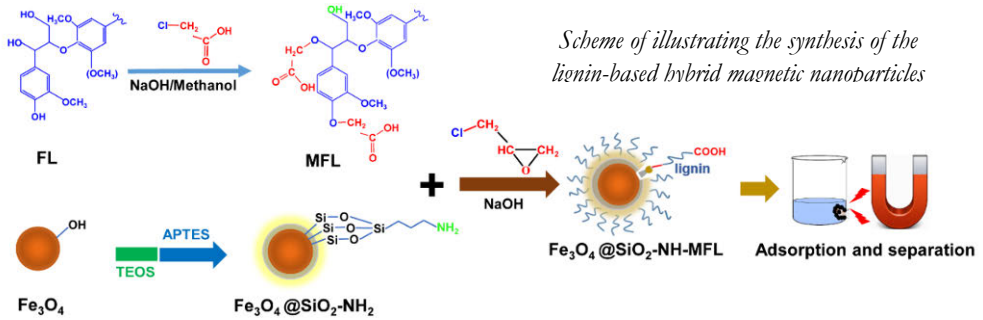
Yongchao Zhang, Weihua Zhang, Xiaoju Wang, Stefan Willför, Chunlin Xu

Water pollution has raised a global concern for the last few decades because of their rampant damage to the ecological environment. Water pollutants can be both heavy metals and organic contaminants that are associated to numerous industries and daily disposal by human beings. Here, we present two research highlights that are addressing water pollution problems, using nanostructured biocomposites which were constructed from lignin and nanocellulose, respectively.

Lignin-based hybrid magnetic nanocomposites for heavy metal ion removal

Various adsorbents have been developed for the adsorption of heavy metal ions from aqueous solutions. In an up-to-date research context, nanomaterials are regarded as the most promising novel adsorbents to remove heavy metal ions from wastewater because the unique physical and chemical properties of nanostructured adsorbents provide much higher efficiency and faster rates for the removal of heavy metal ions. Among various nanostructured adsorbents, nanoparticles exhibit unprecedented opportunities for the adsorption of heavy metals ions in high efficiency. Especially, magnetic nanoparticles as well as their composites have emerged to draw considerable interests in the adsorption of heavy metal ions because of their intriguing features, such as easy separation of adsorbent and adsorbate by an external magnetic field, large surface area, uniform structure, and diversity in surface functionalization.

Lignin is one of the most abundant renewable aromatic polymers in nature. We have recently developed a fractionation process based on formic acid hydrolysis of non-wood to allow an efficient separation of lignocelluloses into the three major components without severe degradation. In this process, formic acid lignin with a yield of 31.5% was isolated and carboxymethylated. Thereafter, novel hybrid nanoparticles were prepared by a facile method involving epichlorohydrin as a cross-linker between carboxymethylated lignin and amino-functionalized magnetic nanoparticles (see Scheme). Both the special nanostructures and the abundant active sites produced from the carboxymethylated lignin are beneficial for the adsorption of heavy metal ions. The as-synthesized magnetic hybrid nanoparticles exhibited adsorption capacities of 152.4 and 71.4 mg/L for Pb^{2+} and Cu^{2+}, respectively. More importantly, the adsorption equilibrium of Pb^{2+} and Cu^{2+} onto hybrid nanoparticles were achieved within 30 s, which was among the fastest of those previously reported for Pb^{2+} and Cu^{2+} adsorbents. The binding mechanism of Pb^{2+} and Cu^{2+} by hybrid nanoparticles was attributed to ion exchange and hydrogen bonding. The tailored nanostructured hybrid nanoparticles with exceptional adsorption effectiveness and efficiency are low-cost and eco-friendly, which potentially meets the cost-effective criteria for producing the water treatment adsorbents on a large scale.



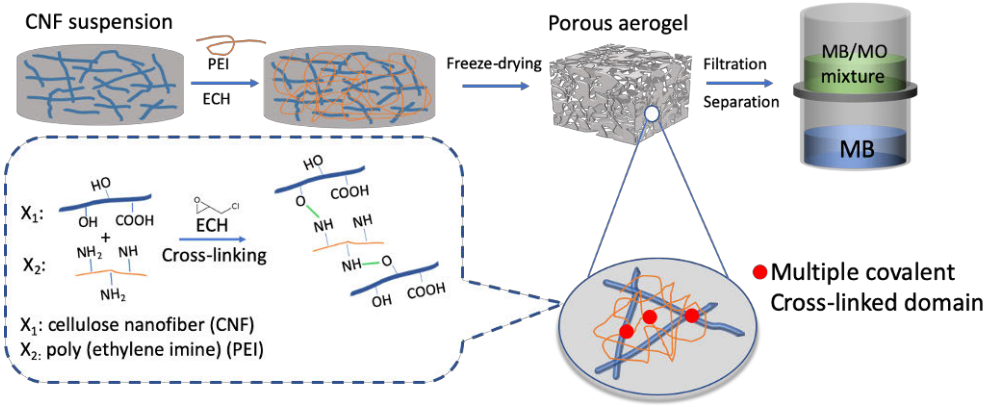
Scheme of illustrating the synthesis of the lignin-based hybrid magnetic nanoparticles

Nanocellulose-based composites for applications in the removal of organic dyes

Water-soluble organic dye is one essential pollutant source of organic pollutants for their extensive applications in the printing and textile industries for producing paints, textiles, leather, and paper. These dye-polluted streams are threatening the quality of water on this planet, influencing the ecological balance, and will eventually cause severe harm to all human beings. In order to treat dye-contaminated water efficiently, vast technologies, such as physical adsorption, membrane filtration, photo-catalytic degradation, oxidation, catalytic reduction, and biodegradation, have been developed and used in recent years. As the most abundant renewable natural polymer on earth, nanocellulose has been considered as a potential raw material to fabricate functional composite materials for organic dye contaminated water treatment.

In this work, nanocellulose-based porous composites were developed for treating organic dyes from industrial wastewater. Firstly, we prepared cellulose nanofibers (CNFs)/poly (ethylene) (PEI)/silver nanoparticle composite aerogels. The as-prepared composite aerogel membrane showed excellent continuous catalytic discoloration of aqueous cationic and anionic dye solutions in batch and flow filtration tests. Moreover, the aerogel membrane exhibited very stable catalytic activity with discoloration efficiency at as high as 98% after 10 times reuse and the water transport was high, up to 5×10^4 L/m^2·h. Interestingly, the aerogel membrane showed excellent shape recovery in water and no obvious deterioration of the structure was observed during long time testing and reuse.

Secondly, we prepared ultralight porous CNF/PEI composite aerogels cross-linked with epichlorohydrin (ECH) as adsorbent to remove organic dyes from wastewater by adsorption (see Scheme). The prepared composite aerogel membrane showed excellent water stability, water activated shape recovery, and fast water transport. In addition, the aerogel also showed excellent performance of recyclability, dynamic filtration–purification, selective adsorption for anionic dyes from mixed dye solutions and smart filtration–separation for cationic and anionic dyes. We envision that this work will not only provide a new strategy to construct low-cost and highly efficient adsorbents, but also demonstrate their potential applications in the removal of organic dyes on a large scale.



A schematic process flow diagram illustrating the synthesis of the nanocellulose-based composite aerogel

Cooperation:
Tianjin Key Laboratory of Pulp & Paper, Tianjin University of Science & Technology, China; Department of Chemical Engineering, Lakehead University, Canada.

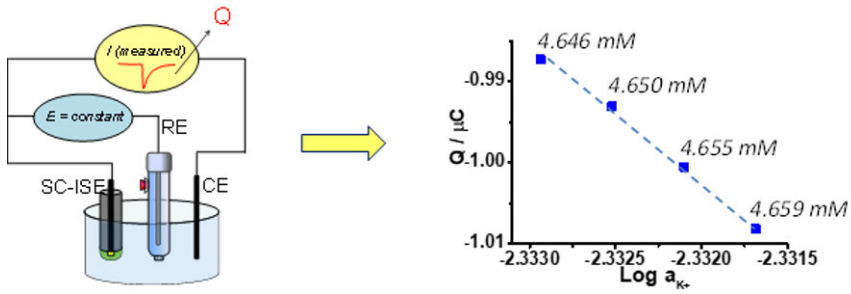
Novel Signal Transduction Principle Enabling High-Precision Ion Sensing

Main funding: Academy of Finland

Tingting Han, Ulriika Mattinen, Zekra Mousavi, Johan Bobacka

Potentiometric ion sensors (ion-selective electrodes, ISEs) are among the most versatile electrochemical sensors known today. ISEs traditionally involve potentiometric signal transduction, which means that ion concentration (activity) is related to the equilibrium potential of the ISE vs. the reference electrode. Since the potential is proportional to the logarithm of ion activity in the sample solution (Nernst equation), ISEs show an impressive dynamic range of 5-8 orders of magnitude. The drawback is the limited precision, i.e. a potential difference of 1 mV means a 4 % change in ion activity for a monovalent ion (8 % for a divalent ion). This is a fundamental limitation of ISEs, which is addressed in this research project by exploring a new coulometric transduction principle.

The coulometric transduction method allows inherent amplification of the analytical signal for solid-contact ion-selective electrodes (SC-ISEs). This approach enables the determination of very small changes in ion concentrations, i.e. it improves the sensitivity and precision of ion sensing. This is of importance e.g. when determining electrolytes (Na^+, K^+, Cl^-) in clinical analysis and when determining small pH changes in seawater. The proof-of-concept for the coulometric transduction method has been demonstrated for several cations (Na^+, K^+, H^+, Ca^{2+}, Pb^{2+}) and anions (Cl^- , NO_3^-, ClO_4^-, SO_4^{2-}). The figure below shows an example of the results obtained for a K^+-selective SC-ISE.



The coulometric transduction principle allows high-precision ion sensing. The calibration curve to the right was obtained using a solid-contact K^+-selective electrode

Exploration of the new signal transduction principle is a generic approach that is expected to have a scientific impact in the fields of electrochemistry, sensor science and analytical chemistry. In particular, the results will improve the analytical performance of SC-ISEs for clinical analysis, including classical in-vitro diagnostics as well as wearable sensors for personal health monitoring. The approach may also be useful for on-line process analysis.

Cooperation:

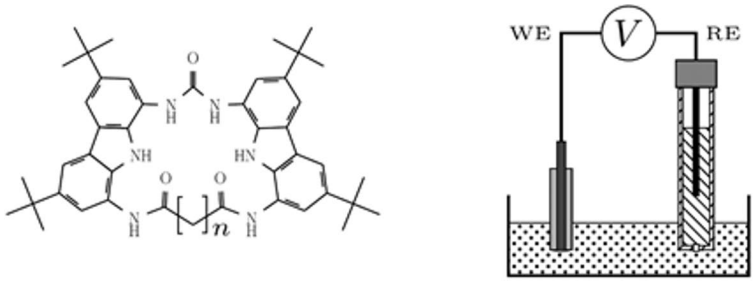
University of Geneva (Switzerland), University of Memphis (USA), Thermo Fisher Scientific (Finland)

Anion-selective electrodes based on novel ionophores

Main funding: Magnus Ehrnrooth Foundation

Ville Yrjänä, Indrek Saar, Johan Bobacka

Ion-selective electrodes (ISEs) have been used for over one hundred years to determine concentrations of numerous different analytes such as H^+, Na^+, K^+, Pb^{2+}, Cl^- and F^-. The advantages of ISEs include low cost, ease of manufacturing, ease of use, and portability. These properties make ISEs an attractive alternative to many other analytical methods for certain applications. ISEs have established themselves a position in e.g. clinical chemistry where they are used for routine analysis of blood samples and achieve the high throughput that is required for such an application. ISE research has for several decades focused on polymeric ion-selective membranes and solid-state ion-to-electron transducers to enable the manufacturing of smaller, more robust ISEs with membranes that can be tuned more easily than e.g. glass or crystal membranes. Ionophores, which are receptor molecules that can reversibly and selectively bind target analytes, play an essential role in the selectivity of polymeric ion-selective membranes. The design of ionophores that are selective to specific anions is particularly challenging and this is addressed in this work. The goal of the present work is thus to design and synthesize tailor-made ionophores for anions and to produce solid-contact anion sensors based on these novel ionophores.



Macrocyclic receptors (left) for carboxylates were prepared and characterized. A subset of these new receptors was used to prepare solid-contact ion-selective electrodes (right) for acetate

Novel macrocyclic receptors for carboxylates were designed and synthesized by collaborators at the University of Tartu. The number of units in the methylene bridge, which links the two ends of the 1,3-bis(carbazolyl)urea backbone, was systematically varied to produce a series of receptors with cavities of different sizes. The receptors' binding affinities for several carboxylates of varying sizes were determined in DMSO-d_6:H_2O (99.5 %:0.5 % m/m) and two local maxima for affinities were observed in receptors with seven and nine units in the methylene bridge. The receptors with five, nine, and twelve units in their methylene bridges were chosen for sensor prototyping based on the binding affinity results. ISEs with membranes based on poly(vinyl chloride) (~32 wt.%)

plasticized with bis(2-ethylhexyl) sebacate (~65 wt.%) were prepared with 2 wt.% ionophore and 50 mol.% anion exchanger (relative to the ionophore) at PCC.

The sensors, which were studied as acetate-selective electrodes, were found to be selective for carboxylates and were able to reduce the selectivity coefficients of interferents by up to four orders of magnitude when compared to the control sensors, which did not contain any ionophore. The selectivity towards acetate improved with increasing number of units in the methylene bridge. However, the sensors did also show selectivity towards carboxylates in general and the selectivity towards the carboxylates was determined primarily by the lipophilicity of the carboxylate (i.e. the sensors were more selective towards benzoate than pivalate and lactate). Further sensor development using these three macrocyclic receptors and an acyclic receptor, which is also based on 1,3-bis(carbazolyl)urea, is ongoing.

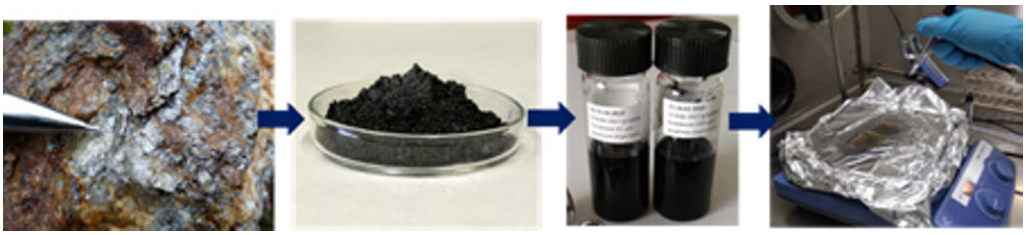
Cooperation:
The group of Prof. Ivo Leito at the University of Tartu, Estonia.

Exfoliation of Finnish flake graphite and fabrication of electrically conductive few-layer graphene films and composites with nanocellulose

Main funding: Academy of Finland (MISU Programme) and K.H Renlunds stiftelse

Sara Lund, Saara Sirkiä, Elisabeth Björnvik, Rose-Marie Latonen, Tom Lindfors, Jan-Henrik Smått, Jouko Peltonen, Jenny Palosaari and Olav Eklund

There is a growing demand for the development of new sustainable and disposable materials due to the Earth's limited resources. Materials derived from graphite and cellulose such as graphene and nanocellulose can answer to that demand for several different reasons. Graphene is a highly conductive nanomaterial which can potentially substitute some commonly used rare heavy metals (e.g. Ga, Pt and In) in many electronic applications. Cellulose nanocrystals (CNC) are extracted from the natural biopolymer cellulose which is a biodegradable and nontoxic material readily available from renewable sources, cellulose being the most abundant polymer on the Earth.



The evolution of materials from the flake graphite bearing rock sample in Haapamäki (on the left) to purified graphite powder, few-layer graphene dispersions and finally, to the spray-coated few-layer graphene films (on the right)

In this project, Finnish flake graphite is exfoliated in liquid-phase by high-shear mixing using a suitable dispersing agent to produce dispersions of few-layer graphene and CNC composites. Firstly, we have exfoliated graphite in a sodium cholate (SC) surfactant solution and investigated different aspects of the exfoliation process such as the graphite flake size, exfoliation temperature and dialysis of the dispersions. For this study, the graphite ore obtained from Haapamäki was enriched in an in-house process to contain 99.3 ± 0.5% m/m carbon and the purified graphite was sieved into 6 different size fractions (from ≤45 μm to 250 μm – 1 mm). Spray-coated films were fabricated from each size fraction and from the dialyzed and non-dialyzed dispersions. We found that it is not necessary to use the more expensive large flakes to produce dispersions with high concentration and good quality. We also found that dialysis is an effective method to remove excess SC from the dispersions and that it improves the conductivity of the films (ca 8000 S/m vs 13 000 S/m). Overall, we have produced dispersions containing over 3 mg/ml few-layer graphene and the films show conductivities as high as 17 000 S/m, which is higher than previously reported for similar materials.

We have also fabricated electrically conductive graphene/CNC composites by directly exfoliating graphite in a CNC suspension and spray-coating the dispersion on thin glass substrates. This is a simple, fast and environmentally friendly method since there are no extra chemicals or processing steps needed. The biocompatibility of the composites have been investigated with algae in a collaboration with Department of Biochemistry, Molecular Plant Biology from the University of Turku. The idea is to use the graphene/CNC composite as a conductive substrate for the algae in a photosynthetic electrochemical cell.

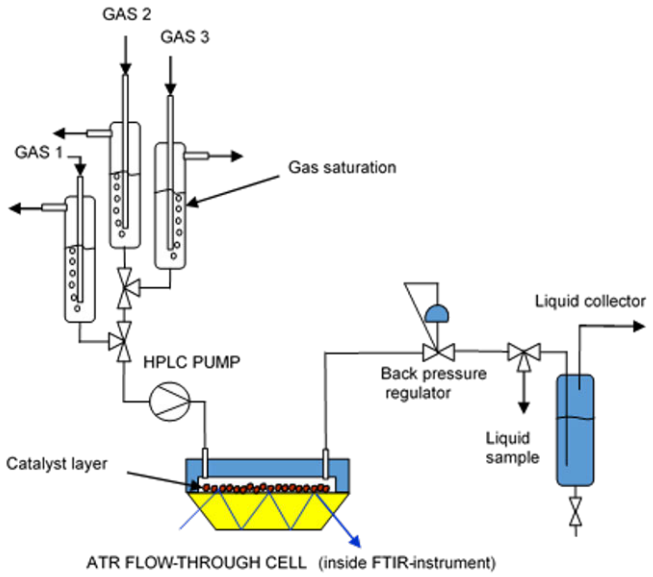
Cooperation: This work is a part of a project called FennoFlakes (lead by prof. Olav Eklund) which identifies potential flake graphite ores in Finland and produces purified graphite which is to be used in proof-of-concept applications to demonstrate the usefulness of the graphite raw material. The FennoFlakes project is an interdisciplinary collaboration between Geology and Mineralogy, Laboratory of Molecular Science and Engineering (Analytical and Physical Chemistry groups) with Fennoscandian Resources Oy and Beowulf Mining as industrial partners. The Laboratory of Natural Materials technology (Wood and Paper Chemistry group) has provided the nanocellulose suspensions needed for the composite production.

Towards a deep understanding of multiphase molecular processes by application of transient experimental techniques and mathematical modelling

Main funding: Academy of Finland (Academy Professor's project 2019-2023), Åbo Akademi

Tapio Salmi, Kari Eränen, Pasi Tolvanen, Adriana Freites Aguilera, Ole Reinsdorf, Matias Alvear, Christoph Schmidt, Wander Perez-Sena, Jani Rahkila, Dmitry Murzin, Johan Wärnå, Vincenzo Russo, Sébastien Leveneur

For molecular-level understanding of chemical processes, particularly reaction mechanisms, measurement of the rates of chemical processes, i.e. chemical kinetics, plays a central role. Conventional methods for investigating chemical kinetics are based on the measurement of concentration changes as a function of reaction times in batch and semibatch reactors. For rapid reactions, continuous reactor technology is preferred because it enables kinetic measurements in very short reaction times. Conventional kinetic methods are, however, not sufficient for studying chemical processes in which solid heterogeneous catalysts and several phases (gas-liquid-solid) are involved. Numerous industrially relevant catalytic processes are much more difficult to investigate on a deeper molecular level, because they are multiphase systems involving both gas and liquid phases. In situ and transient experiments in the liquid phase are much more demanding than for gas-phase experiments. Attenuated total reflection infrared spectroscopy (ATR) is a strong tool for the investigation of surface species for liquid-phase catalytic reactions. A new approach and new techniques are needed in this area not only to get a better understanding on reaction mechanisms but to establish adequate kinetics and design significantly improved chemical reactors, for instance by using solid structures (e.g. solid foams, monoliths, milli- and microreactors) and 3D printing technology. The objective is to get a deep understanding of reaction mechanisms in multiphase catalytic systems. This will result in the preparation of much more efficient catalysts in the future, in establishing reaction kinetics models relevant for fundamental science and in the development of industrial applications.

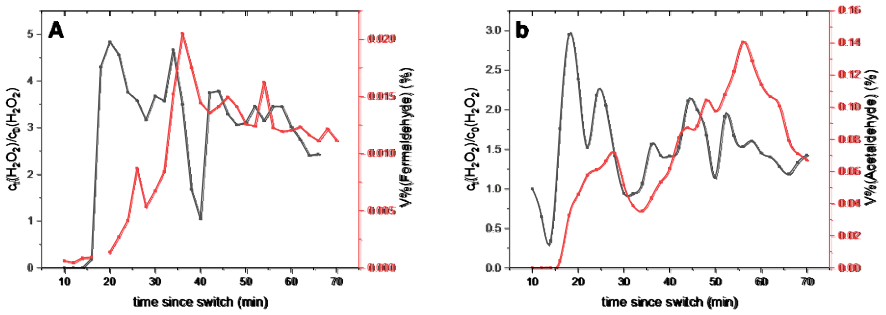


The molecules to be studied will be biodegradable and originate from biomass. The aim is to investigate environmentally friendly processes with current and particularly potential industrial relevance. The key molecules are monomers from biomass, hydrogen, oxygen, water and hydrogen

peroxide. The main focus will be on heterogeneously catalyzed oxidation and epoxidation processes. Oxidation of carbonyl and hydroxyl groups in molecules originating from biomass is of significant industrial importance, presenting many challenges related to the understanding of reaction mechanisms and kinetics. The project has been commenced with studies of the reaction mechanisms of hydrogen peroxide direct synthesis and epoxidation of alkenes and fatty acids. Hydrogen peroxide is used as the epoxidation agent. The research equipment has been constructed: three laboratory-scale trickle-bed reactors for step and pulse experiments and an in-situ reactor system inbuilt in an ATR spectroscopic device.

Direct synthesis of hydrogen peroxide

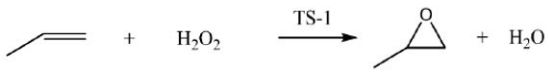
The direct synthesis of hydrogen peroxide from hydrogen and oxygen is an attractive reaction pathway, because the process is clean and simple compared to the established indirect anthraquinone process. The experimental set up for the direct synthesis consisted of a concurrent downflow tubular trickle bed reactor (30 cm, 1.5 cm I.D.) Transient experiments were carried out at 15°C and 20 bar using a commercial 5%Pd/C catalyst the step experiments after reaching steady state the solvent feed were switched from water to an alcohol (methanol, ethanol or isopropanol) using a two-way valve. The hydrogen peroxide concentration was analyzed offline by HPLC with UV/Vis detection. In all solvent-step experiments, it was found that after a switch to the alcohol mixture, an increased concentration of hydrogen peroxide was detected. The change of the solvent feed resulted in a sharp step in the concentration of methanol, suggesting minimal of axial dispersion in the catalyst bed. After the switch from water to alcohol, the concentration profile of hydrogen peroxide started to undergo a pattern of four maxima. The concentration pattern was repeated, but with a declining amplitude approaching a steady state. A similar oscillatory behavior was detected in the presence of ethanol and iso-propanol. The oscillations were confirmed in the ATR equipment. A reaction mechanism was proposed based on these observations.



Oscillatory behavior of direct synthesis of hydrogen peroxide on a Pd/C catalyst. Solvents: (a) methanol (b) ethanol

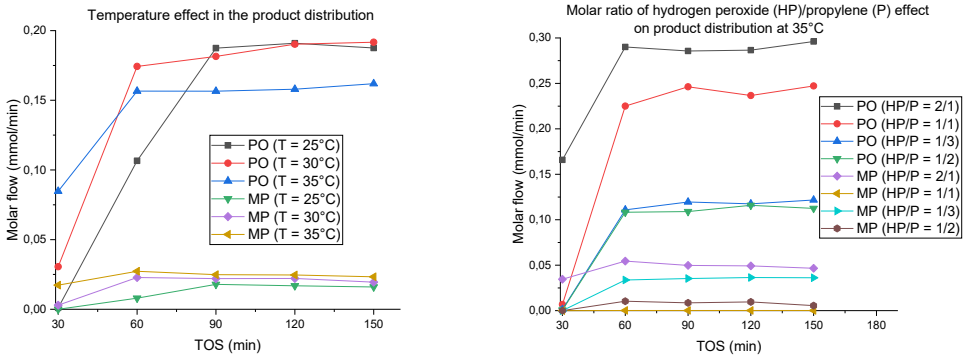
Epoxidation of alkenes by hydrogen peroxide

Alkenes can be epoxidized by hydrogen peroxide in the presence of a heterogeneous catalyst. The epoxidation mechanism and kinetics of ethylene, propylene and butylenes to corresponding alkene oxides are studied in this project. The research effort related to the development of an eco-friendly propene oxide process has led to HPPO (Hydrogen Peroxide Propene Oxide) process, where titanium silicalite (TS-1) is used as heterogeneous catalyst and methanol is a typical solvent,



Titanium silicalite (TS-1) is used as the heterogeneous catalyst in a laboratory-scale fixed bed reactor which is coupled to an online gas chromatograph. The reaction temperature can be varied between 25°C and 80°C and a broad range of inlet molar ratios of propene and hydrogen peroxide can be used in the experiments. The water-to-methanol ratio is studied to observe the changes in the product distribution.

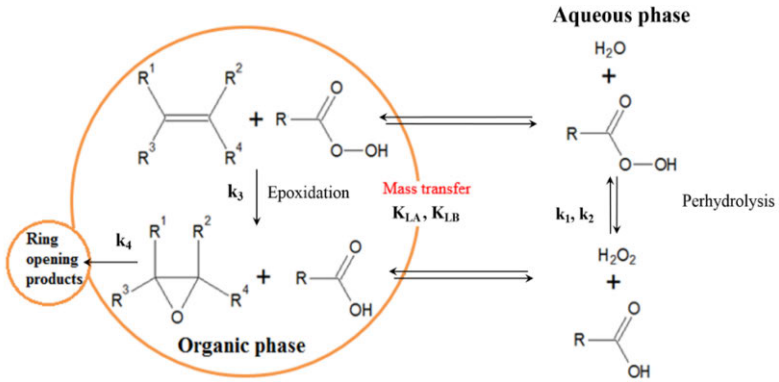
Besides the main product, several by-products are mentioned in literature, but in our experiments only 1-methoxy-2-propanol (MP) was detected as a by-product. Propene oxide (PO) was always the main product, but the steady-state ratio between propene oxide and 1-methoxy-2-propanol varied with the conditions. The results of transient experiments indicate that the main and the by-product are formed through consecutive reactions. The reaction temperature has an important effect on selectivity. The increase of the excess of H_2O_2 in the feed improves the yield of propene oxide. By increasing the H_2O_2-to-propene ratio from 1:1 to 2:1, an increase of the propene conversion from around 70% to 95% is observed in the range 25-35°C.



Product distribution in the synthesis of propene oxide on TS-1 catalyst a) temperature and b) molar ratio influence

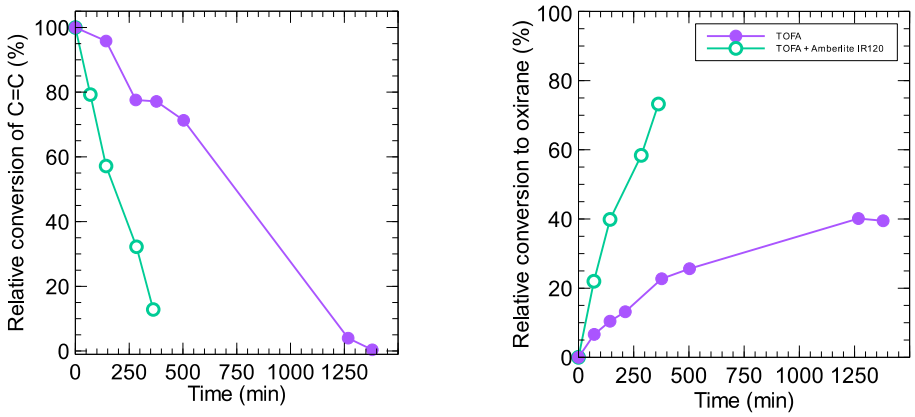
Epoxidation of fatty acids and fatty acid esters by hydrogen peroxide

Tall oil fatty acids are a by-product from Kraft pulping process and they represent a renewable and inexpensive alternative with a high potential as a renewable feedstock. Epoxidized tall oil fatty acids have a great potential as chemical intermediates. The epoxidation process is a complex reaction system, where an oil phase, an aqueous phase and a solid catalyst phase co-exist. Besides the epoxidation, ring opening reactions of the epoxide proceed simultaneously.

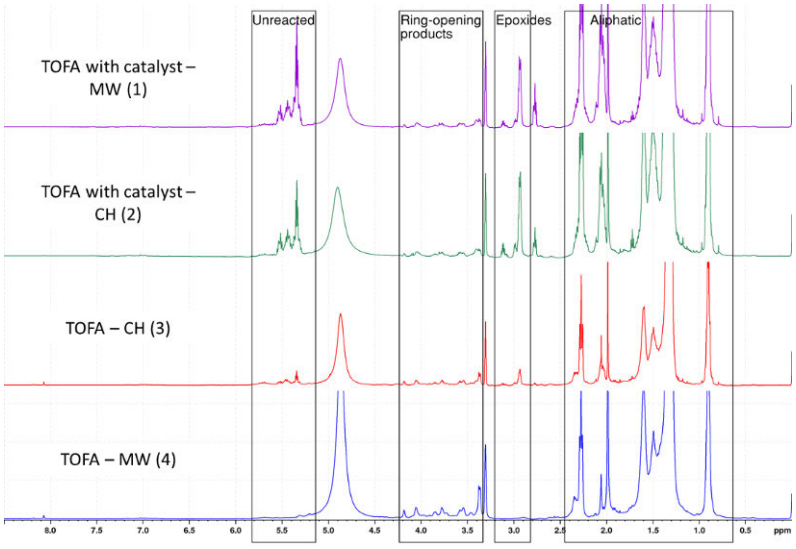


Simplified reaction scheme for fatty acid epoxidation in the presence of hydrogen peroxide, carboxylic acid and a heterogeneous acid catalyst

Epoxidation of oleic acid, tall oil fatty acids (TOFA) and distilled tall oil (DTO) is conducted in an isothermal batch reactor with in-situ-formed peracetic acid using hydrogen peroxide as reactant and acetic acid as reaction carrier. Amberlite IR-120 was used as the solid heterogeneous catalyst. The catalyst loading effect, the reactant ratios, the reaction temperature (40-70°C) and the influence of microwave irradiation on epoxidation and ring opening were studied. The application of microwave irradiation resulted in an improvement of the epoxidation rate in the absence of the catalyst. At higher temperatures, the selectivity to oxirane decayed due to ring opening. Titration analysis and NMR analysis confirmed that microwave irradiation induces the ring opening reactions for TOFA epoxidation and it accelerates this process for DTO. The rapid nature of the microwave heating might have unchained a series of ring opening reactions between neighboring oxirane groups and with the nucleophilic agents in the reaction mixture.



Relative conversion of double bonds (left) and relative conversion to oxirane (right) for the epoxidation of TOFA in the presence and absence of Amberlite IR-120 at 50°C



^{1}H-NMR spectra for epoxidized TOFA samples

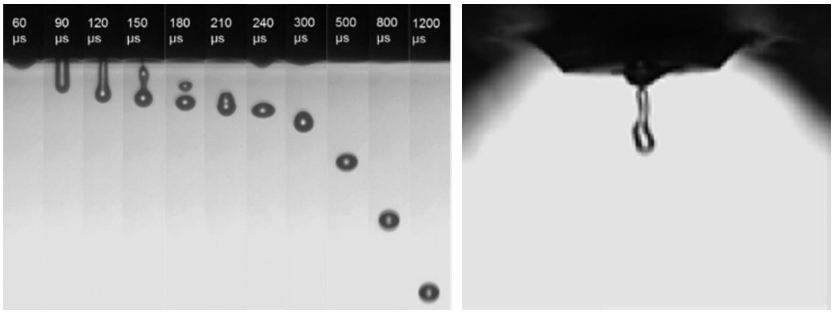
Process intensification I: Microreactor technology

Main funding: Graduate School in Chemical Engineering (GSCE), Academy of Finland

Kari Eränen, Erfan Behravesh, Rossana Suerz, Zuzana Vajglová, Narendra Kumar, Teuvo Kilpiö, Vincenzo Russo, Yaseen Khan, Juha Lehtonen, Johan Wärnå, Roland Dittmeyer, Dmitry Murzin and Tapio Salmi

Gas-phase microreactors provide a safe and efficient way to study the kinetics of rapid reactions, to screen catalysts and to produce chemicals even in large scale. Gas-phase microreactors have been successfully implemented to prepare chemical intermediates, such as ethylene oxide, methyl chloride, ethyl chloride, acetaldehyde, ethyl acetate, ethylene and diethyl ether. In recent times, the project has focused on the use of microreactors for oxidation, dehydration and etherification of bio-ethanol as a sustainable raw material. The activities focus all the essential elements of microreactor technology, from coating and characterization of the microreactor elements to catalyst screening and characterization, kinetic studies as well as mass transfer and flow modelling.

A new coating technology was introduced, inkjet printing in collaboration with Karlsruhe Institute of Technology. With this method, very thin and even coatings of microreactor channels is achieved which suppresses the mass transfer limitations and guarantees a well-reproduced performance of the microreactor. Extremely small droplets can be distributed on the channels by inkjet technology.



A uniform (a) and non-uniform (b) catalyst ink droplet formation

Extensive kinetic studies were carried out for ethanol oxidation to acetaldehyde on gold catalysts implemented in microreactor plates. Ethyl acetate and ethylene were obtained as by-products in minor amounts.

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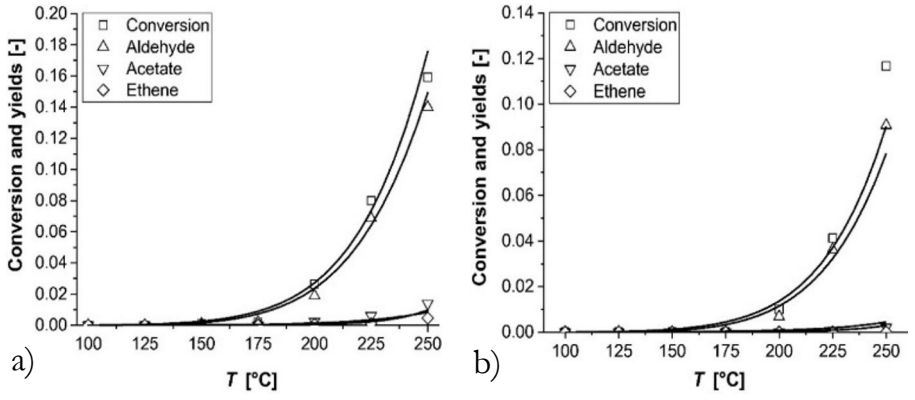
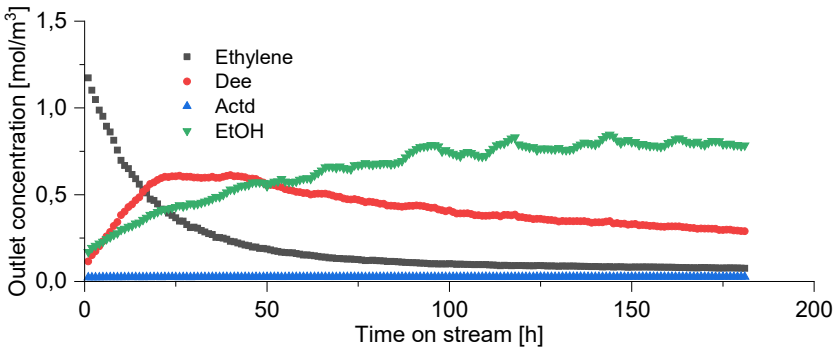


Ethanol conversion and products yields versus temperature at flow rate of (a) 25 and b) 50 ml/min. The lines show the modelling and the marks show the experimental results

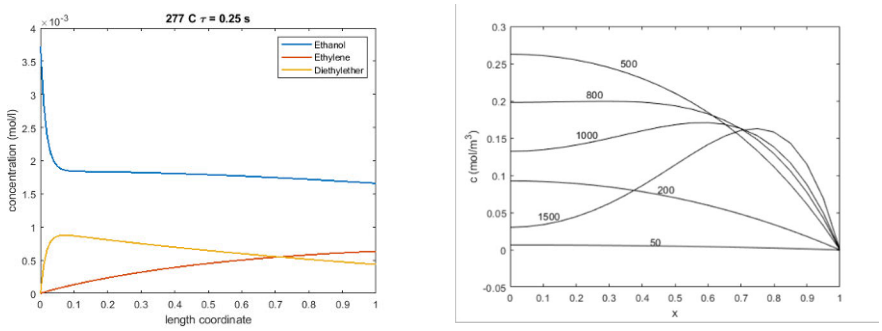
Furthermore, microreactors are strong tools in the investigation of the long-term stability of a catalyst layer, as was demonstrated in the dehydration and etherification of ethanol.

Dehydration and etherification of bio-ethanol was studied in a microreactor using γ-alumina, H-Beta-38 and Sn-Beta-38 as catalysts. An extensive series of kinetic experiments was carried out in the microreactor device operating at ambient pressure and temperatures 225-325°C. The H-Beta-38 catalyst coated microplates exhibited the highest production rate of ethene. While the fresh H-Beta-38 catalyst allowed complete conversion of ethanol and very high selectivity towards ethene, the catalyst deactivated significantly with time-on-stream. Diethyl ether was the dominating co-product, whereas trace amounts of acetaldehyde were detected in the experiments. The fundamental hypothesis of the reaction mechanism was the co-existence of two kinds of active sites on the catalyst surface. The Brønsted sites deactivate, whereas the Lewis sites are more stable, which leads to a shift of the product distribution during long-term experiments, from ethene to diethyl ether.



Shift of product distribution in the dehydration and etherification of ethanol on H-Beta-38 catalyst

Big steps forward in the demanding field of mathematical modelling of milli- and microscale reactors were taken by using the very advanced and user-friendly modelling software gPROMS. A generalized mathematical model was developed for catalyst layers in micro- and millireactor structures. The model describes the reaction-diffusion phenomena in the porous structure very well. With the advanced modelling approach, the concentration profiles inside the thin catalyst layers can be computed and the concentration profiles along the microreactor channels are obtained. The project resulted in the doctoral thesis of Erfan Behravesh.



Concentration profiles in a microreactor channel (ethanol dehydration, left) and concentration profiles inside the catalyst layer (ethanol oxidation, different layer thicknesses 50-1500 micrometer, right)

Cooperation: University of Umeå, Sweden, Karlsruhe Institute of Technology (KIT), Germany, Aalto University, Finland; Università di Napoli 'Federico II', Italy

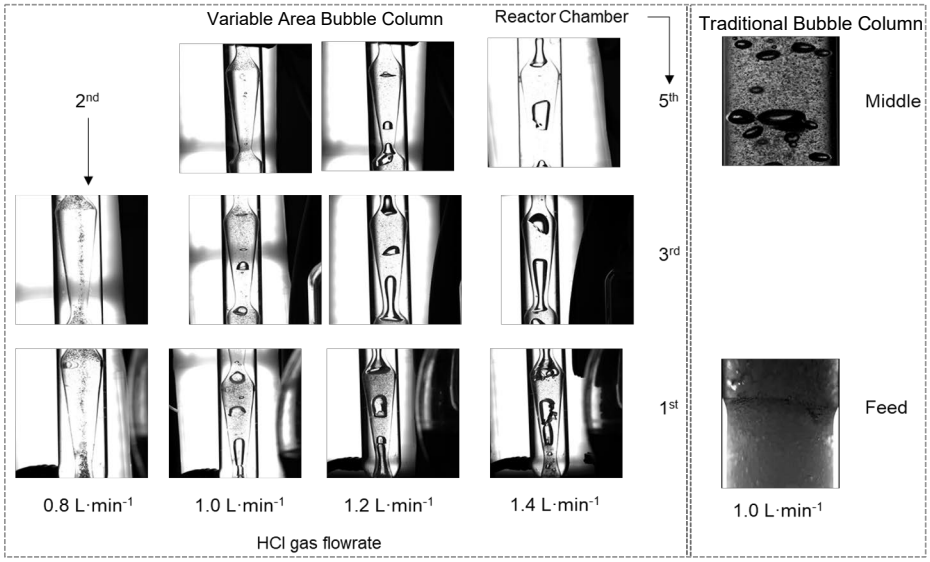
Process intensification II: Novel multiphase reactors

Main funding: PCC, Graduate School in Chemical Engineering (GSCE), Academy of Finland, Magnus Ehrnrooth Foundation, Åbo Akademi

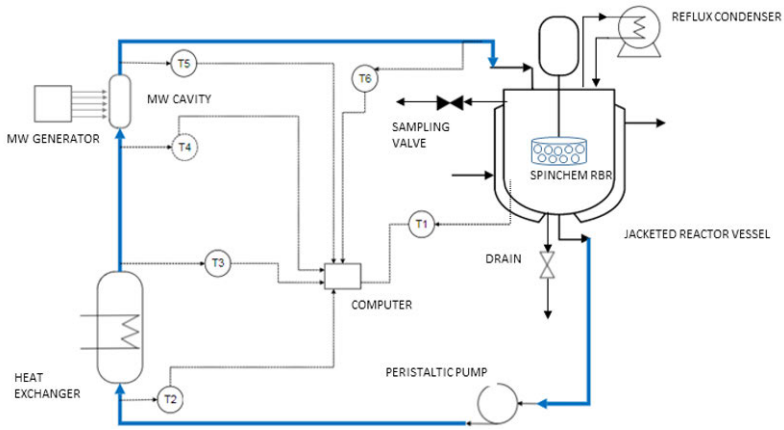
Johan Wärnå, Teuvo Kilpiö, Pasi Tolvanen, Cesar de Araujo Filho, Adriana Freites Aguilera, Atte Aho, Wander Perez-Sena, Sébastien Leveneur, Leolincoln da Silva Correia, Javier Ibanez Abad, Ananias Medina, Gregory Hamel, Debanga Mondal, Vladimir Shumilov, Ali Najarnezhadmashhadi, Sebastian Franz, Maria Herrero Manzano, Mouad Hachhach, Markus Schubert, Uwe Hampel, Juan Garcia Serna, Jyri-Pekka Mikkola, Dmitry Murzin, Tapio Salmi

Development and advanced modelling of multiphase reactors and structured catalysts, such as solid foams is the topic of the project, involving various flow models in the bulk phases of the reactor as well as modelling of simultaneous reaction and diffusion in porous catalyst structures. The main applications are catalytic three-phase hydrogenation, oxidation, epoxidation and catalytic liquid-phase hydrochlorination. Production of epoxidized vegetable oils under the presence and absence of microwaves and heterogeneous catalysts was studied extensively. The most recent research is devoted to the effect of acoustic irradiation (ultrasound) on epoxidation of double bonds in fatty acids and fatty acid esters. The products are valuable chemical intermediates and bio-lubricants and they can be carbonated with CO_2 to obtain polyurethanes.

A variable-diameter bubble column was introduced to investigate oxidation and hydrochlorination processes under continuous operation. The influence of liquid flow rate, gas flow rate, temperature and catalyst concentration on the glycerol conversion and the product distribution was studied. High-speed camera images and residence time distribution experiments were conducted to collect relevant information about the flow conditions inside the column reactor. A model based on the axial dispersion concept was developed and compared with experimental data. The new column reactor gave a clearly better performance than the classical bubble column, the reason being the suppression of backmixing in the liquid phase.

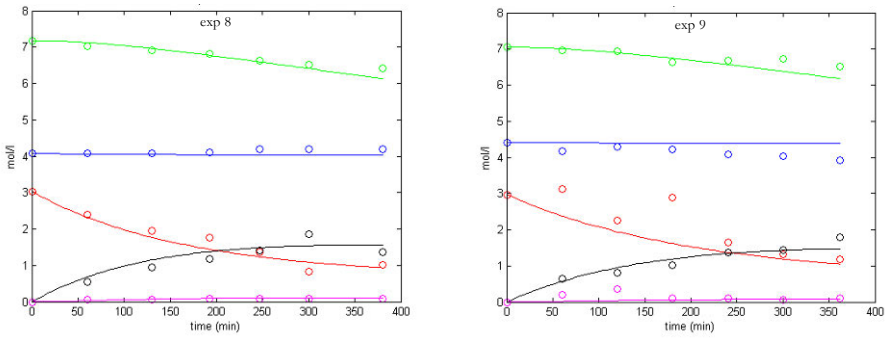


Glycerol hydrogenation in the presence of homogeneous catalyst. Images recorded at steady state at HCl flowrates in the range 0.8 – 1.4 L·min^{-1}, 6 mL·min^{-1} of glycerol, 80 ºC At the right the corresponding images of the traditional bubble column at 1.0 L·min-1, 105 ºC, 6 mL·min of glycerol and 3% catalyst concentration by weight



Loop reactor system for studies of microwave and ultrasound effects on solid-catalyzed liquid-liquid reactions

The results obtained with the tailored loop reactor system equipped with a novel mixing technology (SpinChem Rotating Bed Reactor) showed that epoxidation of fatty acids, such as oleic acid occurs spontaneously in the absence of added catalyst, but the product yield can be considerably improved by exposing the system to microwave irradiation and incorporating a solid catalyst. Several heterogeneous catalysts (cation exchange resins with sulphonic acid groups) were screened to find the highest performance. Mathematical modelling of the multiphase system was carried out, starting from first principles. Detailed kinetic models based on reaction mechanisms were derived and the model parameters were estimated by non-linear regression analysis. The models for epoxidation with conventional heating and microwave irradiation in the presence and absence of a solid catalyst had a good correspondence between the experimental and calculated concentrations of the reaction components. The rate constants and activation energies for the perhydrolysis, epoxidation and ring opening reactions were obtained as a result of the parameter estimation. The project resulted in the doctoral thesis of Adriana Freites Aguilera.



Fitting of the model to the experimental data for oleic acid epoxidation. In black: ***epoxyoleic acid****, pink: peracetic acid, red: oleic acid, green: hydrogen peroxide and blue: acetic acid*

Cooperation: Università di Napoli 'Federico II', Italy; Normandie Université -INSA Rouen, France; Universidad de Valladolid, Spain; Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany; University of Umeå, Sweden.

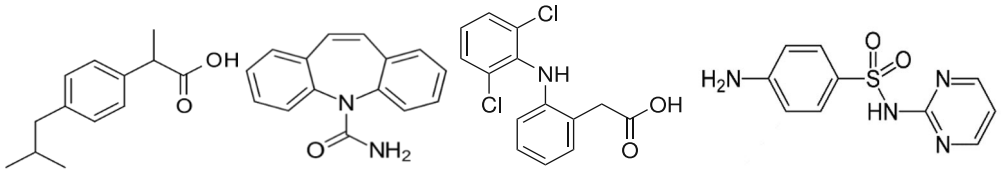
Removal of pharmaceuticals from waste waters by combined ozonation and heterogeneous catalysis

Main funding: Åbo Akademi University, GSCE

Soudabeh Saeid, Matilda Kråkström, Pasi Tolvanen, Narendra Kumar, Kari Eränen, Janne Peltonen, Markus Peurla, Jyri-Pekka Mikkola, Alexia Lahaye, Laurent Maël, Sophie Ozanne, Andreas Franz, Vincenzo Russo, Leif Kronberg, Patrik Eklund, Tapio Salmi

The slip of pharmaceuticals from wastewaters to aquatic environment is a serious and growing environmental problem. In spite of the very advanced wastewater treatment technologies of today, many pharmaceutical components remain in the cleaned water and end up in rivers, lakes and seas. The crowded and highly industrialized Baltic Sea region is a very woundable ecosystem because of the very shallow rivers and lakes and the tiny contact of Baltic Sea to Atlantic ocean. In general, pollution of waters by pharmaceutical rests is a global problem due to the increasing consumption of pharmaceuticals; a cocktail of drugs emerges in surface waters and effluents of communities. Some pharmaceuticals possess a high-risk to the aquatic life and humankind, because they interact heavily with the ecosystem, for instance influencing the reproduction of aquatic fauna. For a completele destruction of the pharmaceuticals, the development of an advanced oxidation process (AOP) is necessary. In this project, a combined ozonation and catalytic technology was developed for removal of pharmaceuticals from water, because ozonation alone is not able to quantitatively remove pharmaceuticals and partially oxidized intermediates.

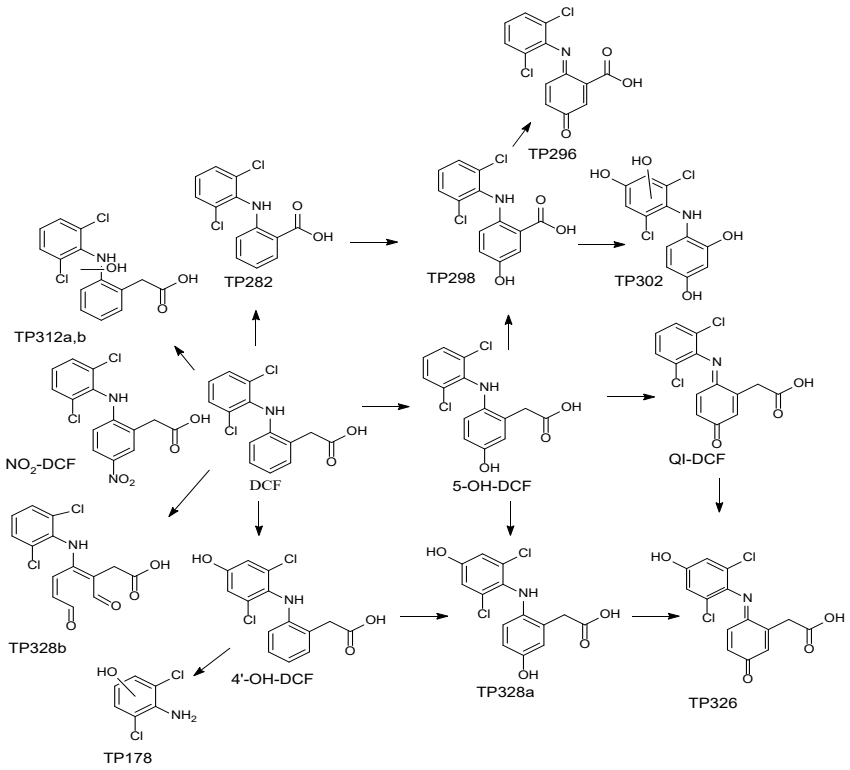
Four commonly used pharmaceuticals are studied in detail in the project: ibuprofen (IBU), carbamazepine (CBZ), diclofenac (DCF) and sulfadiazine (SDZ).



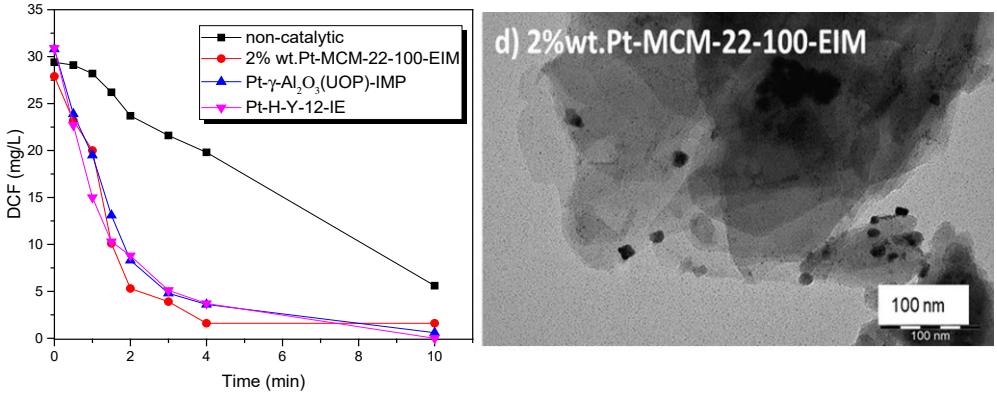
IBU CBZ DCF SDZ

A tailored laboratory-scale equipment was designed to conduct catalyst screening and kinetic ozonation experiments. The solid catalyst was placed in Spinchem™ rotating bed stirrer and ozone was created in situ by an ozonator. Very well reproduced kinetic results were obtained. Solid metal catalysts with various amounts of Lewis and Brønsted acid sites were screened and the influence of metal particle sizes of Cu, Pd, Fe and Ni in ozone degradation was revealed. The catalyst characterization methods included nitrogen adsorption-desorption, scanning electron microscopy, transmission electron microscopy and Fourier-transform infrared spectroscopy. Inductive coupled plasma spectrometry was used to study potential leaching of Fe, Cu, Ni, Pd during the reaction. Liquid chromatography-mass spectrometry was used for quantification of the by-products from ozonation. NMR spectroscopy was used for detailed product identification to reveal the role of intermediate products in the ozonation process.

The project has a very important fundamental aspect: detailed decomposition schemes of pharmaceuticals were proposed, thanks to the sophisticated chemical analysis by LC-MS and NMR, as shown below for diclonofenac (DCF).



Extensive catalyst screening and characterization enabled to find the optimal conditions, which minimize the reaction time and enhance the destruction of harmful, partially oxidized intermediates. The positive effect of heterogeneous catalysts was prominent for most of the model molecules studied, as illustrated in the figure for DCF. Catalyst characterization was done in collaboration with University of Turku and kinetic modelling was applied on the oxidation process, in collaboration with Università di Napoli 'Federico II'. The project has resulted in two doctoral theses (Matilda Kråkström and Soudabeh Saeid).



Degradation of DCF by ozonation and heterogeneous catalysis at room temperature. The catalysts 2wt%.Pt-MCM-22-100-EIM, Pt-γ-Al₂O₃ (UOP)-IMP and Pt-H-Y-12-IE (left), TEM image of Pt-MCM-22-EIM: metal is visible as black spots (right)

Metal-acid bifunctional catalysts - developing novel shaped extrudates for various reactions

Main funding: Academy of Finland

Narendra Kumar, Päivi Mäki-Arvela, Kari Eränen Zuzana Vajglová, Markus Peurla, Leena Hupa, Mark Martinez Klimov, Tapio Salmi and Dmitry Murzin

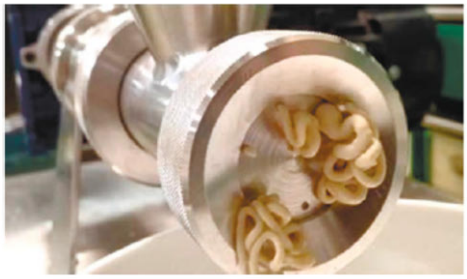
The metal-acid bifunctional catalysts are widely used in many industrially significant chemical processes, e.g. hydrocracking of heavy oils, dewaxing, reforming, selective ring opening, hydroisomerization or synthesis of menthol from citral/citronellal. Such reactions include several steps such as for example dehydrogenation of alkanes, skeletal isomerization of olefins and hydrogenation of the latter is hydroisomerization of C_5-C_6 *n*-alkanes to improve the fuel quality (increase of octane number). The de/hydrogenation steps occur on the metallic sites while isomerization or hydrocracking steps proceeds on the acid sites (e.g. amorphous silica-alumina oxides, zeolites, mesoporous aluminosilicates).

Diffusion of the intermediates between the metallic and acidic sites is very important and therefore design of the metal-acid bifunctional catalysts plays a key role. The controlled acidity (Brønsted and Lewis) in terms of strength and the number of the acid sites, the metal-acid balance and proximity between these two types of active sites should mainly be taken into account for optimal performance of bifunctional catalytic systems.

Many studies of metal-acid bifunctional catalysts are performed with the powder catalysts under the kinetic regime. However, in industry where shaped catalytic bodies containing binders are used, the mass transport limitations are almost unavoidable. Not only mass transfer limitations but also changes of physicochemical properties of a catalyst due to its scale-up process can lead to a significantly different product distribution as well as catalyst deactivation compared to fine catalyst powders. During the scale-up of zeolite-based catalysts by extrusion, the organic and inorganic binders are typically added to improve plasticity of the extruded paste and to improve the mechanical resistance of shaped zeolites, respectively. Chemical interactions between the catalyst and the binder, and the shaping process *per se* can have a significant effect on the physicochemical properties of the final extrudates.

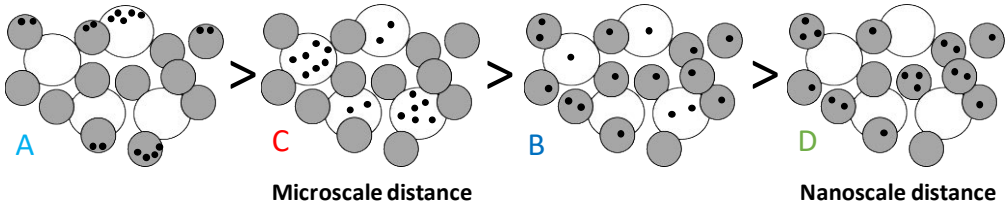
The current project is aimed at improvement of the fundamental knowledge on the scaling-up of metal-acid bifunctional catalysts for a range of reactions: straight chain paraffins hydroisomerization; hydrogenation of citral/citronellal with subsequent cyclization of isopulegol to menthol and selective hydrocracking of hexadecane. This project is focused on the effect of the preparation of metal/zeolites bifunctional extrudates with controlled metal deposition on the catalyst deactivation and regeneration in continuous fixed-bed reactors. Zeolites and mesoporous materials and different acidity were used. Binders of different type (e.g. bentonite, colloidal silica) were applied.

It was demonstrated that extrusion is extremely sensitive to the moisture content of suspensions for shaping; in some cases, the shaping of a catalyst by extrusion is completely infeasible as illustrated in the Figure below



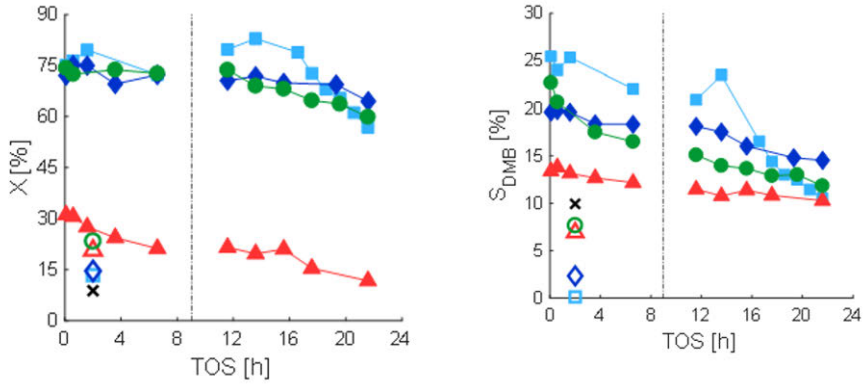
Extrusion of a too wet paste

Different synthesis procedures resulted in the controlled metal deposition in the shaped catalysts in different locations giving materials with different metal-to-acid site ratios (see Figure).



A schematic picture of the catalysts employed in this study, showing different metal location (black circles) and distances between the metal and acid sites located on the binder (white) or the zeolite (grey)

For different reactions research done at PCC unequivocally demonstrated importance of the metal location in extrudates on activity, selectivity and stability in the model reactions of practical relevance. In for example hydroisomerization of n-hexane, the most stable catalytic activity was obtained with the catalyst where Pt was distributed uniformly in the entire shaped body randomly on both H-Beta-25 zeolite and on the Bindzil binder. Selectivity to dimethylbutanes (DMB, Figure below) decreased, while selectivity to methylpentanes increased with time on TOS. Such behavior can be explained by gradual catalyst deactivation influencing selectivity in the network comprising consecutive reactions from *n*-hexane to methylpentane and further to dimethylbutanes.



Conversion and selectivity to dimethylbutanes as a function of TOS. Legend: Pt/(H-Beta-25+Bindzil), post synthesis (light blue square); Pt/(H-Beta-25+Bindzil), in-situ synthesis (dark blue diamond); (Pt/Bindzil)+H-Beta-25 (red triangle); (Pt/H-Beta-25)+Bindzil (green circle)

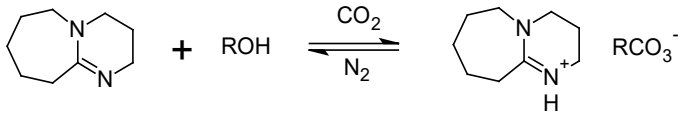
Wood valorization – cellulose derivatization in novel switchable ionic liquids and supercritical fractionation of wood

Main funding: TanDem Forest Value, Sweden and Fortum Foundation

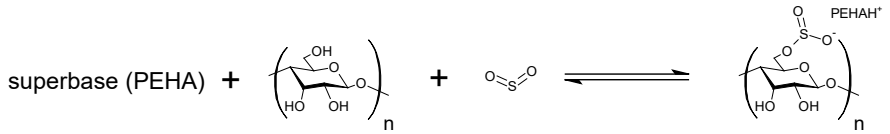
Pasi Virtanen, Ramakrishna Jogi, Päivi Mäki-Arvela, Narendra Kumar, Jyri-Pekka Mikkola and Tapio Salmi

The demand of renewable resources for production of energy and chemicals has become more and more important. Cellulose, which is the most abundant renewable resource with affordable price, high availability and good mechanical properties, is evaluated as one of the most potential sustainable raw material for this purpose. Properties of cellulose itself can be modified by different derivation reactions, to widen its utilization in industrial applications, pharmaceuticals, membranes, textile fibers, coatings and paints. The utilization of cellulose in various applications is limited, because it cannot be melted and is very hard to dissolve because of its stiffness and close chain packing through many inter- and intra-molecular hydrogen bonds. Efficient dissolution of cellulose enhances the research of cellulose chemistry and development of cellulose-derived materials having special properties and functionalities. Organic solvents and hazardous chemicals have been utilized for derivation of cellulose, e.g.DMAc/LiCl, NMMO, $LiClO_4$ $3H_2O$ molten salt hydrate, ionic liquids and NaOH-urea.

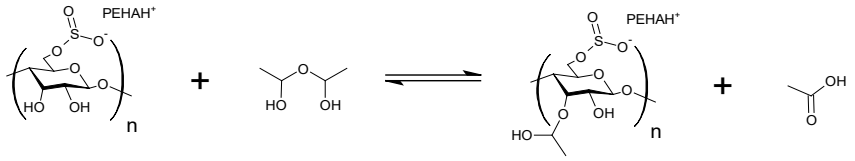
Switchable Ionic Liquids can be formed by exposing an equimolar mixture of two neutral liquids, for instance an amidine such as 1, 8-diazabicyclo-[5.4.0]-undec-7-ene (DBU) with an alcohol such as 1-hexanol to gaseous CO_2, under ambient pressure at room temperature, causing an exothermic transformation of the neutral liquid mixture into an ionic liquid, Scheme below. The formed viscous ionic liquid phase can be converted back to neutral liquid mixture upon the removal of CO_2 by bubbling nitrogen or applying vacuum at room temperature. The rate for back transformation of the ionic liquid to neutral ones can be increased by increasing the temperature to around 55-65°C.



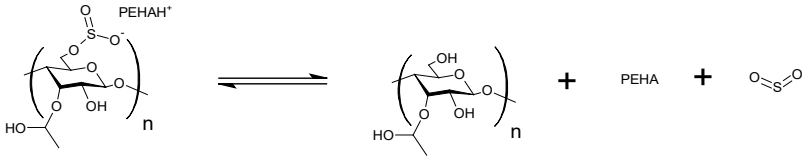
A 'switchable' solvent system is capable of ionic/non-ionic *e.g.* molecular-to-ionic switching by the addition or removal of another compound, a so-called "trigger". CO_2 can be applied as a trigger for the formation of a bicarbonate salt according to scheme above, whereas upon the removal of CO_2 by bubbling N_2, the bicarbonate salt is switched back to its original form being an alcohol and an amidine. Thus, re-use and recycling of ionic liquid components become much easier. The main objective is to utilize this switching reaction so that instead of alcohol, the compound containing OH-group would be cellulose and cellulose would then dissolve into the mixture containing also a co-solvent such as DMSO. In all previous studies, the base has been either DBU or 1,1,3,3 tetramethylguanidine (TMG) and switching gas has been CO_2. The idea is to study other superbases, such as *e.g.* pentaethylenehexamine (PEHA) or 1,5-Diazabicyclo[4.3.0]non-5-ene (DBN) and other acidic "trigger" gases, such as N_2O or SO_2 in dissolution of cellulose and further derivation with *e.g.* acetic anhydride to cellulose acetate.



Cellulose reaction with superbase and SO_2 to soluble form

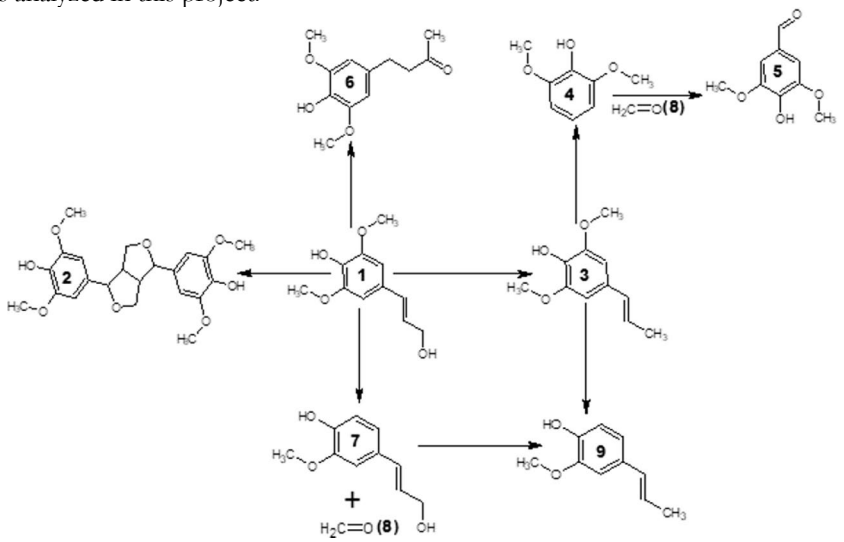


Soluble cellulose reaction with acetic anhydride to cellulose acetate



Recycling of super base and SO_2 as well as product separation

Lignocellulose contains cellulose, hemicellulose and lignin as its main fractions. Degradation of lignocellulose produces aliphatic and aromatic fractions, which can be used as a main ingredient for fuel production in our pursuit towards sustainability. The current study focuses on the aromatic fraction, which principally originates from lignin. The goal is to obtain a better understanding on the formation of phenolic monomers during fractionation of birch wood under supercritical ethanol over iron based catalysts. The deconstruction of lignin components into valuable aromatic compounds by the cleavage of aromatic (C-C) and ether (C-O) bonds is catalytically quite challenging. One possible way for birch lignin degradation is over a palladium based catalyst supported on activated carbon in methanol at 250 °C, for 3 h under H_2 (30 bar) atmosphere. Under these reaction conditions, aryl methoxide undergoes β- elimination over Pd catalyst forming aryl hydrates as the primary products. In the next step, C-O bond cleavage occurs in aryl hydrates resulting in the formation of propylguaiacol and propylsyringol with high conversions and selectivity. The formation of different phenolic compounds as a function of time during catalytic birch fractionation with supercritical ethanol (at supercritical point, ethanol acts as a hydrogen donor) is analyzed in this project.



Reaction network for fractionation of phenolic compounds in birch fractionation under supercritical ethanol. 1. sinapyl alcohol, 2. syringaresinol, 3. 4-propenyl syringol, 4. syringol, 5. syringyldehyde, 6. syringol acetone, 7. coniferyl alcohol, 8. formaldehyde, 9. isoeugenol

Cooperation: Umeå University, Sweden

Engineering extraction of hemicellulose-lignin complexes for obtaining emulsion stabilizing hydrocolloids

Main funding: Academy of Finland

Jussi V. Rissanen, Maarit Lahtinen, Lucas Lagerqvist, Elina Lius, Patrik Eklund, Kirsi Mikkonen, Atte Aho, Henrik Grénman

The performance of hemicellulose-based compounds from lignocelluloses in the potential products is determined largely by the chemical composition and the structure of the molecules. The objective in the extraction processes has mostly been to obtain completely pure fractions of hemicellulose, lignin, and cellulose. However, a controlled mixed structure of the compounds can be an advantage in certain applications.

Recently research has shown, that galactoglucomannan (GGM) based compounds have the potential to replace the "golden standard" food stabilizer gum Arabic (GA) in food, pharmaceutics, and cosmetics. In these studies, GGM displayed exceptional capacity to inhibit lipid oxidation and act as a multifunctional stabilizer, enhancing both the physical and oxidative stability of emulsions. The higher content of phenolic residues in GGM compared to GA was concluded to contribute to GGM's excellent oxidation inhibition capacity. The exact mechanisms behind the beneficial influence of lignin residues in the GGM are unclear, as is the influence of the structure and composition of the lignin-hemicellulose complexes (LCC) on their performance. The basic phenomenon has been established, but many details are in the dark.

In our recent study, hemicelluloses from spruce were extracted with pressurized hot water (PHWE) using a well separable additive, which is suitable for the alimentary and cosmetics industry. The results clearly demonstrated that the extraction rate was considerably enhanced with the additive (Fig. 1 left) and about 10-15% more lignin (Klason lignin in solid) was dissolved compared to normal PHWE. Moreover, the NMR results indicated that lignin stays covalently bound to the dissolved hemicelluloses forming amphiphilic water soluble LCC. The extraction method also influenced e.g. the molar mass of the obtained macromolecules, see Figure 1 (right). However, the detailed mechanisms of dissolution should be understood to be able to influence the properties of the extracted compounds by varying the experimental conditions.

The current interdisciplinary research focuses on building on a newly developed extraction method for enhancing hemicelluloses extraction, which enables tuning the lignin content and properties of the LCC. The complexes are utilized for emulsion stabilization studies in collaboration with specialists in alimentary research and emulsions. Different wood species combined with varying reaction conditions have been tested and their performance as emulsion stabilizers and anti-oxidizing agents was evaluated. The results clearly show that there are significant differences in the LCC extracted from different wood species in the formation of oil-water emulsions as well as their stability (Figure 2). The smallest drop size was obtained initially with pine, however, the emulsion was not stable. With birch and aspen extracts, larger droplets were initially forms, but the stability was much better compared to pine. The detailed reasons for the differences caused by physico-chemical properties of the macromolecules is ongoing.

The work bridges the state of the art knowledge in the safely enhanced extraction of hemicelluloses-lignin compounds and the related reaction engineering (chemical engineering) and the utilization of the LCC for alimentary purposes (alimentary chemistry). Moreover, the potential utilization is by no means limited to the alimentary industry, but fields such as cosmetics and health products are highly viable.

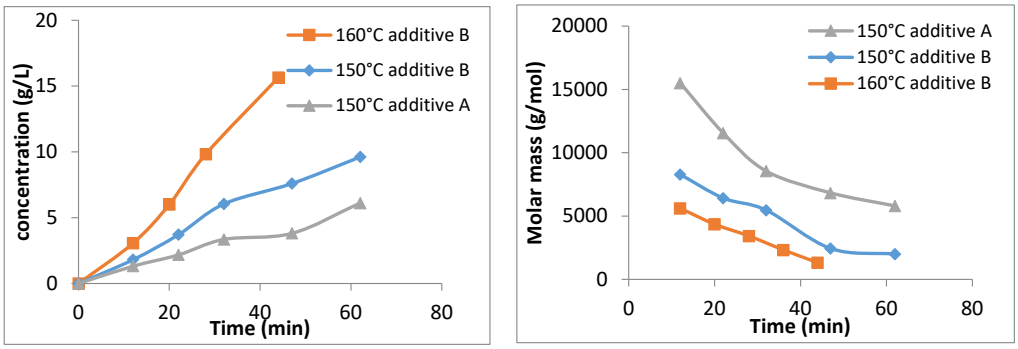


Figure 1 *The enhancement of the extraction rate by selected additive (left), the influence of additive addition to the molar mass of the macromolecules (right)*

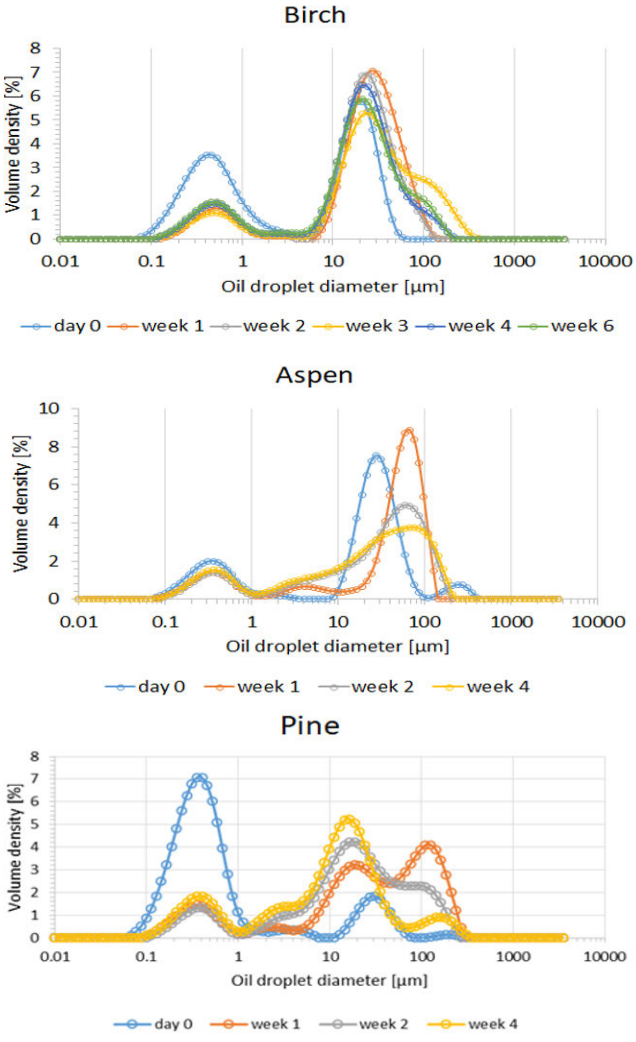


Figure 2. *The formation of oil-water emulsions with LCC extracted from birch, aspen and pine*

Cooperation: Department of Food and Nutrition, University of Helsinki

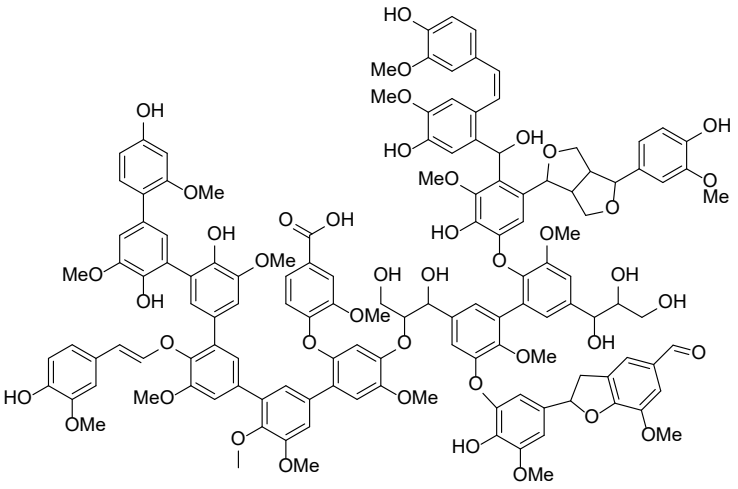
Structure, Reactivity and Valorization of a Novel Type of Mild Alkali Pressurized Hot-Water Extracted Lignin

Main funding: Suomen Luonnonvarain Tutkimussäätiö, Fortumin Säätiö

Lucas Lagerquist, Andrey Pranovich, Jani Rahkila, Stefan Willför, Patrik Eklund

In this project we have worked with lignin obtained from a novel bio-refinery process, developed by CH-Bioforce Oy. This process fractionates different biomass by pressurized hot-water extraction, followed by mild alkali pulping. Both steps are performed in oxygen starved conditions and the lignin fraction can be obtained as black liquor or as precipitated. Our initial studies were focused on developing practical methods to obtain and purify the lignin from the black liquor. Also further fractionation based on molar mass and chemical structure was studied and developed. The isolated lignin fractions were fully characterized by the spectroscopic methods ^{13}C NMR, ^{13}C DEPT experiments, ^{31}P NMR, 2D HSQC, and FTIR as well as with other methods such as size exclusion chromatography, elemental analysis, pyrolysis-gas chromatography-mass spectrometry, methoxy group determination, carbohydrate determination after methanolysis and thermal gravimetric analysis.

Lignins from hardwood, softwood and wheat straw has been studied and compared to structurally intact milled wood lignin, supplied by collaborators. The lignin obtained by this process, was similar to soda-type technical lignins, in terms of structure, molar mass, degree of condensation, hydroxyl groups etc. In addition to the characterization, our study on softwood lignin has also focused on the thermal properties, as well as chemical derivatization. The modifications were performed to see if the thermal stability could be increased by simple reactions.



Schematic structure of softwood "soda-type" lignin from the Bio-refinery process

It was concluded based on the structural characterization that the isolated sulfur-free lignin from the bio-refinery process had relatively few of the traditionally occurring alkyl-aryl ether linkages remaining, and that the process caused fragmented of the lignin with subsequent re-condensation. We also identified multiple structural anomalies caused to the lignin by the process for example, the uncommon arylglycerol end group linkages and new condensed syringyl structures. The lignin contained only small amounts of carbohydrate impurities. Our thermal studies showed that the

lignins were stable up to 270-300 °C, varying on tree species, and had considerable char residue left at 600 °C. The thermal properties could be tailored by simple chemical reactions, such as acetylation and methylation, were the acetylated lignin reduced the stability and methylated increase it.

During this project we have also developed an improved method for the quantitative determination of hydroxyl groups in lignin by ^{31}P NMR. The traditional method uses internal standards for the concentration determination and our method is based on ^{31}P PULCON (pulse length-based concentration determination). PULCON determines the concentration of a sample based on that the signal strength obtained with an NMR probe is inversely proportional to the 90° pulse length for the probe. The method simplifies the sample preparation and removes the necessity of using an internal standard, thereby eliminating problems such as overlapping signals, stability of the internal standard, and potential data processing errors.

As the process cause fragmentation of the native lignin and an enrichment of carbon via condensation reactions, the lignin is more suitable to be used in applications in its polymeric form instead of degradative valorization, as degradative methods often rely on the cleavage of the alkyl-aryl ether bonds. Applications areas for this lignin could for example be as a macromonomer component in copolymers, in polymer blends or in composites, either to reduce the price of expensive polymers or to change/improve the material properties. The high amount of free phenolic hydroxyl groups allows for easy chemical modification that can be used to further modify the material properties. The reactivity of the lignin was studied by various chemical modifications, such as mild hydrogenation, ozonation, oxidations and simple chemical modifications. The mild hydrogenations were performed using catalytic amount of Pd/C at relatively low temperatures and hydrogen pressure. The intent of the hydrogenation study was to study the structural changes to the lignin without excessive depolymerization/reductive cleavage, however, the lignin was shown to be stable under these conditions without any noticeable changes. Multiple oxidation methods have also been studied on the lignin such as a pulsed corona discharge oxidation that was tested on the lignin in cooperation with Lappenranta University of Technology. This method modifies the lignin into highly oxidized structures, containing large amounts of carbonyl functions and carboxylic acid salts. The lignin has also been subjected to ozonation to yield highly oxidized structures but also more selective methods using PIFA have been explored in cooperation with other projects. In an effort to valorize the lignin different chemical derivatizations has also been studied. One such method is the allylation or propargylation followed by Claisen rearrangement, to introduce reactive double or triple bonds that could be further polymerized into new materials.

This project is also part of other lignin related collaborations within the PCC with topics such as: 3D printing using blends of modified lignin and PLA, cyclic voltammetry of lignin and modified lignin, using lignin for phenol formaldehyde resins and reductive hydrogenolysis of lignin.

Cooperation:
Dr. Tarja Tamminen, VTT Technical Research Centre of Finland Ltd; Professor Ilkka Kilpeläinen, Laboratory of Organic Chemistry, Department of Chemistry, University of Helsinki; Sebastian von Schoultz and Dr. Lari Vähäsalo, CH-Bioforce Oy; Professor Marjatta Louhi-Kultanen, School of Chemical Engineering, Aalto University. Dr Marleny Caseres-Najarro, Århus University, Denmark.

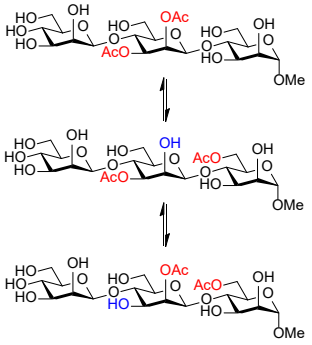
Acyl group migration in mono-, oligo- and polysaccharides

Main Funding: Magnus Ehrnrooth Foundation, Waldemar von Frenckells Foundation.

Robert Lassfolk, Jani Rahkila, Michael Johansson, Filip Ekholm, Johan Wärnå, Reko Leino

Polysaccharides are a key component in plants and the large variety of polysaccharides gives them variating properties. Many polysaccharides are acetylated on various positions and for example can glucans, xylans and mannans be partly acetylated in the plants. The degree to which the polysaccharides are acetylated is dependent on where in the plant the polysaccharides are located. For most of the naturally acetylated polysaccharides the acetylation is critical for the biological activity and mutations to decrease the degree of acetylation can have detrimental consequences for the plant. The main polysaccharides in focus so far for this project has been the β-(1→4)-linked mannans. There are many different types of mannans, for example linear mannan, glucomannan, galactomannan and galactoglucomannan. The mannans have many biological roles in nature, but one of the more interesting ones are that they act as signaling molecules for plant growth and development. Besides their biological role in nature the mannans also exhibit other biological activities such as inhibit the growth of cancer tumors and display antioxidant activities. It is well known that acyl groups migrate in monosaccharides, but extensive investigations in oligo- and polysaccharides are lacking. In nature, acetyl groups are used to activate and deactivate various substrates, suggesting that acetyl group migration in polysaccharides could have a role regarding the biological activity of polysaccharides. The aim of this project is to investigate the acyl group migration in mono-, oligo- and polysaccharides. So far β-(1→4)-linked mannan model compounds has been investigated.

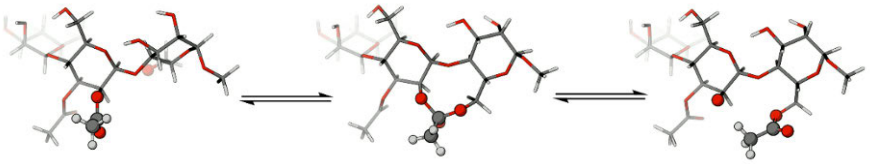
Investigation into the possible acetyl group migration towards *O*-6 of the same monosaccharide unit or a free hydroxyl position at another saccharide unit was done using a trisaccharide model compound where no migration to a neighboring group was possible. After 6 weeks of migration some new migration products could be analyzed. Using NMR-spectroscopy it could be unambiguously concluded that one of the acetyl groups in the middle carbohydrate unit of compound **2** had migrated across a glycosidic bond to the *O*-6 position of either the reducing or non-reducing end of the trisaccharide. With further analysis it could be concluded that the acetyl group had migrated towards the reducing end.



The newly observed acetyl group migration over monosaccharide units in the trisaccharide model compound

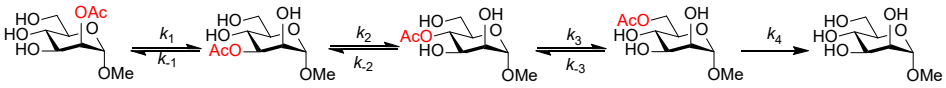
To understand this new migration phenomenon better, computational calculations were performed. Based on the calculations, it is evident that the migration process proceeds by initial deprotonation of the acetyl-accepting hydroxyl group; without prior deprotonation, the migration barrier is computed to be prohibitively high, amounting to hundreds of kJ/mol. This is consistent with the earlier work where migration is fast at high pH, slow at neutral pH and at acidic pH only hydrolysis of the acyl group takes place. At the transition state, the distance between the oxygen

atoms has decreased to ca 2.7 Å and a nine-membered ring has been formed, including the saccharide-bridge. After crossing the barrier the distance is reduced to below 2.5 Å. The activation energy for the migration is calculated to be 56 kJ/mol at room temperature, which corresponds to a reaction half-life of less than a millisecond. The reaction rate is therefore limited by the dynamics of the saccharide chain. After deprotonation of the correct accepting hydroxyl group, the trisaccharide still needs to reorient and rotate appropriately in order for the acetyl group and O^- to come in sufficiently close contact for the migration to take place. Therefore, even if the migration itself requires surprisingly little in the form of activation energy, the preordering of the adjacent monosaccharide groups takes time; weeks, as shown by the NMR spectroscopic data in this work.



The acetyl group migration between the saccharide units in the trisaccharide coumpound.

To further understand the acetyl group migration phenomenon, kinetic isotope effects were investigated. In order to investigate the deprotonation process, an alternative buffer solution was prepared using H_2O instead of D_2O. The H_2O buffer was otherwise similar to the earlier used D_2O buffer, but contained the corresponding non-deuterated acid and base in order to obtain the same properties. In the initial D_2O buffer all protons of the carbohydrate hydroxyl groups will be exchanged to deuterium. Thus, for studying the ^1H isotope in the hydroxyl groups such exchange possibilities should be limited. The migration in the H_2O buffer followed otherwise a similar pattern as observed in the other monosaccharide experiments, but was considerably faster. The rate constant for ^1H is always higher compared to deuterium, except for the hydrolyzation step. The average $^1H/^2H$ ratio is approximately 2.5, without considering the k_4, where the protons are not involved in the rate determining step. The observed primary isotope effect in the monosaccharide model compound thus provided clear experimental evidence for deprotonation being the rate limiting step in acetyl group migration in polyhydroxyl compounds. This is further supported by the earlier studied migration processes where the migration rate was dependent on the pD of the buffer solution.



Migration path and rate constants in both an D_2O and H_2O buffer. Conditions: pD/pH = 8 and 25 °C in buffered D_2O or buffered H_2O with 10% D_2O

	D_2O (h^{-1})	H_2O (h^{-1})	$k(^1H)/k(^2H)$
k_1	0.566 ± 0.0068	0.990 ± 0.0364	1.75
k_{-1}	0.395 ± 0.0058	0.672 ± 0.0292	1.70
k_2	0.036 ± 0.0015	0.066 ± 0.0028	1.83
k_{-2}	0.091 ± 0.0127	0.200 ± 0.0262	2.21
k_3	0.300 ± 0.0125	1.146 ± 0.1632	3.82
k_{-3}	0.019 ± 0.0020	0.072 ± 0.0140	3.80
k_4	0.002 ± 0.0001	0.002 ± 0.0001	0.97

This study has so far demonstrated for the first time that acyl group migration between different saccharide units is possible. The conditions used in the study are similar to natural conditions in the cytoplasm of cells, where the pH resides between 7 and 8, giving the new phenomenon a great possibility to take place in natural conditions. Also, during plant growth the pH is increased, increasing the migration rate. This could have a big impact on the mannans that are responsible for the cell signaling for plant growth and development. The exact implication of the phenomenon is not fully clear at the moment and further studies are required to give better understanding.

Bioactive glasses for biomedical applications

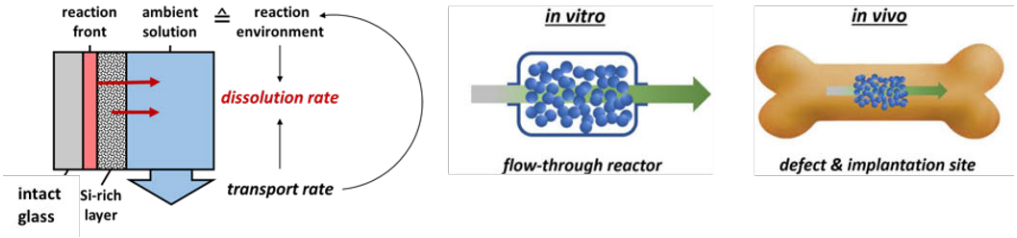
Main funding: Graduate School of Chemical Engineering (GSCE ÅA), Business Finland, Companies

Laura Aalto-Setälä, Minna Siekkinen, Polina Sinitsyna, Adrian Stiller, Markus Engblom, Oskar Karlström, Leena Hupa

We characterise the *in vitro* properties of bioactive glasses for medical devices in soft and hard tissue engineering. We also study the hot-working properties of the glasses with the goal to enable a controlled fabrication of continuous fibres from glass melt or manufacture of porous products through free-form sintering, additive manufacturing and template sintering of bioactive glass particulates. One recent effort has been an enhanced understanding of the interactions of biodegradable polymers and bioactive glasses in composite implants and tissue engineering scaffolds.

Controlled, predetermined ion release and gradual total dissolution of the glass are critical characteristics for the bioactive glass –based devices. Ideally, after implanting the device inside the human body, the inorganic ions are released in concentrations needed to stimulate and support the regeneration of damaged or diseased tissue. We compare the dissolution of the ions in various *in vitro* conditions with the cellular responses of the same glasses in cell culture and in vivo studies done by the experts in medicine, cell and molecular biology. Our research strives for achieving detailed knowledge of dissolution kinetics and the molecular level reaction mechanisms of bioactive glass –based implants in living tissue. This information is crucial for tailoring the glasses for controlled performance in the target application.

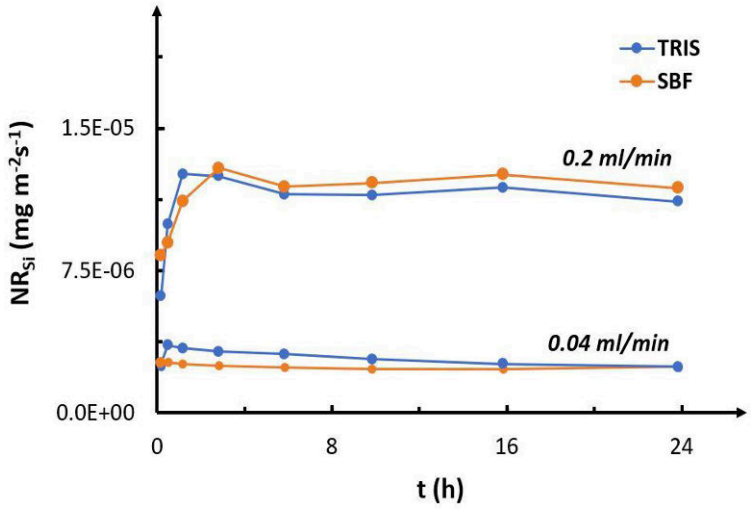
We study the dissolution and reaction layer formation in dynamic in vitro conditions using buffered solutions such as the so-called simulated body fluid. The information gained from the changes in the composition of the solution and the reactions layers at the dissolving glass surface in different conditions are utilized to predict the overall fate of the glass in the aqueous systems mimicking the body environment (see figure below).



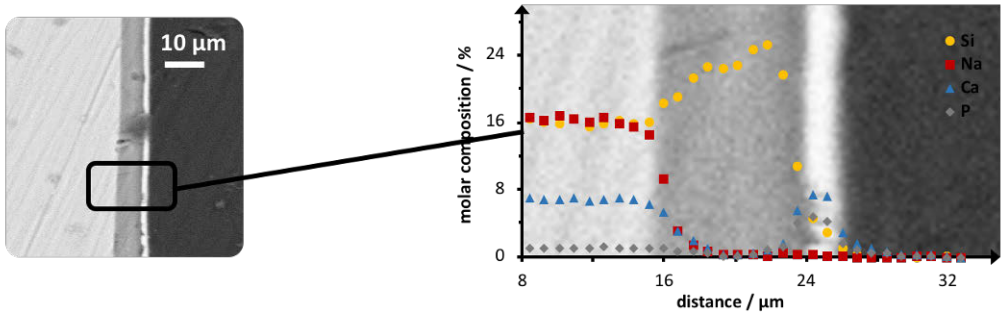
The dissolution and layer development depend on the glass composition and the transport rate of the released species through the layers that develop at the glass surface. The continuous flow-through reactor concept is developed to mimic the conditions the implanted bioactive glass-based implant experiences in the dynamic body environment

The figure below illustrates the impact of fluid flow rate on normalized release rate of Si species from the bioactive glass S53P4 in Tris-buffer solution and the Tris-buffered simulated body fluid (SBF) containing inorganic ions in similar conditions as those in blood show. The release of Si-

species from the glass are of the same level in both solutions. These results imply that there are no fundamental differences between the glass network dissolution in Tris-buffer and SBF.



The impact of fluid flow rate on the dissolution of bioactive glass S53P4 and saturation of the Si species released from the glass into solution



Analysis of layer composition with SEM-EDX

Cooperation: University of Turku, Helsinki University, Aalto University, Tampere University, Friedrich Schiller University of Jena (Germany), Friedrich-Alexander University of Erlangen-Nuremberg (Germany)

Metals and corrosion

Main funding: Academy of Finland (AoF), Business Finland (BF), European Union (EU), Swedish Energy Agency (SEA), Finnish Recovery Boiler Committee (FRBC), Nordic Energy Research (NER), Enova, European Regional Development Fund (ERDF), Graduate School of Chemical Engineering (GSCE), Industrial Partners (IP), PCC

Elisa Hupa, Nina Bruun, Oskar Karlström, Juho Lehmusto, Fiseha Tesfaye, Maria Zevenhoven, Patrik Yrjas, Emil Vainio, Mikko Hupa, Leena Hupa

CLUE, which is an acronym for **CLean and efficient Utilization of demanding fuEls**, is an umbrella project focusing on several research topics on sustainable fuel conversion in the period 1.11.2017-31.10.2019. It got continuation in the CLUE^2-project with a similar agenda that runs in the period 1.12.2019-30.11.2022. The purpose of the CLUEs is to perform and present industrially relevant research based on a fundamental understanding of detailed chemistry. An important aspect is to maintain the long-term co-operation between industry and academia for mutual benefits. The text here and the two following project descriptions contain research topics included in this project. Here below, we present topics related to metals and corrosion.

By 2020, Finland targets to obtain at least 38 % of its energy from renewable sources. Solid biomass fuels are the most important energy source for meeting these targets. However, fouling, slagging, and corrosion threaten long-term operation availability and costs of biomass power plants. A high concentration of potassium in biomass fuel tends to result in the formation of compounds with low melting points. Significant amounts of highly corrosive alkali chloride in the flue gases emanate through these processes.

We aim to provide new and unique information on high-temperature corrosion primarily in power plants firing biomass and waste, focusing on the onset chemistry of the corrosion reactions. We do this by making use of new innovative experimental techniques, not previously applied, to high-temperature corrosion studies. The research focuses on the details of corrosion onset chemistry, on the role of different oxygen carriers in high-temperature reactions, and the gas-phase chemistry during the corrosion reactions. New insight on reaction mechanisms will broaden the view on corrosion research, paving the road for further studies in the field. The work will help material designers, boiler designers, and plant operators to address and master corrosion-related problems.

One rule of thumb is to maintain superheater steel temperatures below the ash deposits' first melting temperature, T_0. This way to control corrosion is known from before. However, it is less well known how the corrosion rate depends on the amount of melt formed at T_0, in particular at low amounts of melt formed. The objective is to understand better how superheater corrosion depends on the amount of melt (share of melt fraction) at temperatures at or slightly above the deposit first melting temperature T_0.

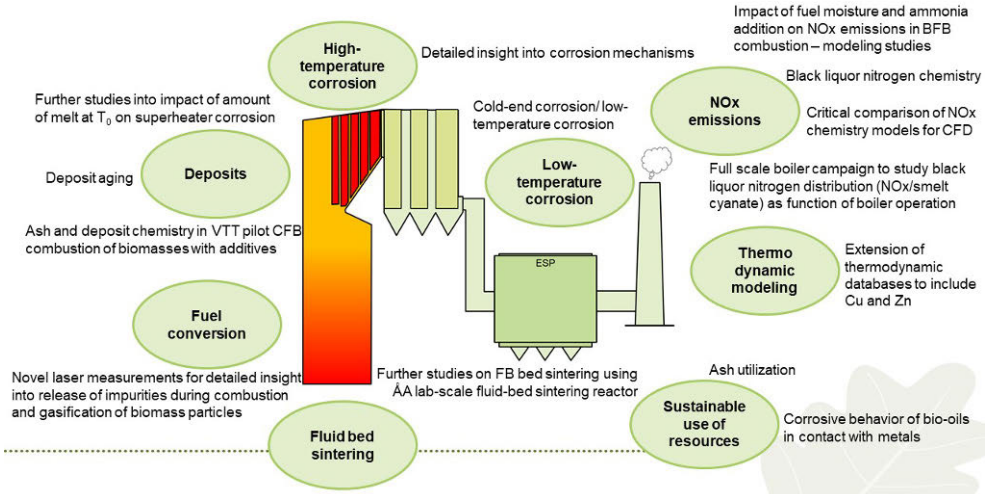
Slags on superheaters constitute a mix of complex inorganic phases. The melting behaviour and the thermodynamic properties of such complex mixtures and their combined effect with gaseous chlorides are poorly studied or not available. Our research will give new information concerning properties of the metallic sulphates, chlorides and their phase mixtures, which will help to predict slagging and high-temperature corrosion-related problems.

Development of thermodynamic databases relevant for industrial high-temperature processes will contribute with new data regarding the thermodynamic properties of phases and phase mixtures in the systems $MSO_4 – M_2SO_4 – MCl$, where M = K, Fe, Ca, Mg, Cu, Zn. This work provides industry

with new information for solving problems related to high-temperature processes utilizing biomass.

Another important topic studied is ash deposit aging, i.e. changes in deposit chemistry and morphology with time. These studies provide information for prediction of superheater corrosion and deposit removability. We study intra-deposit alkali chloride enrichment using several approaches: in laboratory-scale by a temperature-gradient setup of synthetic ash deposits, and in industrial-scale by ash deposit sampling of boiler superheater's using boiler deposit probes.

Hygroscopic and deliquescent salts in ash deposits have been found to cause cold-end corrosion in the combustion of biomass and waste-derived fuels. The hygroscopic properties of various salts, e.g. ammonium sulphates and chlorides, are studied in the laboratory in controlled conditions to determine the temperature and humidities where the salts absorb water. Corrosion tests with various steel qualities and salt mixtures help us to understand the different corrosion mechanisms.



CLUE²-project research topics

Another field of metal and corrosion research concerns locally produced bio-oils (fish oils and used cooking oils). Their physico-chemical and thermal properties determine their applicability as possible fuels for marine engines. The bio-oils are infamous for their corrosive behaviour. The objective for us is to investigate the corrosive properties of the bio-oils that are in contact with ferrous metals. We develop new methods to estimate and measure the corrosion mechanisms of the bio-oils during their use and storage.

Cooperation: Aalto University, Seoul National University (South Korea), Stellenbosch University (South Africa), Umeå University (Sweden)

Fuels and emissions in biomass combustion

Main funding: Academy of Finland (AoF), Business Finland (BF), European Union (EU), Swedish Energy Agency (SEA), Finnish Recovery Boiler Committee (FRBC), Nordic Energy Research (NER), Enova, European Regional Development Fund (ERDF), Graduate School of Chemical Engineering (GSCE), Industrial Partners (IP), PCC

Roland Balint, Meheretu Dirbeba, Arturo Keim, Paulo Santochi, Daniel Schmid, Stefan Heberlein, Raju Viswamoorthy, Markus Engblom, Oskar Karlström, Patrik Yrjas, Mikko Hupa, Leena Hupa

Research on black liquor nitrogen chemistry involves volatile flame chemistry and aims on a better understanding of the existence/stability of an envelope flame during droplet pyrolysis in boiler conditions. Earlier results imply that, as a modelling approach, the chemical form of the black liquor volatile nitrogen that reaches the bulk gas can be either mainly NH_3 (no flame) or a mixture of NO/N_2 (with flame). We perform single droplet experiments and modelling to understand better flame stability, including dependence on slip velocity and oxygen concentration.

Full-scale boiler campaign at the UPM Pietarsaari mill recovery boiler provides data for black liquor nitrogen distribution (NOx/smelt cyanate) as function of boiler operation. This will show how black liquor nitrogen splits between gaseous NOx and smelt cyanate, and how the distribution and overall emission depends on boiler operation.

Fluidised bed sintering and agglomeration formation tendency is studied using the lab-scale fluid-bed sintering reactor at Åbo Akademi University. In the future, less peat is expected to be utilized as fuel. Consequently, fluidised bed agglomeration could become a growing problem. The work carried out within this work package aims to understand better the effect of peat/peat ash on alkali-induced fluidized bed agglomeration. Studies will include alternative bed materials, like blast furnace slag and kaolin. Results from tests using phosphorus-rich fuels are reported.

Novel laser measurements for detailed insight into release of impurities during biomass combustion and gasification involves collaboration with Lund University, Sweden. Through them, we have access to sensitive nonintrusive laser measurements, which quantify gaseous lead, zinc, nitrogen, sulphur and possiblyphosphorus compounds in the very proximity of single fuel particles under combustion and gasification conditions. These types of measurements can give new and relevant information on how these minor elements behave during combustion and gasification of waste and biomass.

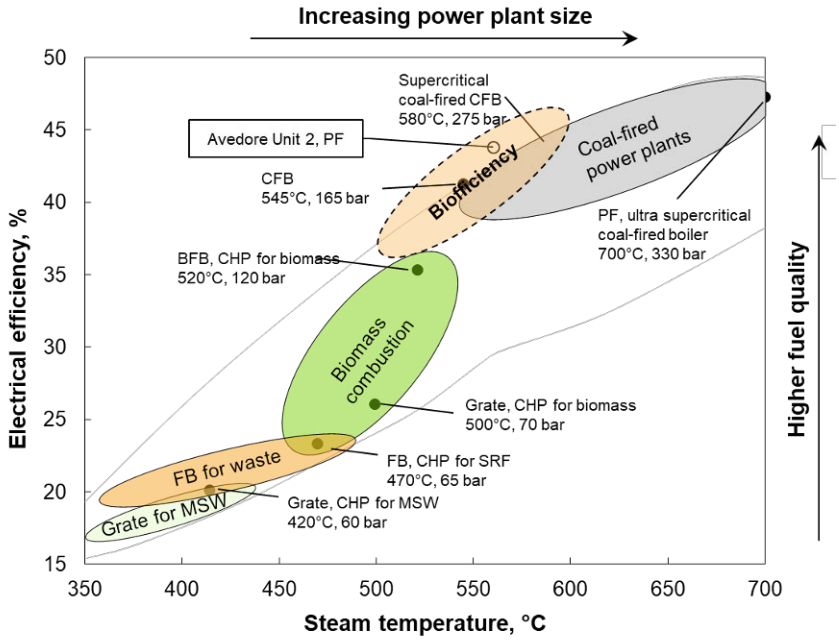
Biomass fuel moisture influence how to inject ammonia in the most efficient way to minimize final NOx emissions during bubbling fluidised bed (BFB) combustion. This study combines three different modelling tools in a unique way to predict NOx emissions from biomass combustion in a BFB boiler. Parameters to study are i) fuel moisture content, ii) NH_3 injection strategies, and iii) their influence on final NOx emissions. The fuel moisture content influences the concentrations of the primary nitrogen species such as NO, HCN and NH_3, the temperature of the flue gas and the moisture content of the flue gas.

Comparing different gas-phase reaction mechanisms for NOx-chemistry sub-models in CFD-modelling allows determining their NOx-chemistry prediction accuracy. This will show which mechanisms are suitable for CFD boiler NOx modelling, taking into account the prediction accuracy as well as the computational cost and issues with solution convergence. A practical goal is to find a mechanism(s) suitable for boiler simulations, including understanding of the limitations

of the mechanisms. The main industrial application for these studies will be the black liquor recovery boiler. However, some BFB modelling cases can be included in the study.

EU-Biofficiency

The main objective and goal of the EU-financed Biofficiency project (November 2016 – October 2019) was to develop the next generation of biomass-fired CHP (Combined Heat and Power) plants at medium to large scale (10 to 200 MWth). This meant to allow elevated steam temperatures up to 600 °C through solving and understanding of ash-related problems – slagging, fouling and corrosion and widen the feedstocks for pulverised fuel (PF) and fluidised bed (FB) combustion using pre-treatment methods to reduce inorganic elements: chlorine, sulphur and alkali metals in the fuel.



The Biofficiency project's target area of steam-temperatures, efficiency and power-plant sizes

Energy from biomass is a suitable technology for medium- and large-scale units where many utility and industrial applications are in Scandinavia. The main challenge for efficient CHP and high temperature steam production from biomass are ash-related problems, i.e. ash fouling and corrosion that limits both steam temperature and heat transfer. By solving these issues, large-scale boilers offer a huge potential for efficiency increase and emission reduction during CHP generation at cost competitive and environmentally friendly conditions. In order to reach these goals and to enable a secure and carbon-neutral heat and power generation, several measures have to be undertaken.

Cooperation: Lund University, Technical University of Munich, Technical University of Denmark, VTT Technical Research Centre of Finland, Technical University of Athens, ECNpoTNO, Engie Laborelec

Fuel ash and circular economy

Main funding: European Union, European Regional Development Fund (ERDF), Uudenmaan liitto, 6 Aika, Enova - Research Council of Norway

Thomas Kronberg, Christoffer Sevonius, Jan-Erik Eriksson, Juho Lehmusto, Fiseha Tesfaye, Oskar Karlström, Emil Vainio, Johan Werkelin, Patrik Yrjas, Maria Zevenhoven, Leena Hupa

The research on ash utilization aims at finding new ways to utilize biomass and waste-based ashes. Current research includes studies of using ash as one component to stabilize clay-rich soil at construction sites. Also, stabilization of dredging masses to be filled in construction sites is explored. The goal is to enhance the understanding of the ash composition and ash collection site as well as the impact of additives in combustion on the suitability of the ashes as secondary raw materials instead of used as land-filling.

CircVol is a 2.5-year project that runs until the end of 2020. Turku Science Park is the coordinator, and the partners include large Finnish cities, research institutes and academia. It promotes a business that subscribes to the ideas of circular economy and the utilization of large volumes of industrial side streams and earth masses in earthworks.

More than 90 % of accumulated waste volumes come from the extractive and manufacturing industries. Side streams from the manufacturing sector are not utilized sufficiently as of yet, even though collection and refining technologies are already highly developed. The efficient reuse of earth masses can be harnessed to achieve significant economic savings and promote the carbon neutrality objectives of cities.

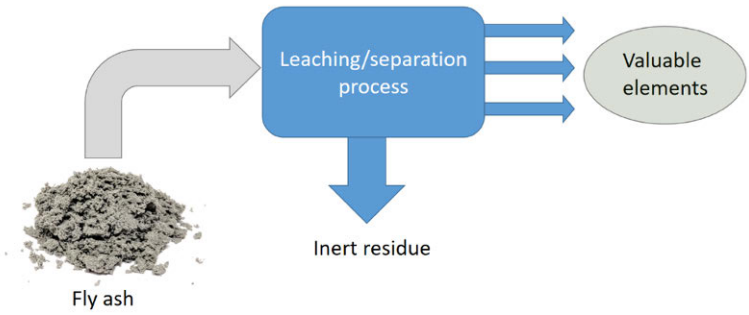
The primary research efforts at Åbo Akademi have dealt with the stabilization of dredged marine clay by fly ash and other recycled industrial by-streams. As sea dumping of dredged marine clay is no longer permitted, new ways to utilize the dredged material are needed. Our goal has been to use these clays in land constructions together with various stabilizers based on industrial by-streams. As stabilizers, we have used various fly ashes and other industrial waste or by-streams to reduce the amount of cement needed for the stabilization. From the 20 recipes developed in laboratory tests, nine were selected to pilot-scale stabilization of dredged clay in the Naantali Housing Fair 2022 area.

Pilot scale experiments of mixing fly ash from Naantali multifuel power plant and other industrial by-streams to stabilize earth in Naantali Housing Fair 2022 area

The stabilized earth should fulfil the strength criteria for earth construction. Our research goals have been to find new and safe ways to utilize industrial by-streams and waste materials. In earth construction, the properties must fulfil all the requirements given in the legislation (Environmental Protection Act 527/2014 and Mara degree - Degree on the Recovery of Certain Wastes in Earth Construction; 843/2017).

We have used hydrothermal methods for separating valuable resource elements or harmful elements from ashes. The information gained on the ash composition aids in evaluating the suitability of particular ash as a fertilizer or as a geopolymer. Work will also address the removal of cadmium and other EU dirty dozen heavy metals from the black liquor recovery boiler and the pulp mill process.

The objective of the **Waste-to-Energy 2030** project is to improve the competitiveness of the sector by increasing the efficiency and performance of existing installations while improving circular economy practices. The project is co-funded by the Research Council of Norway, Enova and industry partners. Our part in the project is in the "Ash valorization" task. Fly ash from waste incineration contains several valuable elements and is an interesting secondary source of metals and other elements. Due to the volatility of many metals in incineration, they are enriched in the fly ash. These heavy metals and other minor impurities make it problematic for disposal, and fly ash from waste incineration is therefore regarded as a hazardous waste. Instead of landfill of fly ashes, the recovery of valuable elements and stabilization of the ash is of interest. In this task, we will look at the occurrence of valuable elements or elements problematic for disposal. We develop methods to enrich and recover the elements. The ultimate goal is to find a concept for recovering target elements from fly ashes while producing a non-hazardous inert residue.



Schematic of separation process of valuable elemens from fly ash

Cooperation:

Geological Survey of Finland GTK, Oulu University of Applied Sciences, City of Oulu, Finnish Environment Institute SYKE, TTY Foundation/Tampere University of Technology, Turku University of Applied Sciences, SINTEF (Norway)

5. PCC publications 1.1.2018–31.12.2018

5.1 Theses (2018)

5.1.1 Doctoral Theses (4)

Hachemi, Imane, Catalytic transformation of algae, tall-oil fatty acids and triglycerides to renewable fuels and chemicals (18.6.2018)

Meierjohann, Axel, Application of LC-MS/MS for environmental analysis (7.9.2018)

Nisula, Linda, Wood extractives in conifers – A study of stemwood and knots of industrially important species (23.2.2018)

Rahkila, Jani, Multivalency in Carbohydrate Chemistry : From oligosaccharides to oligovalency and beyond (16.2.2018)

5.1.2 Masters's theses (15)

Alda-Onggar, Moldir, Hydrodeoxygenation of bio-oil model compounds using alumina, zirconia and carbon supported catalysts

Arandia, Kenneth, Analysis of silicon oil in tall oil products

Blidi, Slim, Solid-state composite reference electrodes: evaluation in different applications

Gamaethiralalage, Jayaruwan Gunathilake, Determination of carbonic acid species using carbonate- and novel bicarbonate-selective electrode

Graeffe, Daniela, Studium av extraherbara näringsämnen i markprover med jonkromatografi och ICP-OES

Li, Changbai, Determination of acetate in wine: comparison between ion chromatography and ion-selective electrodes

Nynäs, Emma, Thermal conversion and treatment of plastic residues from biogas plants (in Swedish)

Oña, Jay Pee, Towards calibration-free solid-contact ion-selective electrodes: study and improvement of the standard potential stability

Rantala, Joni, Determination of bio-oil induced corrosion

Schmid, Daniel, Influence of biomass pre-treatments on the formation of NO and NO-precursors in the different combustion stages

Sergeeva, Anna, Preparation of iron phosphate by precipitation from pickling acid residue

Siekkinen, Minna, Effect of ion concentration on the chemical durability of bioactive glasses in a cascade reactor system (In Swedish)

Sjögren, Frida, Karakterisering av CH-Bioforce dissolvingmassa

Vega, Pablo, Modifying nanocellulose hydrogels with O-acetyl-galactoglucomannan derivatives: tuning the surface hydrophilicity of the fiber surface

Yrjänä, *Ville*, Potentiometric sensors for the determination of glyphosate concentration

5.2 Publications 2018 (158)

5.2.1 Articles in refereed international scientific journals and series (138)

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5. Ahn, K., Schedl, A., Zweckmair, T., Rosenau, T., Potthast, A., **Fire-induced structural changes and long-term stability of burned historical rag papers**, *Scientific Reports* 8 (2018) 1, art. no. 12036

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5.2.2 Review articles in refereed international scientific journals and series (2)

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5.2.3 Books (1)

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5.2.4 Book chapters (9)

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5.2.4 Articles in refereed international edited volumes and conference proceedings (8)

151. Huttula, M., Patanen, M., Piispanen, R., Ohigashi, T., Kosugi, N., Swaraj, S., Belkhou, R., Pranovich, A., Jyske, T., Kilpelainen, P., Karkonen, A., Korpinen, R., Laakso, T., Valkonen, S., Saranpää, P., **STXM chemical mapping of Norway spruce knotwood lignans**, *Microscopy and Microanalysis* (Proceedings of the 14th International Conference on X-ray Microscopy (XRM2018)) 24 (2018) S2, 482–483

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5.3 Edited conference proceedings and reports

Virtanen, P., Latonen, R-M., Lagerquist, L., Långvik, O., Mäki-Arvela, P., Sundberg, A., Werkelin, J. (eds) Åbo Akademi Johan Gadolin Process Chemistry Centre Annual Report 2017-2018, Åbo Akademi University, 2018, ISSN: 1459-8213, Painosalama, Turku, Finland, 2018

5.4 Patents and invention disclosures (2018)

Nowicki, J., Muszynski, M. Mikkola, J.-P., **Process for preparing fluorinated basic ionic liquids** PL 224608 B1 20170131

Sokalski, Tomasz, Lewenstam, Andrzej, Mousavi, Zekra, Granholm, Kim, **A reference electrode and an arrangement for an electrochemical measurement**, EP2932249B1 20181107, US10094798B2 20181009, (2018)

5.5 Awards granted (2018)

Aalto-Setälä Laura and Uppstu, Peter, 1st prize in the Åbo Akademi Innovation Catalyst innovation competition for "Bone savers – Enhanced treatment of large bone defect" 2018

Aalto-Setälä, Laura, Winner of the writing competition of scientific and research articles to the magazine "Tiede": Bioactive glass transforms into bone and battles against bacteria 2018

Balint, Roland, Johan Gadolin Process Chemistry Centre Poster and Flash Talk Award 2018

Behravesh, Erfan, Johan Gadolin Process Chemistry Centre Poster Award 2018

Bobacka, Johan, First Class Knight of the White Rose of Finland 2018

Freites, Adriana, Johan Gadolin Process Chemistry Centre Poster and Flash Talk Award 2018

Korotkova, Ekaterina, Johan Gadolin Process Chemistry Centre Poster and Flash Talk Award 2018

Murzin, Dmitry, Gadd Prize of Chancellor of Åbo Akademi 2018

Salmi, Tapio, Award of Finlandssvenska folktinget, 2018

Sinitsyna, Polina, Johan Gadolin Process Chemistry Centre Poster Award 2018

Tesfaye, Fiseha, Young Leaders Professional Development Award of The Minerals, Metals & Materials Society (TMS) 2018

Xu, Wenyang, Best oral award on 15th European Workshop on Lignocellulosics and Pulp (EWLP), Aveiro, Portugal 2018

6. PCC publications 1.1.2019–31.12.2019

6.1 Theses (2019)

6.1.1 Doctoral Theses (6)

Godina, Lidia, Aqueous-phase reforming of renewable polyols for sustainable hydrogen production (22.02.2019)

Kinnunen, Hanna, Influence of lead and zinc compounds on superheater corrosion in fluidized beds firing demolition wood (30.08.2019)

Niemi, Jonne, The role of temperature gradient in ash-deposit chemistry and superheater corrosion (22.11.2019)

Pérez Nebreda, Andrea, Valuable monomers and oligomers from hemicelluloses (03.05.2019)

Sui, Jingxin, An electrochemical approach to high-temperature corrosion (24.05.2019)

Xu, Wenyang, Three-dimensional printing of wood-derived biopolymers towards biomedical applications (22.02.2019)

6.1.2 Masters's theses (17)

Alvear, Matias, Aqueous phase reforming of renewables for hydrogen production in presence of supported platinum and palladium catalysts (presented at Politecnico di Milano)

Azkaar, Muhammed, One-pot transformation of citronellal to menthol using shaped bifunctional catalysts. Role of metal (Pt and Ru) influence of acid sites, structures and textural properties of solid catalysts

Forstén, Jon, The role of calcium on deposit chemistry and corrosion in fluidized bed combustion of biomass

Kaka Khel, Taimoor Ahmad, Hydrocarbon conversion of long-chain paraffins. Role of metal (Pt, Ru, Ni) and influence of acid sites, structures and textural properties of solid catalysts

Karlemo, Camilla, Foreign element balances in black liquor boilers

Kemp, Emily, Optimization of modification of glassy carbon electrodes with nitrogen-doped reduced nano-graphene oxide for DNA biosensor applications

Lindfors, Christoffer, Hydrodeoxygenation of lignin-derived phenol compound isoeugenol over nickel- and cobalt-based catalysts

Mun Man, Hiu, pH sensors with high sensitivity utilizing coulometric transduction method – comparison of solid-contact ionselective electrode and polyaniline-based ion-selective electrode

Obradović, Nikola, Solid-contact ion-selective electrodes with high sensitivity – Comparison of potentiometric and coulometric signal transduction

Rudnäs, André, Impact of potassium salts on the fate of oxygen carriers in chemical looping combustions

Sirén, Ralf, Evaluation of optimal chemical aids and process parameters in oil refinery wastewater flocculation and flotation

Suerz, Rossana, Ethanol dehydration in microreactor (presented at Università di Padova)

Tediashvili, Davit, Influence of conditioning and surface modification of PEDOT used as solid-contact in K^+selective electrodes

Tuomisalo, Matias, Analys av AdBlue–lösningens hållbarhet och dess inverkan på försvarsmaktens distributionslogistik

Törmä, Sofia, Diesel fuel particle emissions from a constant-volume combustion chamber

Wrzosek Cabrera, *Jose Antonio*, Water resistant electrospun nanofibers composed of nanocellulose and conducting polymer with electrical properties

Örn, Anton, Degradation studies on polymethylsiloxane

6.2 Publications 1.1.–31.12.2019 (140)

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127. Zheng, J. L., Tolvanen, P., Eränen, K., Taouk, B., Salmi, T., Leveneur, S., **Synthesis of carbonated vegetable oils: Investigation of microwave effect in a pressurized continuous-flow recycle batch reactor**, *Chemical Engineering Research and Design* 132 (2019) 9–18

128. Zweckmair, T., Rhakila, J., Willför, S., Xu, C., **TEMPO-oxidized O-acetyl galactoglucomannan oligomers: Isolation and comprehensive structural elucidation**, *Wood Science and Technology* 53 (2019), 71–85

6.2.2 Review articles in refereed international scientific journals and series

129. Konwar, L. J., Mäki-Arvela, P., Mikkola, J.-P., **SO_3H-containing functional carbon materials: Synthesis, structure, and acid catalysis**, *Chemical reviews*, 2019, doi: 10.1021/acs.chemrev.9b00199

130. Murzin, D. Yu., **On the scientific heritage of Mikhail Isaakovich Temkin**, *Kinetics and Catalysis* 60 (2019) 388–397

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6.2.3 Books

132. Salmi, T., Mikkola, J.-P., Wärnå, J., **Chemical reaction Engineering and Reactor Technology**, 2nd edition, CRC Press Taylor & Francis Group, Boca Raton Fl. 2019, 627p

6.2.4 Book chapters

133. Gaustad,G., Fleuriault, C., Gökelma, M., Howarter, J.A., Kirchain, R., Ma, K., Meskers, C., Neelameggham, N., Olivetti, E., Powell, A.C., Tesfaye, F., Zhang, M., (Eds), REWAS 2019 - **Manufacturing the circular materials economy**, *Minerals, Metals & Materials Series*, 2019, pp. XII, 338. DOI: 10.1007/978-3-030-10386-6

134. Hamuyuni, J., Tesfaye, F., **Advances in lithium-ion battery electrolytes: Prospects and challenges in recycling**, in *"REWAS 2019: Secondary and Byproduct Sources of Materials, Minerals, and Metals"*, Eds. Gabrielle Gaustad et al., The Minerals, Metals & Materials Series, 2019. DOI: doi.org/10.1007/978-3-030-10386-6_31

135. Hupa, L., Wang, X., Eqtesadi, S., **Bioactive glasses** in "*Springer Handbook of Glass",* Eds. Musgraves, J.D., Hu, J., Calvez, L. Springer, 2019, (ISBB-978-3-319-93726-7), April 2019

136. Moroz, M., Tesfaye, F., Demchenko, P., Prokhorenko, M., Lindberg, D., Reshetnyak, O., Hupa, L., **Thermal stability and thermodynamics of the Ag_2ZnGeS_4 compound**, in "*Materials Processing Fundamentals 2019*", Eds Guillaume Lambotte, Jonghyun Lee, Antoine Allanore, Samuel Wagstaff, The Minerals, Metals & Materials Series, https://link.springer.com/chapter/10.1007/978-3-030-05728-2_20

137. Salminen, E., Bridier, S., Mäki-Arvela, Kumar, N., Fahl, J., Roine, J., Salmi, T., Mikkola, J.-P., **Design of metal-modified zeolites and mesoporous aluminosilicates and application in the synthesis of fine chemicals**, Chapter 4: Nanoparticle Design and Characterization for Catalytic Applications in Sustainable Chemistry, pp.115–131. DOI: 10.1039/9781788016292-00115

138. Simakova, I., Murzin, D., **Ruthenium nanoparticles: An overview of recent developments in colloidal synthesis, properties, and potential applications**, 2019, 99–141. Elsevier, DOI: 10.1016/B978-0-12-814807-5.00004-8

139. Tesfaye, F., Jung, I.-P., Paek, M.-K., Moroz, M., Lindberg, D., Hupa, L., **Thermochemical data of selected phases in the FeO_x–$FeSO_4$–$Fe_2(SO_4)_3$ system**, in "*Materials Processing Fundamentals 2019*" Eds. Guillaume Lambotte, Jonghyn Lee, Antoine Allanore, Samuel R. Wagstaff, 1–214, https://doi.org/10.1007/978-3-030-05728-2_21

140. Tesfaye, F., Moroz, M., Reshetnyak, O., Lindberg, D., Taskinen, P., Hupa, L., **The fast silver ion conducting solid-state electrolytes for deriving thermodynamic data**, in "*Thermophysical Properties of Complex Materials*", Ed. Shahzad, A., InTechOpen, 1–19, http://dx.doi.org/10.5772/intechopen.86878

6.2.5 Other articles

Salmi, T., **Mikroreaktorteknologi – en ny och överlägsen väg?**, *Redox* 72 (2019)

6.3 Edited conference proceedings and reports

Virtanen, P., Latonen, R-M., Lagerquist, L., Långvik, O., Mäki-Arvela, P., Sundberg, A., Werkelin, J. (eds) Åbo Akademi Johan Gadolin Process Chemistry Centre Annual Report 2017–2018, Åbo Akademi University, 2018, ISSN: 1459-8213, Painosalama, Turku, Finland, 2018

6.4 Patents and invention disclosures (2019)

6.4.1 Patents

Bergelin, M., Eriksson, J-E., Ylänen, H.O., Xu, C., Leppänen, A-S., Willför, S., Köppä, S., Kekonen, A., Johansson, M., Viik, J., Hyttinen, J., (2019) **An arrangement for facilitating wound healing, a method for measuring wound healing and a wound dressing,** US Patent, US 10 206 604 B2

Mikkola, J.-P., Murzin, D. Yu., Salmi, T., Wärnå, J., Fagerholm, M., Snåre, M., Aldea, S., Eränen, K., Grenman, H., **Preparation of salt particles from precipitated calcium carbonate**, Finn. Patent FI 1217761 B 20190215, 2019

Sokalski, Tomasz, Lewenstam, Andrzej, Mousavi, Zekra, Granholm, Kim, **A reference electrode and an arrangement for an electrochemical measurement**, EP2932249B1 20181107, US10094798B2 20181009

6.4.2 Invention disclosures

Mikkonen, K., Tenkanen, M., Xu, C., Willför, S., BITE-project, "**Use of non-starch, non-cellulosic plant polysaccharide-rich extracts to stabilize alkyd oil emulsion in paint formulation**"

6.5 Awards granted (2019)

Bruun, Nina, Johan Gadolin Process Centre Poster Award 2019

Junghans, Paula, Johan Gadolin Process Centre Poster Award 2019

Mattsson, Ida, Johan Gadolin Process Centre Poster and Flash Presentation Award 2019

Mendez, Carolina, Johan Gadolin Process Centre Poster and Flash Presentation Award 2019

Salmi, Tapio, Gadd Prize of Chancellor of Åbo Akademi 2019

Salmi, Tapio, Nobel laureate A.I. Virtanen Prize in chemistry, Finnish Chemical Society 2019

Stiller, Adrian, Johan Gadolin Process Centre Poster and Flash Presentation Award 2019

Tolvanen, Pasi, Colleague of the Year Award 2019

Véliz, Diosángeles Soto, Johan Gadolin Process Centre Poster Award 2019

7. External interactions 2018

7.1 Organization of conferences/courses/meetings 2018

REWAS 2019 – Manufacturing the Circular Materials Economy, conference. A co-organizer, *Fiseha Tesfaye*

Computer-Aided Chemical Reaction Engineering, International postgraduate course, May 2018, Turku/Åbo

Reaction Kinetics, International postgraduate course, December 2018, Turku/Åbo

7.2 Visits and visitors

Visits

Boeva, Zhanna, Budapest University of Technology and Economics, Hungary, June 2018

Boeva, Zhanna, Georgia Tech, USA, September-October 2018

Grénman Henrik, visiting researcher, Delft University of Technology, Process and Energy, The Netherlands, January 2018

Ivaska, Ari, Beijing Graphene Institute, China, October 2018

Ivaska, Ari, Guangzhou University, China, October 2018

Lehmusto, Juho, Oak Ridge National Laboratory, Tennessee, USA, July – December 2018

Lindfors, Tom, Budapest University of Technology and Economics, Hungary, May – June 2018

Korotkova, Ekaterina, TSTU, 29-30.03.2018, 27.04.2018

Pranovich, Andrey, St. Petersburg Forest Technical University, Faculty of Chemical Technology and Biotechnology, Russia, April 2018

Savela, Risto, Technical University of Dortmund, Germany, April – June 2018

Sokalski, Tomasz, The University of Warsaw Biological and Chemical Research Centre (CNBCh UW), Poland, December 2018

Sundberg, Anna, RISE, Sweden, August 2018

Tesfaye, Fiseha, Seoul National University, South Korea, March – August 2018

Zhang, Yongchao, Lakehead University, Canada, January – July 2018

Zhang, Yongchao, TUST, China, November – December 2018

Visitors

Alexis Lebeau, Rouen France, Erasmus student (6 months), May – November 2018

Attah-Kyei, Desmond, Stellenbosch University, South Africa, April – May 2018

Badazhkova, *Veronika*, St. Petersburg State Chemical and Pharmaceutical University, Russia, August-September 2019

Balint, Roland, Technische Universität München, Germany, October 2017 – March 2018

Bembaron, Julia, INSA Rouen, France, June – August 2018

Benamar, Benotmane, University M'Hamed Bougara of Boumerdes, 13.12.2018-18.12.2018

Bollella, Paolo, University of Rome "La Sapienza", Italy, August-September 2018, **Johan Gadolin Scholarship**

Cai, Xiaoshuang, Institut National des Sciences Appliquées (INSA) Rouen, France, October 2018 – February 2019, **Johan Gadolin Scholarship**

Chaperon, Sarah, École Nationale Supérieure de Chimie de Rennes, France, 2018, 3 months

Cisse, Maperda, INSA Rouen, France, June – August 2018, 3 months

Daigue, Emilieu, INSA, Rouen, France, November 2017 – May 2018, 6 months

Eliason, Felicia, Chalmers University of Technology, Sweden, February – May 2018

*Fuchtner, Sophi*e, University of Copenhagen, Denmark, 2 weeks, 2018

Galasheva, Sofia, St. Petersburg State Chemical and Pharmaceutical University, Russia, October – December, 2018, 3 months

Godino, Andres Morato, University Carlos III of Madrid, Spain, October 2017 – January 2018 and August – September 2018

Gonzalez Carlos Rosales, University of Vallidolid, Spain, August 2017 – May 2018, 9 months

Hemery, Remi, INSA Rouen, France June – August 2018, 3 months

Ho-Wen-Tsa, *Anthony,* INSA Rouen, France, June – August 2018, 3 months

Ibanez Abad, Javier, Université de Lille 1, France, April – August 2018, 5 months, **Johan Gadolin Scholarship**

Itterheimová, Petra, Masaryk University, Czech Republic, January – June 2018

Ke, Xiwei, Tsinghua University, China, August – December 2018, **Johan Gadolin Scholarship**

Khaydukova, Maria, Saint-Petersburg State University, Russia, August 2017 – October 2018, **Johan Gadolin Scholarship**

Krauß, Annabelle, University of Stuttgart, Germany, 2018

Lamine Bouhoun, Mohammed, University of Science and Technology Houari Boumediene, Algeria, October – November 2018

Le Guillant, *Amadelie*, INSA Rouen, France, June – August 2018, 3 months

Lozachmeur, Chlóe, INSA Rouen, France, June – August 2018, 3 months

Mendez, Carolina, Universidad de Chile, Chile, April – November 2018, **Johan Gadolin Scholarship**

Moro Lobo, Alberto, University of Vallidolid, Spain, September 2107 – June 2018, 10 months

Nuri, Ayat, University of Mohaghegh Ardabili, Iran, February – October 2018, 8 months

Näykki, Teemu, Finnish Environment Institute (SYKE), Finland, May 2018

Ospina, Marcela Arango, Institute of Biomaterials, Friedrich Alexander Universität Erlangen-Nuremberg, Germany, 01.08.2018-31.10.2018, **Johan Gadolin Scholarship**

Ozanne Sophie, INSA, Rouen, France, May – August 2018, 3 months

Papp, Soma, Budapest University of Technology and Economics, Hungary, August-November 2018, **Johan Gadolin Scholarship**

Riabukhin, Dmitry, Saint-Petersburg State Forest Technical University, Russia, June 2017 – February 2018, **Johan Gadolin Scholarship**

Rossello, Teresa Marti, University of Strathclyde, Glasgow, United Kingdom, May – June 2018

Shchukina, Anastasia, St. Petersburg University, Russia, August – September 2018

Sitdikov, Ruzal, Kazan Federal University, Russia, August 2017 – April 2018, **Johan Gadolin Scholarship**

Stiller, Adrian, University of Ulm, Germany, January – May 2018

Tieuli, Sebastiano, Ca'Foscaro, Venezia, Italy, December 2017 – March 2018, 3 months

Torres, Gaetan, INSA Rouen, France, February – April 2018, 2 months

Truffier-Blanc, Julius, INSA Rouen, France, June – August 2018

Wei, Lingyuan, Delft University of Technology, the Netherlands, March – July 2018, 4 months

Xu, Huanfei, Quingdao University of Science and Technology, China, September – December 2019, **Johan Gadolin Scholarship**

Yin, Tanji, Yantai Institute of Coastal Zone Research, China, August – November 2018, **Johan Gadolin Scholarship**

Zergane, Hichem, University of Science and Technology Houari Boumadiene (USTHB), Algeria, September – December 2018

7.3 Evaluation of candidates

Reviewer for application of Associate senior lecturer in wood material science and engineering, Swedish Agricultural Sciences, 2018, *Anna Sundberg*

7.4 External evaluations and reviews

External evaluations

Evaluation of proposals in the EU H2020, 2018, vice chair, *Päivi Mäki-Arvela*

Evaluation of Haldor Topsoe PhD scholarship programme, 2018, *Dmitry Murzi*n

Evaluation of Applications in French National Agency of Science, *Dmitry Murzin*

Evaluation of Applications in Danish Science Foundation, *Dmitry Murzin*

Evaluation of Applications in Kazakhstan Science Foundation, *Dmitry Murzin*

Evaluation of Applications in UK Science Foundation, *Dmitry Murzin*

Evaluation of proposals, FONDECYT, Research council in Chile, July 2018, *Päivi Mäki-Arvela*

Evalaution of proposals, vice chair, Swedish Research Council, 2018, *Päivi Mäki-Arvela*

Evaluation of ISCRE conference abstracts, *Henrik Grénman, Tapio Salmi*

Evaluation of proposals in the EU H2020 Marie-Sklodowska-Curie Actions-IF-2017, *Z. Boeva*

Evaluator of research proposal for ARRS Slovenian Research Agency, Latvian Council of Science, Belgian Fund for Scientific Research (FNRS), Quatar National Research Fund, *Reko Leino*

Evaluator of research proposals/member of evaluation panels for FCT Fundacao para a Ciencia e a Tecnologia (Portugal), ARRS Slovenian Research Agency, Latvian Council of Science, European Research Council (ERC), Belgian Fund for Scientific Research (FNRS), *Reko Leino*

Referee, ERC Starting Grant, *Dmitry Murzin*

Reviewer for application of Associate senior lecturer in wood material science and engineering, Swedish University of Agricultural Sciences, 2018, *Anna Sundberg*

Vice-chair and independent observer tasks for the EU Research Executive Agency (REA), *Reko Leino*

Vice Chair of H2020-MSCA-ITN-2018 evaluation panel and final evaluation of two FP7-MC-ITN projects for EU Research Executive Agency (REA), *Reko Leino*

Doctoral thesis evaluations

Camacho, A. R., University of Valladolid, reviewer, *Dmitry Murzin*

Gallina, S. Gianluca, Universidad de Valladolid, tribunal member, 2018, Jyri-*Pekka Mikkola*

Goldmann Valdes, Werner, University of Oulu, reviewer, 2018, *Stefan Willför*

Hantzlik (geb. Müller) Anne, Technische Universiteät Dresden, opponent, 2018, *Tapio Salmi*

Ibanez Abad, Javier, Université de Lille, reviewer, 2018, *Dmitry Murzin*

Jaatinen Salla, Aalto University, reviewer, 2018, *Päivi Mäki-Arvela*

Jarvis, Jennifer, University of Memphis USA, opponent, 2018*, Johan Bobacka*

Keskiväli, Juha, University of Helsinki, opponent, 2018, *Leino Reko*

Lauberts, Māris, University of Latvia, Latvia, opponent/reviewer 2018, *Andrey Pranovich*

Paunovic Vladimir, ETH Zurich, 2018*, Dmitry Murzin*

Quesada Sanchez Jorge, University of Oviedo, 2018, *Dmitry Murzin*

Sanchez Álvaro Cabeza, Universidad de Vallidolid, 2018, *Dmitry Murzin*

Swärd, Antonia, KTH, Sweden, opponent, 2018, *Stefan Willför*

Urmes, Caroline, Université de Toulouse ENSIACET, opponent, 2018*, Tapio Salmi*

Xiao Huang, Uppsala University, evaluation committee member, 2018, *Tom Lindfors*

7.5 Editorial Boards

Catalysis today, editorial board member, *Dmitry Murzin*

Catalysis for Sustainable Energy, editorial board member, *Dmitry Murzin*

Chemistry of Plant Raw Material (KHIMIIA RASTITEL'NOGO SYR'IA), editorial board member, *Andrey Pranovich, Bjarne Holmbom*

Bio-Byword Scientific Publishing Pty Ltd (Journal of Electronic Research and Application). Editorial board member, *Fiseha Tesfaye*

Bulletin of Chemical Reaction Engineering and Catalysis, region. edit. for Europe, *Dmitry Murzin*

Bulletin of St. Petersburg State Institute of Technology, editorial board member, *Dmitry Murzin*

Catalysis in Industry, Associate editor and editorial board member, *Dmitry Murzin*

Catalysis Letters, scientific advisory board, editorial board member, *Dmitry Murzin*

Cellulose Chemistry and Technology, editorial board member, *Bjarne Holmbom, Stefan Willför*

Chemosensors (MDPI), Editorial Board member, *Johan Bobacka*

Current Catalysis, editorial board member, *Dmitry Murzi*n

Current topics in electrochemistry (Research Trends), Editorial Board member, *Johan Bobacka*

Electroanalysis, editorial advisory board member, *Andrzej Lewenstam*

Electrochimica Acta (Elsevier), Editorial Advisory Board member, *Johan Bobacka*

Foundations of Science, editorial advisory board member, *Andrzej Lewenstam*

Frontiers in Chemistry, Green and Environmental Chemistry, editorial board member, *Jyri-Pekka Mikkola*

Holzforschung, editorial board member, *Bjarne Holmbom, Stefan Willför*

International Journal of Chemical Engineering, editorial board member, *Dmitry Murzin*

Izvestija Sankt-Peterburgskoj Lesotehnicheskoj Akademii, editorial board member, *Andrey Pranovich*

Jacobs Journal of Materials Science, editorial board member, *Andrey Pranovic*h

Journal of Engineering, editorial board member, editorial board member, *Dmitry Murzin*

Journal of Elementology, co-editor, *Andrzej Lewenstam*

Journal of Elementology, editorial board member, *Tomasz Sokalski*

Journal of Wood Chemistry and Technology, editorial board member, *Stefan Willför*

Kinetics and Catalysis, editorial board member, *Dmitry Murzin*

Magnesium Research, editorial advisory board member, *Andrzej Lewenstam*

Nordic Pulp and Paper Research Journal, member of editorial board, *Anna Sundberg,* member of scientific advisory board*, Stefan Willför*

O´Papel, editorial board member, *Bjarne Holmbom*

Philosophy of Science, editorial advisory board member, *Andrzej Lewenstam*

Progress in Industrial Ecology, editorial board member *Jyri-Pekka Mikkola*

Russian Journal of Chemical Industry, editorial board member, *Dmitry Murzin*

Sensing and Bio-Sensing Research (SBSR), editorial advisory board member, *Tom Lindfors*

Sensors, editorial advisory board member, *Andrzej Lewenstam*

Sensors and Actuators B: Chemical (Elsevier), Editor, *Johan Bobacka*

The Open Catalysis Journal, *Dmitry Murzin*

Topics in Catalysis, scientific advisory board, *Dmitry Murzin*

Wood Science and Technology, editorial board member, *Bjarne Holmbom*

Member of of scientific committees and boards

2nd International Conference and Exhibition on Materials & Engineering, Nov 19-21, 2018, San Diego, USA. A member of the organizing committee, *Fiseha Tesfaye*

25th International Symposium of Chemical Reaction Engineering (ISCRE), Firenze, member of scientific committee, *Tapio Salmi*

Academy of Finland, Research Council for Natural Sciences and Engineering (2016-18), *Reko Leino*

CHISA 2018, Prague, Member of the scientific committee *Tapio Salmi*

Czech Academy of Sciences, Institute of Chemical Process Fundamentals, member of international advisory board, *Tapio Salmi*

CAMURE&ISMR, member of scientific committee*, Tapio Salmi*

Bio4Energy research programme (Swedish government) 2009- (www.bio4energy.se), Steering Group member *Jyri-Pekka Mikkola*

Biocity Turku Research Programme: Diagnostics Technologies and Applications Programme, Board member (vice director), 2018- *Johan Bobacka*

Biocity Turku SmartBio research programme "Advanced Bioresources and Smart Bioproducts – Towards Sustainable Bioeconomy", Vice-chair, *Stefan Willför*

Biofuel Technology Center (www.btk.slu.se), SLU, (Sweden), scientific advisory board member*, Jyri-Pekka Mikkola*

Biorefinery of the Future 2008- (www.bioraffinaderi.se). RISE PROCESSUM AB, Member of the Research & Development Council, *Jyri-Pekka Mikkola*

Chemical Industry, "Kemianteollisuuden tieteellinen neuvottelukunta", Kemianteollisuus ry, scientific advisory board member, *Stefan Willför*

The Chemistry Club "Kemistklubben vid Åbo Akademi r.f.", president, *Johan Bobacka*

Delft Process Technology Institute (DPTI), TU Delft, member of international advisory board, *Tapio Salmi*

Erasmus Mundus Joint Master Degree Programme "EACH – Excellence in Analytical Chemistry", academic board member, *Johan Bobacka*

ERC Consolidator Grant, panel member, *Dmitry Murzin*

EU COST action FP1306, Deputy Member of the Management Committee, *Stefan Willför*

GlucoModicum Oy, Board member, scientific advisor & co-founder of the start-up company, *Johan Bobacka*

Industrial Biotechnology Cluster Finland (IBC Finland), board member, *Stefan Willför*

Institute of Human Rights, ÅAU, board member, *Stefan Willför*

International Conference of Chemical Technology 2016, Member of the scientific committee, Mikulov, Czech Republic, *Dmitry Murzin*

International Conference on the Impact of Fuel Quality on Power Production and the Environment, Executive committee member, *Maria Zevenhoven*

National Bioeconomy, Panel member appointed by the Ministry of Employment and the Economy, *Stefan Willför*

National Research Infrastructure Committee (TIK) (2018), *Reko Leino*

Publication Forum (JUFO) Panel 4 (Chemistry), board member, 2014-2017 *Anna Sundberg*, 2018- *Johan Bobacka*

Research Ethics of ÅAU, board member, *Stefan Willför*

Renewable Resources: Chemistry, Technology, Medicine, International conference in St. Petersburg Russia, scientific advisory board member, *Stefan Willför*, co-chairman and co-organizer, *Andrey Pranovich*

Shareholder Forum and in the Bioeconomy task force for Clic Innovation Ltd, ÅAU representative, *Stefan Willför*

SpinChem AB, Scientific advisory board, *Jyri-Pekka Mikkola*

The Vasa Ship Preservation, member of council, Sweden, *Bjarne Holmbom*

Recycling and Environmental Technologies and Professional Development Committees, TMS - The Minerals, Metals & Materials Society, member of committee, *Fiseha Tesfaye*

Walter Ahlströms foundation, 2018-, Board member, *Anna Sundberg*

8. External interactions 2019

8.1 Organization of conferences/courses/meetings 2019

5th International Congress on Catalysis for Biorefineries – CatBior2019
23.9-27.9.2019, Turku/Åbo (200 participants) www.catbior2019.fi

EACH Winter School, 21–25 January, 2019, Åbo Akademi University, Turku/Åbo

HemiH2 Business Finland project, Final seminar, 10.10. 2019, Turku/Åbo

Nordic Flame Days 2019: 28-29 August; Turku/Åbo

SmartBio Student Symposium, 12.6.2019, Forum Marinum, Turku/Åbo

SmartBio Annual Meeting, 29.10.2019, Auriga Business Center, Turku/Åbo

Summer school in Industrial Chemistry and Reaction Engineering, June 2019, Pargas

Reaction kinetics, International postgraduate course, December 2019, Turku/Åbo

8.2 Visits and visitors

Visits

Joon, Narender Kumar, Malmö University, Sweden, December 2019

Ona, Jay-Pee, TU Delft, The Netherlands, April – July 2019, 3.5 months

Lisak, Grzegorz, Malmö University, Sweden, February 2019

Pranovich, Andrey, St. Petersburg Forest Technical University, Faculty of Chemical Technology and Biotechnology, Russia, January- April 2019, 4 months

Salmi, Tapio, Universitá di Napoli, Chemical Sciences, November 2019, two weeks

Sokalski, Tomasz, The University of Warsaw Biological and Chemical Research Centre (CNBCh UW), Poland, March 2019

Tesfaye, Fiseha, Central South University, Changsha, China, December 2019

Visitors

Alipoormazandarani, Niloofar (PhD candidate), Lakehead University, Canada September – December 2019

Badazhkova, *Veronika*, St. Petersburg State Chemical and Pharmaceutical University, Russia, August-September, 2 months

Bertrand, Emilie, ENSCR Rennes, France, May – August, 3.5 months

Binta, Sylla, Normandie Université INSA-Rouen, France, June – September, 3 months

Bois, Adelina, Sigma Clermont engineering school, France, May – September 2019

Cai, Xiaoshuang (PhD candidate), Normandie Université INSA-Rouen, France, January – March, 2.5 months

Choucard, Theo, Normandie Université INSA-Rouen, France, June – September, 3 months,

Demesa, Abayneh (Postdoc), Lappeenranta University of Technology, Finland, April – June, 3 months, ***Johan Gadolin Scholarship***

Eliason, Felicia (PhD candidate), Chalmers University of Technology, Sweden, January – July, 7 months, ***Johan Gadolin Scholarship***

El Hajam, Maryam (PhD candidate), University of Sidi Mohamed Ben Abdelah, Morocca, 28/08/2019-28/04/2020

Galasheva, Sofia, St. Petersburg State Chemical and Pharmaceutical University, Russia, January 2019-September 2019, 9 months

Glazacheva, Ekaterina, ITMO University, Russia, 10-22.11.2019

Gusev, Konstantin, laboratory engineer, Saint Petersburg State Chemical Pharmaceutical University, Russia, 10-22.11.2019, 2 weeks

Hachhach, Mouad (PhD candidate), Essaadi University, Tangier, Morocco, 1.10-31.12.2019, 3 months, ***Johan Gadolin Scholarship***

Hambly, Bradley, University of Memphis, USA, September – December 2019, 4 months, ***Johan Gadolin Scholarship***

Herrera, René, Universidad del País Vasco, San Sebastian Spain, March – May 2019

Herrero Manzano, Maria, University of Valladolid, August-December 2019

Hichem, Zergane, visiting scientist, USTHB University, Algeria, 28.11.2019 – 31.12.2019, 1 month

Ivanko, Iryna, Charles University, Institute of Macromolecular Chemistry, Czech Republic, September – November 2019

Junghans, Paula, Technische Universität Dresden (TUD), Germany, January – April, 3.5 months

Kalinichev, Andrey, Saint Petersburg State University – June 2019

Kong, Yi, Qingdao University of Science and Technology, China 21.11.2019 – 21.01.2020

Lahaye, Alexia, ENSCR Rennes, France, May – August, 3.5 months

Laluc, Mathias, ENSICAEN, France, May – August, 3.5 months

Li-Zhulanov, Nikolai, Novosibirsk State University, Russia, January – April, 3 months

Long, Li, Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, China, February – July 2019, 5 months

Lu, Xiaojia, Normandie Université INSA-Rouen, France, February – December, 11 months

Makaruk, Roman, Associate Professor, Saint-Petersburg State Institute of Technology, Russia, 10 – 22.11.2019, 2 weeks

Mazri, Sandra, Université de Boumerdes, Algeria, February – May 2019, 3 months

Niidu, Allan, Tallinna Tehnika Ülikool (TalTechcal), Estonia, June - September, 2 months

Perez Sena, *Wander*, Normandie Université INSA-Rouen, France, February – August, 7 months

Pizzolitto, Cristina, Ca' Fostari University of Venice, Italy, February – May, 3.5 months

Razat, Theophile, Normandie Université INSA-Rouen, France, June – September, 2.5 months

Riabukhin, Dmitry, Saint-Petersburg State Forest Technical University, Russia, August – December, 5 months, *Academy of Finland mobility programme*

Rutkowska, Marcelina, MSc student, Erasmus University of Warsaw, Poland, September – December 2019, 4 months

Saar, Indrek, University of Tartu, Estonia, February – May 2019, 4 months

Schindler, Tamara, University of Stuttgart, Germany, April – June 2019, 3 months

Sidorenko, Alexander, Institute of Chemistry of New Materials of National Academy of Sciences of Belarus, Minsk, October, 1 month

Souza de Oliveira, Adriana, Autonomous University of Madrid, Spain, September – December, 4 months

Suerz, Rossana, Università di Padova, Italy, February – August, 7 months

Tan, Liping, Qilu University of Technology, China September – December 2019, 4 months

Terenteva, Oksana, Saint Petersburg State Chemical Pharmaceutical University, Russia, 10 – 22.11.2019

Torozova, Alexandra, Tver Technical University, Russia, September, 1 month

*Trajano, Heathe*r, visiting professor, University of British Columbia, Vancouver, Canada, June – December, 6 months, *Åbo Akademi Mobility Programme*

Weckessen, Stephanie, Technische Universität Dresden (TUD, Germany, August – December, 4.5 month

Xu, Huanfei, Quingdao University of Science and Technology, China, January – February, 2 months, ***Johan Gadolin Scholarship***

Yang, Xiaodeng, Qilu University of Technology, November – December 2019, 1.5 months

Yin, Tanji, Yantai Institute of Coastal Zone Research, China, August – November 2018, ***Johan Gadolin Scholarship***

Zhang, Xuliang, Al-Farabi Kazakh National University, Kazakhstan, October-November, 1.5 months

8.3 External evaluations and reviews

External evaluations

European Science Foundation, post-doctoral project evaluations, *Narendra Kumar*

Evaluator of research proposal for ARRS Slovenian Research Agency, Latvian Council of Science, Belgian Fund for Scientific Research (FNRS), Qatar National Research Fund, *Reko Leino*

Vice-chair and independent observer tasks for the EU Research Executive Agency (REA), *Reko Leino*

Panel member for ERC Consolidator Grant, *Dmitry Murzin*

Expert, Haldor Topsoe PhD scholarship programme, *Dmitry Murzin*

Evaluation of research proposals, EU H2020, Brussels, *Päivi Mäki-Arvela*

Evaluation of research proposal for The Czech Science Foundation, *Ari Ivaska*

Evaluation of research proposal for the National Commission for Scientific and Technological Research (CONICYT), *Ari Ivaska*

Evaluation of research proposals, Slovakia, *Päivi Mäki-Arvela*

Evaluation of research proposals, Fonds de la Recherche Scientifique - FNRS, Belgium, *Päivi Mäki-Arvela*

Evaluation of research proposals in Catalan, Spain, *Päivi Mäki-Arvela*

Evaluation of research proposals, EU H2020-WIDESPREAD-2020-5, 2019, *Rose-Marie Latonen*

Doctoral thesis evaluation

Akuamesu Assoah, Benedicta, Tampere University, reviewer, 2019, *Reko Leino*

Carlson, Annika, KTH Royal Institute of Technology, reviewer, 2019, *Rose-Marie Latonen*

Espensen, Anne Leth, Technical University of Denmark, examiner/opponent, 2019, *Oskar Karlström*

Negin, Amini, Monash University, reviewer, 2019*, Tapio Salmi*

Salminen, Kalle, Aalto University, pre-examiner, 2019, *Johan Bobacka*

Tang, Zhenchen, University of Groningen, reviewer, *Dmitry Murzin*

Ulsamin, *Evgeny,* Eindhoven University of Technology, reviewer, *Dmitry Murzin*

Urmes, Caroline, Université de Toulouse, ENSIACET, reviewer and opponent, *Tapio Salmi*

Verteramo, Luisa Maria, University of Uppsala, thesis committee, 2019, *Reko Leino*

Vet, Tapoi, Vallidolid, Spain, opponent, 2019, *Johan Wärnå*

8.4 Editorial boards

Bulletin of Chemical Reaction Engineering and Catalysis, regional editor for Europe, *Dmitry Murzin*

Bulletin of St. Petersburg State Institute of Technology, editorial board member, *Dmitry Murzin*

Catalysis for Sustainable Energy, editorial board member, *Dmitry Murzin*

Catalysis in Industry, Associate editor and editorial board member, *Dmitry Murzin*

Catalysis Letters, scientific advisory board, editorial board member, *Dmitry Murzin*

Catalysis Today, editorial board member, *Dmitry Murzin*

Cellulose Chemistry and Technology, editorial board member, *Bjarne Holmbom, Stefan Willför*

Chemistry of Plant Raw Material (Khimiia Rastitel'nogo Syri'a), editorial board member, *Andrey Pranovich, Bjarne Holmbom*

Chemosensors, editorial board member, *Johan Bobacka*

Current topics in electrochemistry, editorial board member, *Johan Bobacka*

Electroanalysis, editorial advisory board member, *Andrzej Lewenstam*

Electrochimica Acta, editorial advisory board member, *Johan Bobacka*

Foundations of Science, editorial advisory board member, *Andrzej Lewenstam*

Frontiers in Chemistry, Green and Environmental Chemistry, editorial board member, *Jyri-Pekka. Mikkola*

Frontiers in Chemical Engineering, Chemical Reaction Engineering, Associate Editor, *Henrik Grénman*, *Pasi Tolvanen*

International Journal of Chemical Engineering, editorial board member, *Dmitry Murzin*

Holzforschung, editorial board member, *Bjarne Holmbom, Stefan Willför*

Izvestija Sankt-Peterburgskoj Lesotehnicheskoj Akademii, editorial board member, *Andrey Pranovich*

Jacobs Journal of Materials Science, editorial board member, *Andrey Pranovic*h

Journal American Chemical Engineering, Science Publisher, editorial board member, *Narendra Kumar*

Journal Catalysts, MDPI, Basel, Switzerland, editorial board member, *Narendra Kumar*

Journal of Elementology, co-editor, *Andrzej Lewenstam*

Journal of Elementology, editorial board member, *Tomasz Sokalski*

Journal of Engineering, editorial board member, editorial board member, *Dmitry Murzin*

Journal of Waste and Biomass Valorization, Springer, editorial board member, *Narendra Kumar*

Journal of Wood Chemistry and Technology, editorial board member, *Stefan Willför*

Kinetics and Catalysis, editorial board member, *Dmitry Murzin*

Magnesium Research, editorial advisory board member, *Andrzej Lewenstam*

Nordic Pulp and Paper Research Journal, member of editorial board, *Anna Sundberg,* member of scientific advisory board*, Stefan Willför*

O´Papel, editorial board member, *Bjarne Holmbom*

Philosophy of Science, editorial advisory board member, *Andrzej Lewenstam*

Progress in Industrial Ecology, editorial board member, *Jyri-Pekka Mikkola*

Russian Journal of Chemical Industry, editorial board member, *Dmitry Murzin*

Sensing and Bio-Sensing Research, editorial advisory board member, *Tom Lindfors*

Sensors, editorial advisory board member, *Andrzej Lewenstam*

Sensors and Actuators B: Chemical, co-editor, *Johan Bobacka*

Sensors and Actuators Reports, editorial advisory board member, *Tom Lindfors*

The Minerals, Metals & Materials Society. A member of the Recycling and Environmental Technologies, Professional Development, and Mathewson Leadership IOMMehl-Mehl Awards Committees, *Fiseha Tesfaye*

The Open Catalysis Journal, editorial board member, *Dmitry Murzin*

Topics in Catalysis, scientific advisory board, *Dmitry Murzin*

Wood Science and Technology, editorial board member, *Bjarne Holmbom*

Member of committees and boards

Baltic University Programme, board member, *Tapio Salmi*

Biocity Turku Research Programme: Diagnostics Technologies and Applications Programme, vice director, *Johan Bobacka*

Biocity Turku Research Programme: Advanced Bioresources and Smart Bioproducts Programme, vice director, *Henrik Grénman*

Catalysis in Multiphase Reactors & International Symposium on Multifunctional Reactors (CAMURE 11), Milan, Member of scientific committee, *Tapio Salmi*

CatBior 2019, Turku/Åbo, Chairperson of the scientific committee, *Dmitry Murzin, Jyri-Pekka Mikkola*

Delft Process Technology Institute (DPTI), International Programme Committee, *Tapio Salmi*

EFC Working Party 3: Corrosion by Hot Gases and Combustion Products, Vice-Chairman, *Juho Lehmusto*

Erasmus Mundus Joint Master Degree Programme "EACH – Excellence in Analytical Chemistry", academic board member, *Johan Bobacka*

European Chemical Society (EuChemS), Division of Analytical Chemistry (DAC), delegate, *Johan Bobacka*

Finnish Catalysis Society, Chairman, *Henrik Grénman*

GlucoModicum Oy, co-founder, senior scientific advisor, member of the board of directors, *Johan Bobacka*

GlucoModicum Oy, co-founder, sensor lead, *Zhanna Boeva*

Institute of Chemical Process Fundamentals, Czech Academy of Sciences, member of international advisory board, *Tapio Salmi*

International Conference on the Impact of Fuel Quality on Power Production and the Environment, Executive committee member, *Maria Zevenhoven*

International Symposium on Chemical Reaction Engineering (ISCRE), New Delhi 2020, Member of scientific committee, *Tapio Salmi*

JOM: The Journal of the Minerals, Metals & Materials Society. Advisory Committee member, *Fiseha Tesfaye*

Mechanisms of Catalytic Reactions-XI, Sochi, Russia, Member of scientific committee *Dmitry Murzin*

Nordic Catalysis Society, board member, *Henrik Grénman*

Nordic Symposium on Catalysis 2020, member of organizing committee, *Henrik Grénman, Tapio Salmi*

Publication Forum (JUFO) Panel 4 (Chemistry), member, *Johan Bobacka*

Research Council for Natural Sciences and Engineering (2019-21), Academy of Finland, chair of the council, *Reko Leino*

TMS - The Minerals, Metals & Materials Society, Recycling and Environmental Technologies, Professional Development, and Mathewson Leadership IOMMehl-Mehl Awards Committee member, *Fiseha Tesfaye*

The National Research Infrastructure Committee (TIK) (2019), member of the council, *Reko Leino*

Turku Future Technologies (TFT), chair of steering group, *Tapio Salmi*

9. Ongoing doctoral theses at PCC

Aalto-Setälä, Laura (MSc 2014, University of Helsinki), Gradient-Structured Bio-Engineered Implant Surfaces, FINLAND

Ahamed, Ashiq (MSc 2012, Nanyang Technological University), Material Characterization and Ecotoxicity Assessment of Spent Nanomaterial in Marine Ecosystem, SINGAPORE

Akhmetzyanova, Uliana, (MSc 2013, Tver Technical University & MSc 2015, Åbo Akademi University), Hydroconversion of Biomass Derivatives over Heterogeneous Catalytic Systems Based on Transition Metal Carbides, Nitrides, and Phosphides, RUSSIA

Alvear, Matias (MSc 2019, Politecnico di Milano), Kinetics, Mechanism and Reactor/Catalyst Technology for Epoxidation Reactions, CHILE.

Arroyo Condori, Jesús (MSc 2011, Åbo Akademi University), Electrochemically Controlled Chromatographic Separations, PERU

Balint, Roland (MSc 2018, Technische Universität München), Ash Deposit Aging in Combustion of Biomass GERMANY

Behravesh, Erfan (MSc 2014, Åbo Akademi University), Millistructured Flow Chemistry for Oxidation Processes of Molecules from Biomass IRAN (defended 06.03.2020)

Bruun, Nina (MSc 1984, Åbo Akademi University), Challenge of Bio-Oil in Marine Engines FINLAND

Delgado, Jose Emilio (MSc 2019, INSA-Rouen), Production of γ-Valerolactone – a Green Platform Molecule, double-degree with INSA-Rouen DOMINIC REPUBLIC

Dirbeba, Meheretu Jaleta (MSc 2013, Addis Ababa University), Characterization of Biomass-Containing Industrial Byproducts for Thermochemical Conversion ETHIOPIA

Freites, Adriana (MSc 2015, University of Simon Bolivar), Epoxidation of Vegetable Oils under Microwave Irradiation, Process Intensification for Biomass Conversion VENEZUELA (defended 15.01.2020)

Han, Tingting (MSc 2008, Åbo Akademi University), Novel Signal Readout Principle for Solid-Contact Ion-Selective Electrodes CHINA

Heberlein, Stefan (MSc 2020, Technische Universität München), Energy and Resource Recovery from Waste Using High-Temperature Slagging Gasification GERMANY

Hu, Liqiu (MSc 2019 Tianjin University of Science & Technology), Application of Nanocellulose in Packaging and Bioplastics CHINA

Hupa, Elisa (MSc 2014, Åbo Akademi University), New Approach to Determine Initial Melting of Corrosive Deposits FINLAND

Jogi, Ramakrishna (MSc, 2010, Gitam University, India), An Integrated Process for the Production of Green Aviation Fuel Range Cycloalkanes Through Hydrothermal Liquefaction of Lignocellulosic Biomass INDIA

Joon, Narender (MSc 2016, Åbo Akademi University), Continuous Dynamic Extraction and On-Line Determination of Metals from Solid Environmental Samples INDIA

Keim, Arturo (MSc 2019, Åbo Akademi University), Black liquor Concentration Fouling in Pilot and Industrial Scale CHILE

Kholkina, Jekaterina, MSc 2017, Åbo Akademi University), Synthesis of Value-Added Products from Residual Materials: a Green Approach for the Sustainable Development of Novel Catalytic Materials for Biomass Valorization RUSSIA

Kronberg, Thomas (MSc 1993, Åbo Akademi University), The Properties of Raw glazes - Impact of Composition, Firing and Functional Coatings FINLAND

Kråkström, Matilda (MSc 2015, Åbo Akademi University), Evaluation of Advanced Oxidation Processes for Removal of Antibiotics in Wastewater Treatment Plants FINLAND

Korotkova, Ekaterina (MSc 2011, Åbo Akademi University), Mild-Alkaline Extraction of Spruce Lignin and its Applications RUSSIA

Kortesmäki, Ewelina (MSc 2013, University of Gdansk), Occurrence and Fate of Antibiotics in Wastewater, Wastewater Treatment Plants and Recipient Waters POLAND

Lagerquist, Lucas (MSc 2011, Åbo Akademi University), Exploring the Structure and Reactivity of a Novel Type of Pressurized Hot Water Extracted Lignin FINLAND

Lassfolk, Robert (MSc 2018, Åbo Akademi University), Acyl Migration in Mono-, Oligo- and Polysaccharides FINLAND

Li, Na (MSc 2007, Åbo Akademi University), High-Temperature Corrosion of Ceramics in Biomass Combustion CHINA

Liu, Riu (MSc 2019, Tianjin University of Science & Technology), Exploitation of Lignocellulosic Nanomaterial as Ink Components in 3D Bio printing for Drug Delivery Therapeutics and Tissue Engineering Applications CHINA

Lu, Xiaojia (Msc 2017, Chang´an University), Reductive Fractionation of Lignin with Heterogeneous Catalysts, double-degree with INSA-Rouen CHINA

Lund, Sara (MSc 2013, Åbo Akademi University) Liquid-Phase Exfoliation of Finnish Flake Graphite in Cellulose Nanocrystals and Preparation of Electrically Conducting Composite Films for Sensor Applications FINLAND

Martínez-Klimov, Mark (MSc 2018, Universidad Nacional Autónoma de México), Selective Hydroconversion of Renewable Feedstock into Aviation Fuel MEXICO

Mattsson, Ida (MSc 2015, Åbo Akademi University), Smart Materials from Sweet Molecules: Self-Assembling Polyols Derived from Mannose FINLAND

Medina, Ananias, (MSc 2015, Simon Bolivar University), Development of New Gas-Liquid Reactor Technology, VENEZUELA

Najarnezhasmashhadi, Ali (MSc 2015, Åbo Akademi University), Development of New Structured Catalyst and Reactor Technologies for Biomass Conversion IRAN

Oña, Jay Pee (MSc 2018, Åbo Akademi University), From Fossil to Biohydrogen in Finnish (bio) Industry - Utilizing Electrocatalysis in Aqueous Phase Reforming of Hemicelluloses, double-degree with TU Delft PHILIPPINES

Pérez-Sena, Wander (MSc, Normandie Université INSA Rouen), Green and Safe Production of Monomers from CO_2 and Biomass Feedstock, double-degree with INSA-Rouen DOMINICAN REPUBLIC

Reinsdorf, Ole (MSc, 2018, Rostock Universität LIKAT) Direct Synthesis of Hydrogen Peroxide: Understanding of the Mechanism with Transient Studies, GERMANY

Rendon, Sabine (MSc 2011, Åbo Akademi University), Dyes in Dye-Sensitized Solar Cells FINLAND

Runeberg, Patrik (MSc 2014, Åbo Akademi University), Selective Oxidation of Unprotected Carbohydrates, Polyols and Phenolic Compounds from the Biorefinery Feedstock FINLAND

Saeid, Soudabeh (MSc 2015, Islamic Azad University Tabriz), Elimination of Pharmaceutical Products from Waste Water by Ozonation and Heterogeneous Catalysis - a Systematic Kinetic and Reaction Engineering Approach towards New Technology IRAN (defended 16.03.2020)

Saleem, Farhan (MSc 2013, Åbo Akademi University), Furfural Valorization by H_2O_2: Synthesis of Green Dicarboxylic Acids PAKISTAN

Santochi, Paulo (MSc 2012, Åbo Akademi University), Mathematical Modelling of Nitrogen Oxide Formation in Black Liquor Combustion BRAZIL

Schmid, Daniel (MSc 2019, Åbo Akademi University), Valorization of Biomass Ashes from Power Plants – Towards a Circular Economy, GERMANY

Schmidt, Christoph (MSc 2019, Rostock Universität LIKAT), Transient Studies of Catalytic Three-Phase Reactions, GERMANY

Sevonius, Christoffer (MSc 2012, Åbo Akademi University) Agglomeration Studies in a Laboratory Bubbling Fluidized Bed in Conditions Typical for Biomass and Agrofuel Firing FINLAND

Shumilov, Vladimir (MSc 2014, Åbo Akademi University and Tver State Technical University), Development of Structured Reactors for Transformation of Biomass Components to High-Value Products: Green Process Intensification RUSSIA

Siekkinen, Minna (MSc 2019, Åbo Akademi University), Interaction Between Bio-Active Glass and Bio-Degradable Polymers, FINLAND

da Silva Correia, Leolincoln (MSc 2016, IFP School, France), Health-Promoting Components and Food Additives from Biomass - an Intensified Chemical Engineering Approach, BRAZIL

Sinitsyna, Polina (MSc 2018, Åbo Akademi University), Novel Understanding of Dissolution Kinetics of Bioactive Glasses RUSSIA

Stiller, Adrian (MSc 2019, Universität Ulm), The Impact of Fluid-Flow Rate of Dissolution of Bioactive Glasses GERMANY

Tomasso, Cogliano (M.Sc. Università di Napoli 'Federico II' 2019), Vegetable Oils Epoxidation: From Batch to Continuous Process, double-degree with Università di Napoli 'Federico II', ITALY

Viertiö, Tyko, (MSc 2019, Aalto University) Catalytic Hydrodeoxygenation of Bio-Oil Feed to Transportation fuel FINLAND

Viswamoorthy, Raju (MSc 2004, Annamalai University), CFD-Modelling of Fly Ash Deposition and Deposit Build-Up Dynamics in Upper Furnaces of Black Liquor Recovery Boilers INDIA

Vucetic, Nemanja (MSc 2013, Belgrade University), Preparation of Valuable Organic Chemicals from Homogeneous Catalysis to SILCA and Batch to Continuous Technology SERBIA

Wang, Luyao (MSc 2018, Qingdao Institute of Bioprocess and Bioenergy Technology, Chines Academy of Science, China), Characterization and Modification of Technical Lignin for Sustainable Lignin-Based Wood Adhesive Synthesis, CHINA

Wang, Qingbo (MSc 2018, Kunming University of Science and Technology, China), 3D Bioprinting of Lignocellulosic Nanomaterials and Wood Polysaccharides in Biomedical Applications, CHINA

Yrjänä, Ville (MSc 2018, Åbo Akademi University), Developing Potentiometric Ion-Selective Electrodes for Anions, FINLAND

Zhang, Yongchao (MSc 2015, Qilu University of Technology), Development of a Novel Biomass Fractionation Approach Using Performic Acid Hydrolysis towards Integrated Lignocellulosic Biorefinery, CHINA (defended 14.02.2020)

Zhang, Weihua (MSc 2017, Ocean University of China), Constructing Nanocellulose-Based Advanced Functional Materials for Pollutant Removal in Industrial Waste Waters, CHINA

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