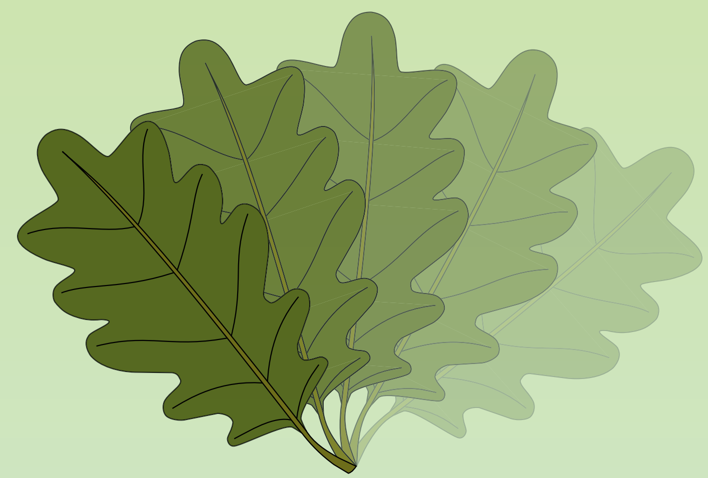
Åbo Akademi
University

Painosalama Oy | Turku/Åbo, Finland 2022

Johan Gadolin Process Chemistry Centre | Report 2020–2021

Åbo Akademi
University
Science and
Engineering

# Report 2020–2021



# Johan Gadolin
## Process Chemistry Centre

# Johan Gadolin
# Process Chemistry Centre

at

Åbo Akademi University

Report 2020-2021


Edited by

Pasi Tolvanen,
Johan Bobacka, Patrik Eklund, Rose-Marie Latonen,
Päivi Mäki-Arvela, Anna Sundberg, Johan Werkelin



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# The Book Editors

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PCC logo: Linus Silvander
Painosalama, Turku/Åbo
2022

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# 1. Overview of PCC activities in 2020-2021

## 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 **mission of *PCC*** is 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***". All our activities are guided by our **fundamental values**, which are:

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

***PCC*** continues a successful tradition of more than 100 years of chemical engineering at Åbo Akademi University. We have 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. Mitigation of the climate change requires defossilisation of industry via innovative process chemistry and technology. Our current research activities include refinement of renewable biomass to chemicals, fuel components and novel bio-based materials, clean energy technology, circular economy, process intensification and on-line chemical analysis. We are committed to promote renewable and clean energy, sustainable industrial production, health and well-being.

The research activities at ***PCC*** are closely integrated with three profiling areas at Åbo Akademi University, *i.e. Technologies for a Sustainable Future (TSF), Solutions for health,* and *The Sea*. For example, Henrik Grénman started as a tenure track professor at *TSF* and is now a full professor at ***PCC***. We participate in several BioCity Turku research programmes and we have close collaboration with TechCampus Turku. Our interactions with society and industry are supported by our *Forum for Society*.

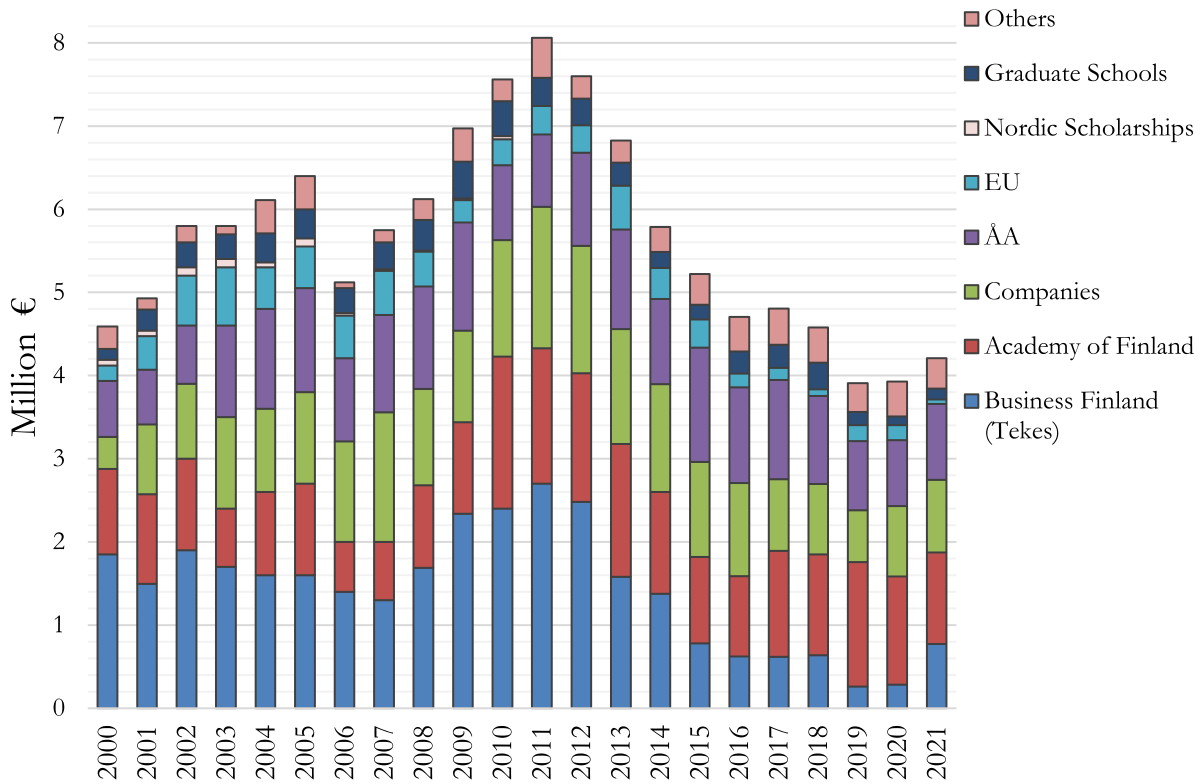
A recent benchmarking of the overall (total) scientific publications of the seven professors at ***PCC*** shows an *average* of 312 publications/person and an *average* personal h-index of 39. To this should be added the scientific achievements of our associate professors, senior researchers, post-doctoral researchers, teaching staff, doctoral students, etc. Thanks to our dedicated personnel and collaborators, ***PCC*** has the critical mass to make a large scientific impact globally.

***PCC*** and its members are continuously applying for external funding, which ensures continuation of our research activities. In this report we highlight some of our achievements during the years 2020 and 2021 (1.1.2020–31.12.2021).

## The years 2020-2021 in numbers

In 2020-2021, more than 150 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 2020-2021 were the Academy of Finland, Åbo Akademi University, Companies and Business Finland.

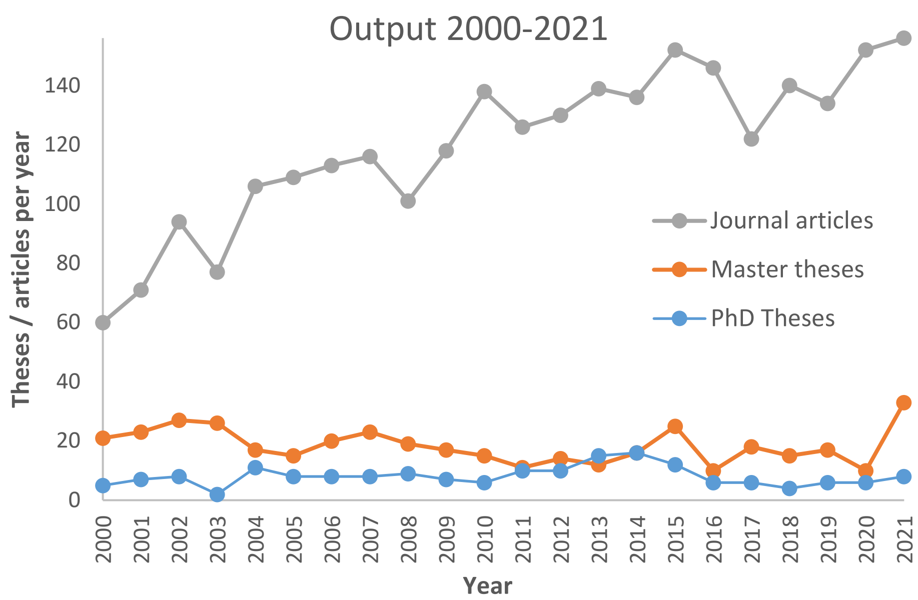



*The funding of the Johan Gadolin Process Chemistry Centre 2000-2021*

From the academic point of view, the years 2020-2021 were productive. The table and figure below show the number of theses and peer-reviewed publications from ***PCC*** since the year 2000. The number of theses show some yearly fluctuations, while the number of peer-reviewed articles are steadily increasing since 2000.

| | 2000 | 2001 | 2002 | 2003 | 2004 | 2005 | 2006 | 2007 | 2008 | 2009 | 2010 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Doctoral Theses** | 5 | 7 | 8 | 2 | 11 | 8 | 8 | 8 | 9 | 7 | 6 |
| **Master's Theses** | 21 | 23 | 27 | 26 | 17 | 15 | 20 | 23 | 19 | 17 | 15 |
| **Journal Articles** | 60 | 71 | 94 | 77 | 106 | 109 | 113 | 116 | 101 | 118 | 138 |
| | **2011** | **2012** | **2013** | **2014** | **2015** | **2016** | **2017** | **2018** | **2019** | **2020** | **2021** |
| **Doctoral Theses** | 10 | 10 | 15 | 16 | 12 | 6 | 6 | 4 | 6 | 6 | 8 |
| **Master's Theses** | 11 | 14 | 12 | 16 | 25 | 10 | 18 | 15 | 17 | 10 | 33 |
| **Journal Articles** | 126 | 130 | 139 | 136 | 152 | 146 | 122 | 140 | 134 | 152 | 156 |

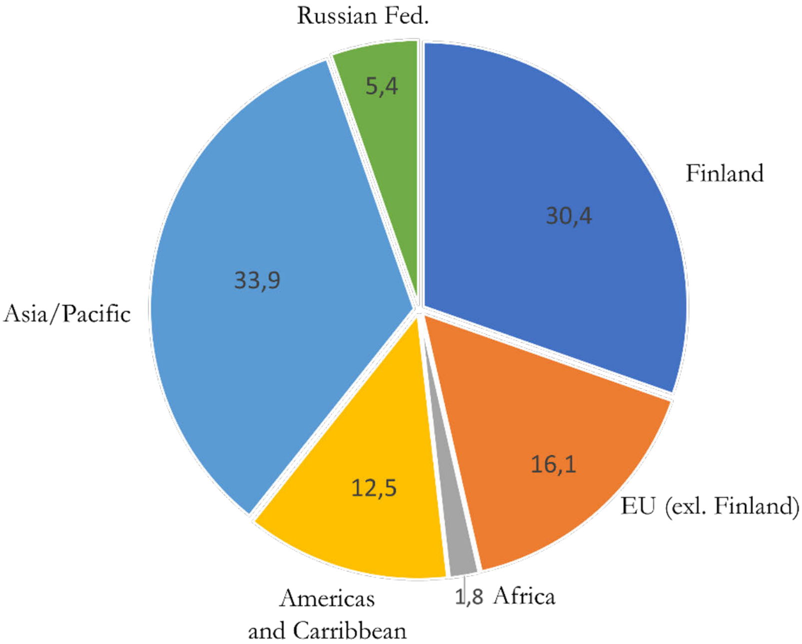
*Theses and peer-reviewed journal articles by the Johan Gadolin Process Chemistry Centre 2000-2021*




*Trendline of theses and peer-reviewed journal articles per year (2000-2021)*

## Doctoral students

A central part of our research activities is done as doctoral theses works. Altogether **57** PhD thesis projects are actively underway at the Centre. Our doctoral students are very international, as almost 70% originate from countries other than Finland (see the graph below). Among our foreign doctoral students in 2020-2021, the top nationalities were China (14), Germany (6), whereas those from Finland are 17 in total. ***PCC*** is certainly one of the most international units at our university.




*Origin of PhD students at Johan Gadolin Process Chemistry Centre during 2020-2021*

## Johan Gadolin International Mobility for Sustainable Chemical Technology

In 2020, PCC introduced a new mobility programme: *Johan Gadolin International Mobility for Sustainable Chemical Technology (IMSCT)*. Funding was obtained from the Åbo Akademi Foundation. The IMSCT mobility programme supports visits of foreign researchers to ***PCC*** as well as research visits of scientists from ***PCC*** to top-level foreign universities and research institutes. Despite travel restrictions imposed by COVID-19, five doctoral students (3-6 months each) and two postdoctoral researchers (7-8 months each) were able to successfully complete their mobility within this programme. One of the visiting postdoctoral researchers continues as a project researcher at ***PCC*** for another four years with funding from the Jane and Aatos Erkko Foundation. This is a good example of the impact of successful international mobility.

## 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 Prof. Chunlin Xu. Furthermore, Dr. Markus Englblom takes care of the coordination of ***PCC*** and functions as secretary of the executive board, while Dr. Pasi Tolvanen coordinates our mobility programme: Johan Gadolin International Mobility for Sustainable Chemical Technology (IMSCT).

The ***PCC*** executive board is supported by a *Scientific Advisory Board* and a *Forum for Society*. 2020-2021 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***.

## Acknowledgements

This report covers the activities of PCC over two calendar years (1.1.2020–31.12.2021). The report was compiled by an Editorial board, including Dr. Pasi Tolvanen (editor-in-chief), Dr. Rose-Marie Latonen, Dr. Päivi Mäki-Arvela, Dr. Anna Sundberg, Dr. Patrik Eklund, Dr. Johan Werkelin, and Prof. Johan Bobacka.

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

### Marta Ramos Andrés

My name is Marta Ramos Andrés and I come from Valladolid (Spain). I am doing my PhD at the Research Institute on Bioeconomy (BioEcoUva, University of Valladolid) on the application of the biorefinery concept at pilot-scale for the production of bioproducts from agri-food residual biomass. The main process of my PhD is the extraction and purification of hemicelluloses and pectins through hydrothermal treatment and ultrafiltration membranes. In October 2020 I had the opportunity to perform a 6-month doctoral stay at the Johan Gadolin Process Chemistry Centre thanks to a scholarship. In my luggage, I included the purified solid samples of hemicelluloses and pectins as well as cellulose nanofibers combined with lignin that I obtained during my PhD at the University of Valladolid. All samples were obtained from discarded carrots. In the Wood and Paper Chemistry group and in the Industrial Chemistry and Reaction Engineering group, under the supervision of Prof. Chunlin Xu and Prof. Henrik Grénman, I had the opportunity to learn the process of forming biodegradable films from the biopolymer fractions of discarded carrots. The films were made with different compositions and were characterized by studying their mechanical and barrier properties in search of potential applications for food packaging. The experimentation performed at Åbo Akademi allowed me to close my PhD by producing a final product based on what was studied and obtained in the previous chapters. During the months I spent in Turku I had the opportunity to learn a lot from excellent researchers, as well as to learn how to use new equipment and new processes. I was able to participate in the many group meetings and learn from all of them. The experience in Finland was extremely enriching as I was able to live in a country so different from my own, full of nature and great people. I will never forget the Finnish winter and the experience in Lapland and I will always be grateful for what I learned and the good results.

### Mahsa Mousavi

My name is Mahsa Mousavi. I got my M.Sc and Ph.D in Organic Chemistry in my home-country, Iran. I was awarded a 7-months Johan Gadolin Scholarship to continue my research as a short-term postdoctoral fellow in Laboratory of Molecular Science and Technology at Åbo Akademi University.

I was working on catalytic oxidation of lignin-based diols, from which interesting results were obtained. The findings could in the future be completed and summarized in two separate publications. The scholarship gave me the opportunity to work with modern analytical instruments used in characterization of organic molecules, as well as other modern lab facilities, new colleagues and new experiences. I appreciate Dr. Reko Leino and Dr. Risto Savela for supporting my research here in Finland during this time.

## Tingting Han

My name is Tingting Han, and I obtained my doctoral degree in analytical chemistry in June 2021 from the Laboratory of Molecular Science and Engineering, Åbo Akademi University, with the thesis entitled Coulometric transduction method for solid-contact ion selective electrode. My doctoral studies is supervised by Prof. Johan Bobacka. Currently, I am working as a postdoctoral researcher at the Center for Advanced Analytical Science, Guangzhou University, supervised by Prof. Dongxue Han. My main research interest focus on the development of electrochemical sensors, especially in the field of solid-contact ion-selective electrodes. I applied 3 months JG international mobility scholarship because I would like to gain new experience, learn and broaden the view of my research. During my stay in Guangzhou University, I learned new skills that strengthened my knowledge and my results are fruitful. I am delighted also friends around are nice, helpful, enthusiastic and feel like warm-family. Moreover, I will continue my research in the same group, which could further deepen the cooperation between Analytical Chemistry Group, Åbo Akademi Univerisy and Center for Advanced Analytical Science, Guangzhou university. I really appreciated for all the help and support, and the most important is that JG scholarship provide me this invaluable opportunity. I highly recommend JG scholarship to everyone. You will not regret it.

## Sara Benalia

Sara Benalia Ph.D. student in Metallurgical Engineering at Polytechnique Montreal, Canada. I am working on development of a thermodynamic model for chromates, molybdates, tungstates and vanadates involved in the corrosion of steels (Fe, Cr, Ni, Mo, W, and V) at high temperature in atmospheres containing O-H-S-C-Cl and alkaline salts. The experimental data required for the calibration of the model are derived from the literature and from the collaboration with research groups of Assoc. Prof. Fiseha Tesfaye (Faculty of Science and Engineering, Åbo Akademi University, Turku, Finland), Prof. Daniel Lindberg (Department of Chemical and Metallurgical Engineering, Aalto University, Espoo, Finland) and Prof. Leena Hupa (Faculty of Science and Engineering, Åbo Akademi University, Turku, Finland). I obtained a mobility grant from Johan Gadolin Process Chemistry Centre (PCC) for 5 months of stay. I started on August 20$^{th}$, 2021; mainly, I am performing phase diagram measurements by Differential Scanning Calorimetry (DSC) at Åbo Akademi University, and Scanning Electron Microscopy (SEM) at the University of Turku (Turun yliopisto). At the end of my stay, on April 25$^{th}$, 2022, more experimental data will be available to calibrate the thermodynamic model. Since my installation in Åbo, I have always felt the kindness of the people that I have been in contact with. Working in such friendly and dynamic environment will be always memorable. Keep in mind to apply!

## Hao Zhang

I am Hao Zhang, coming from China. In 2021 I completed my PhD in Light Industry Science and Technology at Tianjin University of Science and Technology (TUST), China. Currently, I am working as a postdoc in the interdisciplinary research of wood chemistry and electrochemistry, supervised by Prof. Chunlin Xu from Lab of Natural Materials Technology and Prof. Johan Bobacka from Lab of Molecular Science and Engineering. My research focuses on the material design from biomass for energy storage device. I was awarded a Johan Gadolin Scholarship for a period of six months from 01.2022 to 06.2022, providing me with a unique learning and research experience. In Åbo Akademi University (ÅAU), I have been having a fulfilling and enjoyable work on funding application and experiment promotion owing to the outstanding expertise and backgrounds of my professors and their cooperative team. In the past short time with the support of Johan Gadolin Scholarship, I have achieved some output in the files of sustainable material design of Sodium ion battery compounds, and I am confident that I can achieve follow-up fund support and research affirmation for working here longer as expected. In addition, the modern office environment of Aurum, great people from various backgrounds, awesome Finnish culture and attractive landscapes make me linger here. In summary, for me ÅAU is the best place to understand that personal practical work experience abroad. I highly recommend applying for Johan Gadolin Scholarship help me a lot for the starting an abroad life with joyful moments.

## Wander Perez Sena

My name is Wander Perez Sena, and I was born in Santo Domingo, Dominican Republic. I migrated to France in 2016 where I completed my master's degree at the Institute of Applied Science of Rouen (INSA Rouen). Thereafter, I started my career as a PhD candidate at INSA Rouen working in the valorization of vegetables oils derivatives by using knowledge of thermal safety, kinetics and catalysis. This PhD project was later coupled to Åbo Akademi University. By that time, funding for a fourth year at Åbo Akademi University was a big question mark. Thankfully, I was awarded with the Johan Gadolin Scholarship which enable the possibility to come to Finland to finalize my 4th year of PhD and later defend my work for the title of Doctor of science (Tech).

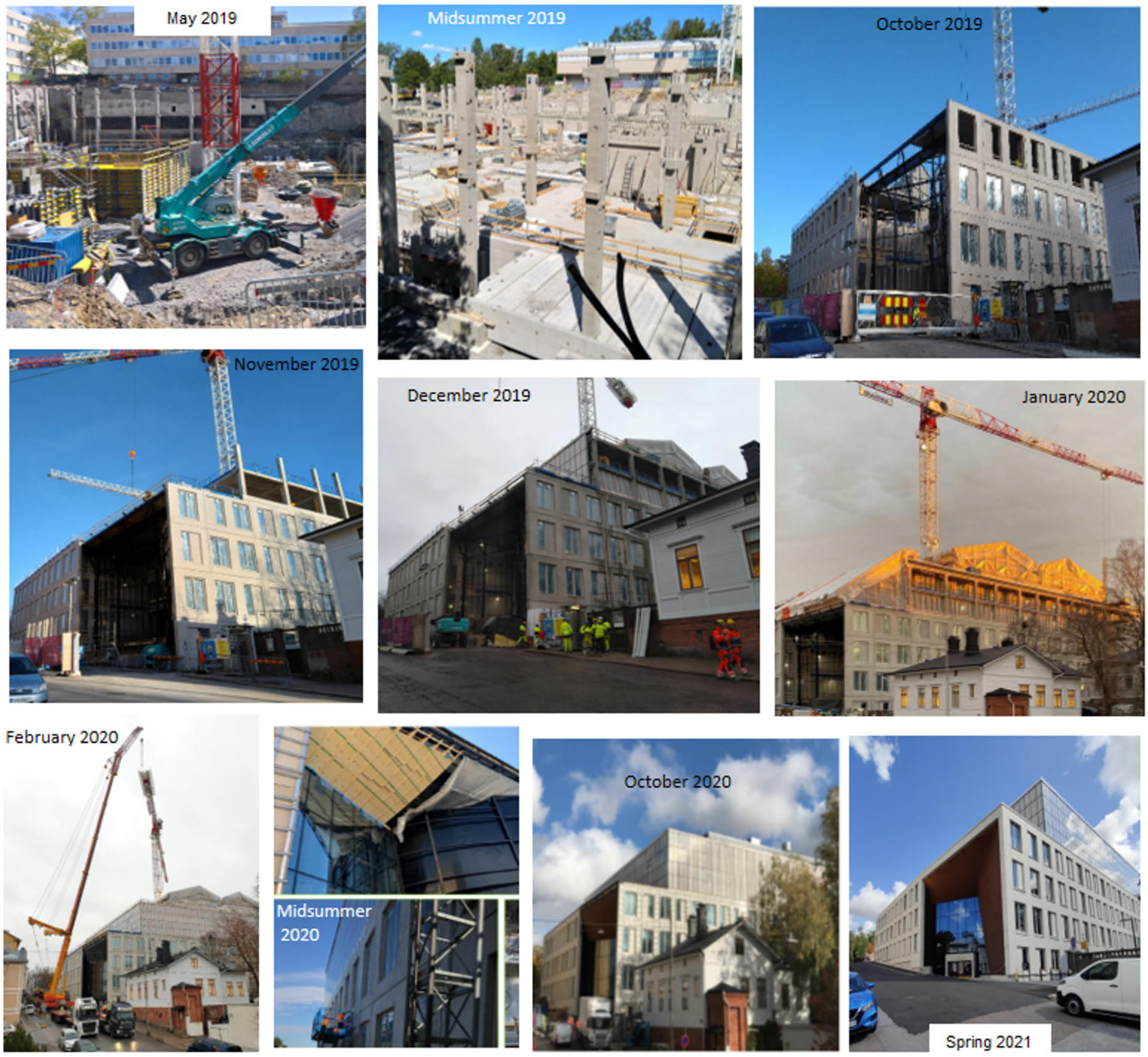
At Åbo Akademi University I had the opportunity to grow profoundly in the field of chemical engineering sciences by working with an excellent and multidisciplinary team with vast knowledge in catalyst synthesis, reaction kinetics, mathematical modelling, and reactor technology at the laboratory of industrial chemistry and reaction engineering (TKR). In fact, the end of my PhD project was just the beginning of my career at Åbo Akademi University, where later, I was appointed to work as Postdoctoral Researcher in an Akademi of Finland project concerning the valorization of hemicelluloses and derivatives through the application of heterogenous catalysis.

## 2.2 From the Old Market Hall to the Golden Aurum

Education in chemistry started in the new Åbo Akademi in 1918 and only two years later, the Faculty of Chemical Engineering (*Kemisk-tekniska fakulteten, KTF*) was established. It was a revolutionary step, because an engineering faculty was invoked in a classical university, which traditionally has faculties in arts and science. The European tradition was to strictly separate classical universities for science and technical universities for engineering. Establishment of chemical and chemical engineering education at Åbo Akademi was preceded by a heated debate in the local newspaper *Åbo Underrättelser*. It was claimed that education in chemistry and physics is too expensive, because it requires laboratory facilities – instead, Åbo Akademi should focus on archeology, because it is easy just to dig down in the historical sites of Turku/Åbo and make exciting discoveries! The young Republic of Finland had, however, a strong driving force for industrialization. The pressure from the local industry was high to expand the engineering education in our country, and the curriculum should be based on chemical technology. Pulp and paper industry and smaller scale chemical industry as well as mining needed skillful engineers. Åbo Akademi received donations for establishing professorships for an engineering faculty and a curriculum for the new faculty was elaborated – the world-famous Swedish chemist, the Nobel Prize winner Svante Arrhenius visited our city and gave advices how the education should be organized. The new faculty, KTF was born 1$^{st}$ of July, 1920 and it had two professorships: one in general chemical technology (the Borgström professorship) and a second one in forest products chemistry and technology. It can well be stated that Johan Gadolin Process Chemistry Centre (PCC) has its roots in these two eminent professorships.

*Laying the foundation (Grundstensmurningen) 8th of May 2019. Speeches by the mayor of Turku, Minna Arve and the university rectors Mikko Hupa and Kalervo Väänänen.*

The education and research in chemical and process engineering has survived over 100 years and it will have a bright future. The story of our education and research is very much a story of buildings. Why? The issue of the facilities for chemistry and chemical engineering education and research at Åbo Akademi has been a continuous dilemma throughout the decades. In the early times, the activities were spread in various buildings in the old town: the Old Market Hall (*Gamla Saluhallen*), Geologicum, Kosmorama, the Reuter Building (*Reuterska huset*). Construction of the New Chemical Building (*Nya Chemicum*) was a great step after World War II. New leaps in the infrastructure was taken as the Gadolinia and Axelia buildings were erected in 1969 and 1977. Axelia became immediately the heart of KTF: a building with a modern spirit, extensive laboratory facilities, space for group work, modern equipment hall and the legendary student club Axelborg. In 1997 Axelia was extended with a new wing called AxeliaII. Finally, the major part of chemistry and chemical engineering was concentrated in one complex, but unfortunately, physical chemistry and the pulp and paper sector, including wood chemistry had to remain in the unfortunate Gadolia building, which declined rapidly. Simultaneously the older part of Axelia needed a renovation. What to do?

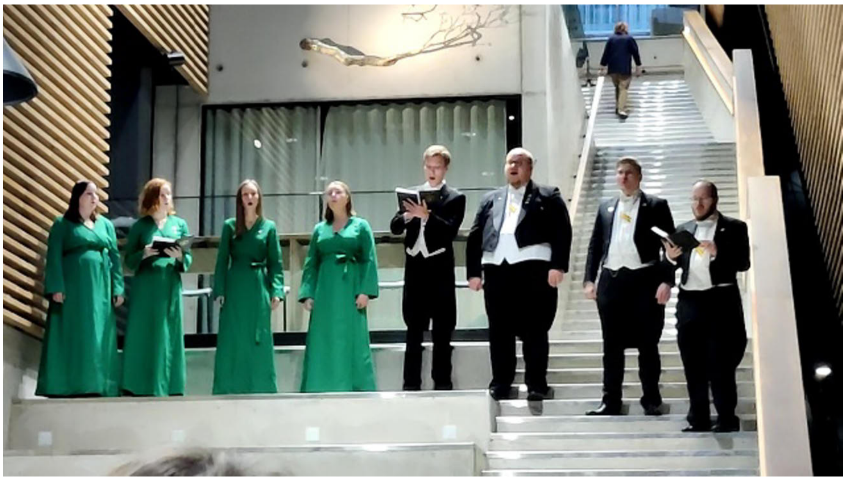



*A construction time lapse of the building of Aurum between years 2019-2021 (Photos by P. Tolvanen and with permission from Skanska Oy)*

Basic renovation of Axelia would have been a very cumbersome and expensive operation, and Rector of Åbo Akademi, professor in organic chemistry, Jorma Mattinen rejected the renovation plan. A spontaneous discussion commenced within the faculty, but nobody had a clear proposal for the solution of the acute issue. Suddenly something like a miracle happened. Professor Tapio Salmi had been elected Dean of the Faculty of Science and Engineering (FNT) 2015 and one day the director of real estate issues of Åbo Akademi Foundation, Mr. Ari Ahokas appeared in the dean's office. He came with very interesting news: the departmental building Juslenia of our neighboring university, University of Turku was in very bad shape and will be demolished. The land area released might be enough for a large building, which could collect all chemistry, chemical engineering, physics, mathematics and industrial management at Åbo Akademi under the same roof. The dean was immediately very enthusiastic about the idea. The idea started to advance in a high speed, and the rector of Åbo Akademi, Mikko Hupa, professor in inorganic chemistry and previous leader of PCC, immediately gave his strong support to the initiative. Soon it became clear that also the Department of Chemistry at University of Turku was eager to join the effort. A preliminary technical planning of the building started and the boards of both universities accepted the initiative. The final planning of the building was given to the hands of *Aihio Arkkitehdit* and the main construction was done by the company Skanska. The leading architect of the project was Piia Viitanen. She put a lasting fingerprint in the history of this beautiful and simultaneously very functional university building.

*Autumn 2022: Official inauguration festivities in the Aurum lobby.*

The planning procedure of the 20000 $m^2$ building was very demanding, particularly because of the special constructions and equipment needed by the chemical laboratories: fume-hoods, ventilation and gas storage systems, storage of explosive and poisonous chemicals as well as high-pressure equipment. Each square meter of the laboratory space was planned together with the corresponding research groups and the laboratory managers. The result is the most modern and most advanced laboratory space for chemical and physical sciences in our country. The building has obtained the environmental certificate 'excellent' in the BREEAM system. Solar energy and ground energy is used in the building, which is important because chemical laboratories are typically very energy demanding. Meeting places for mutual interaction exist, places for students' group work, seminar rooms, a cafeteria, a marvelous big auditorium Argentum built in the spirit of classical lecture theatres. From the open offices of the scientists, a heartbreakingly beautiful view opens over the picturesque old town, towards the medieval cathedral and the observatory hill.



*Quartets of the choirs Florakören and Brahe Djäknar singing at the inauguration.*

What should the name of the building be? A contest was declared, and it was decided unanimously that it should be AURUM. The name which was proposed by two persons, from Åbo Akademi and University of Turku, is Latin and means 'gold', but is has a coupling to the local landscape, too: we are close to the banks of the Aura River, the important landmark of Turku/Åbo. A great house should incorporate impressive artwork. The contest was won by golden sculptures designed by Noora Schroderus, symbolizing the nature, living organisms. She took the impression from oak, the tree symbolizing southwestern Finland. A visitor can see the artwork *Quercus robur* in various places inside AURUM – this marvelous piece of art was the most creative one among the proposals.

*Golden art by Noora Schroderus in the Aurum lobby and cafeteria.*

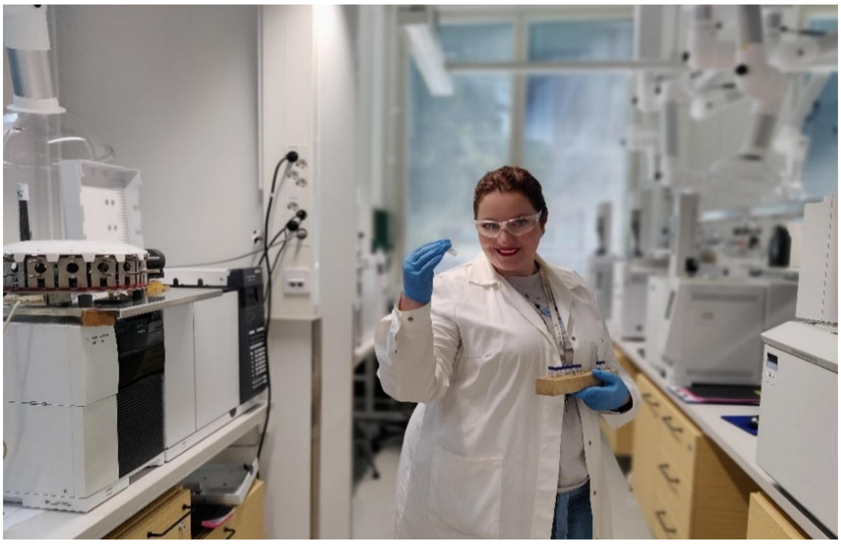
When I enter the building during a late evening or weekend, there are always people, discussing, studying or doing science. The spirit of AURUM has been created and it implies a big leap and a new start for PCC. The critical mass has been concentrated.

Text by *Tapio Salmi*
Photos by *Pasi Tolvanen*

## The moving

Mentally we have been preparing to move already several years, but the actual physical moving from Axelia to the new building Aurum took place between May and November, 2021. Each laboratory had their own time slots to avoid bottlenecks and lost equipment. Overall, the moving has went without any problems, as told below by the personel in charge of the moving. Kari Eränen is very happy about the smooth transfer of the equipment and wants to give credits to the moving company – most of the boxes found the right floor and place. The best about Aurum is according to Kari (TKR) the improved safety compared to the over 40 year old Axelia and even older Gadolinia. New clean surfaces, and safety cabinets for gas bottles, are the major advantages. Teija Tirri (OK/TPK) agrees about the clean sound of Aurum laboratory facilities. She really likes that now there are enough of fume extractors and fume hoods, and that all the chemicals are concentrated and categorized into a separate isolated storage room. The installation of gas lines after moving in has taken quite much effort, according to Teija and Kari. The installation of analytical devices has taken long time, but now most of them are up and running, says Ekaterina Korotkova from NMT. Tor Laurén, the head of laboratory services, is happy of how the moving has gone in practice. Before the move, concerns and worries about the possible logistical problems

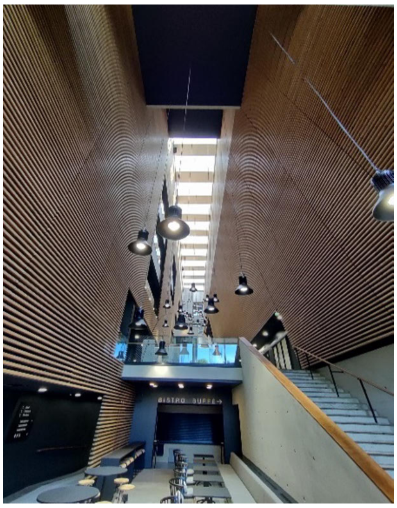




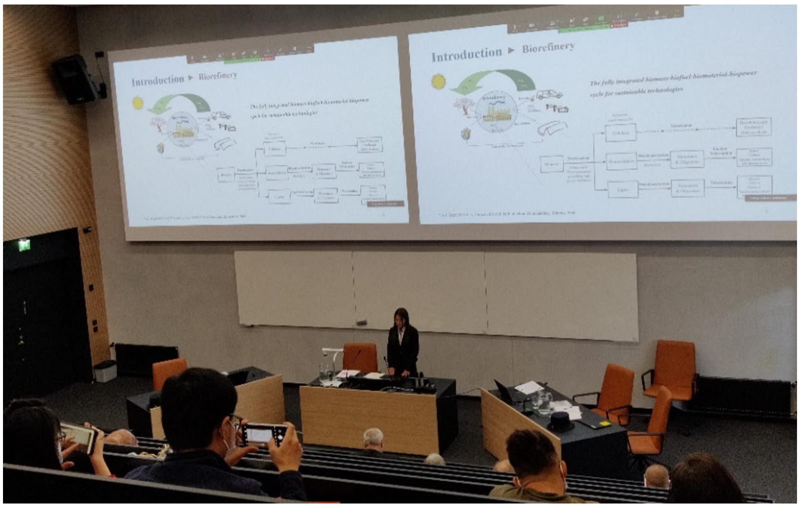

*First thoughts of the moving by the laboratories: Kari Eränen, Eija Tirri, Ekaterina Korotkova and Tor Laurén give their opinions on how the transfer to new Aurum has proceeded.*

were proven wrong – everything went smoothly. Many thanks to all the people that made a huge effort in packing and unpacking all the goods before, during and after the big move. The clean up work before the move was also very important. Reinstallation of the devices has been the most time consuming after the actual move.

**Pictures from the inside of Aurum**

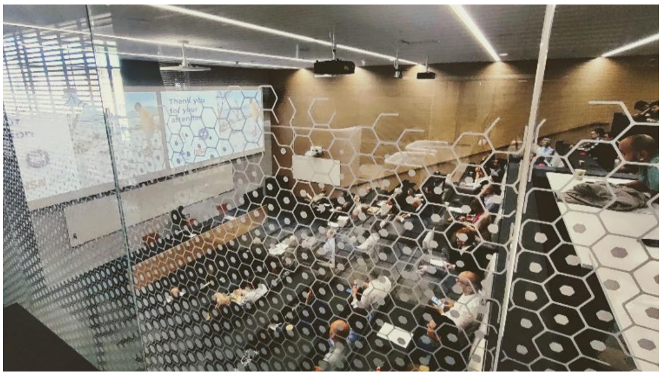


The Aurum lobby



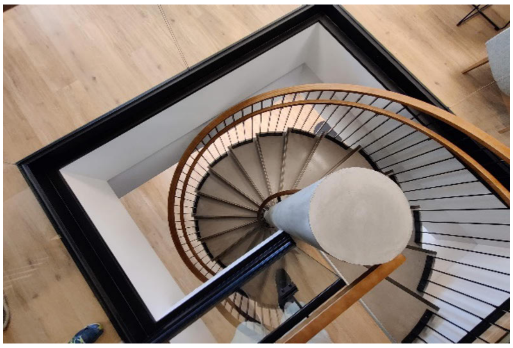

The first doctoral defence in auditorium Argentum

Coffee break at 4th floor



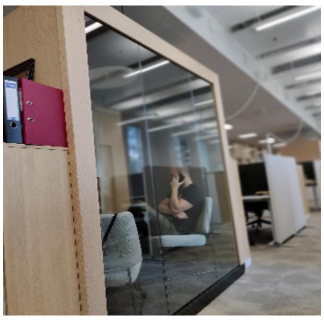
Auditorium Argentum seen from lobby

Long row of laboratory fume hoods



Arcitectonic stairs between floors

Offices equipped with white boards

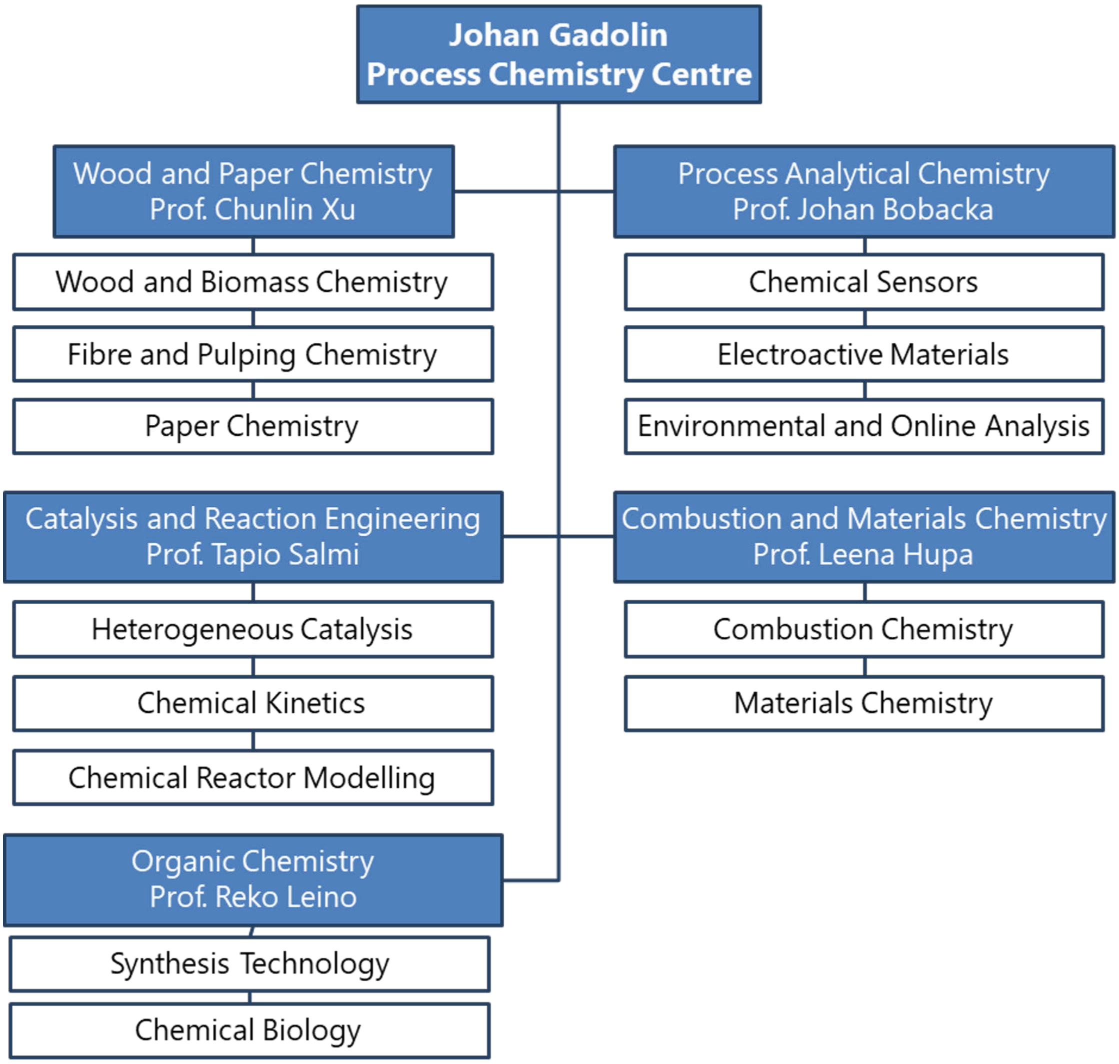


Silent booths for meetings & calls

Open offices with ladscape views

# 3. Our organization and who we are

## 3.1 Organization of *PCC*




### Executive Board

- Professor Johan Bobacka (chairman)
- 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, Lantmännen Agro
- Kenneth Ekman, CrisolteQ – part of Fortum
- Jonas Konn, Kemira
- Linda Fröberg-Niemi, Green Industry Park Ltd
- Christine Hagström-Näsi, CLIC Innovation
- Patrik Holm, Orion Pharma
- Bertel Karlstedt, Valmet
- Kari Kovasin, Metsä Fibre
- Björn Lax, Chemec
- Timo Leppä, T-Media
- Lars Peter Lindfors, Neste
- Pia Nilsson, UPM
- Leena Paavilainen, Luke
- Jarkko Partinen, Metso Outotec
- Leena Sarvaranta, VTT
- Mathias Snåre, Nordkalk
- Kenneth Sundberg, Anison Therapeutics
- Kari Toivonen, Finnsusp Oy
- Petri Vasara, AFRY
- Stefan Wallin, Oy SEW Advisory Ab

## 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, 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 in 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.

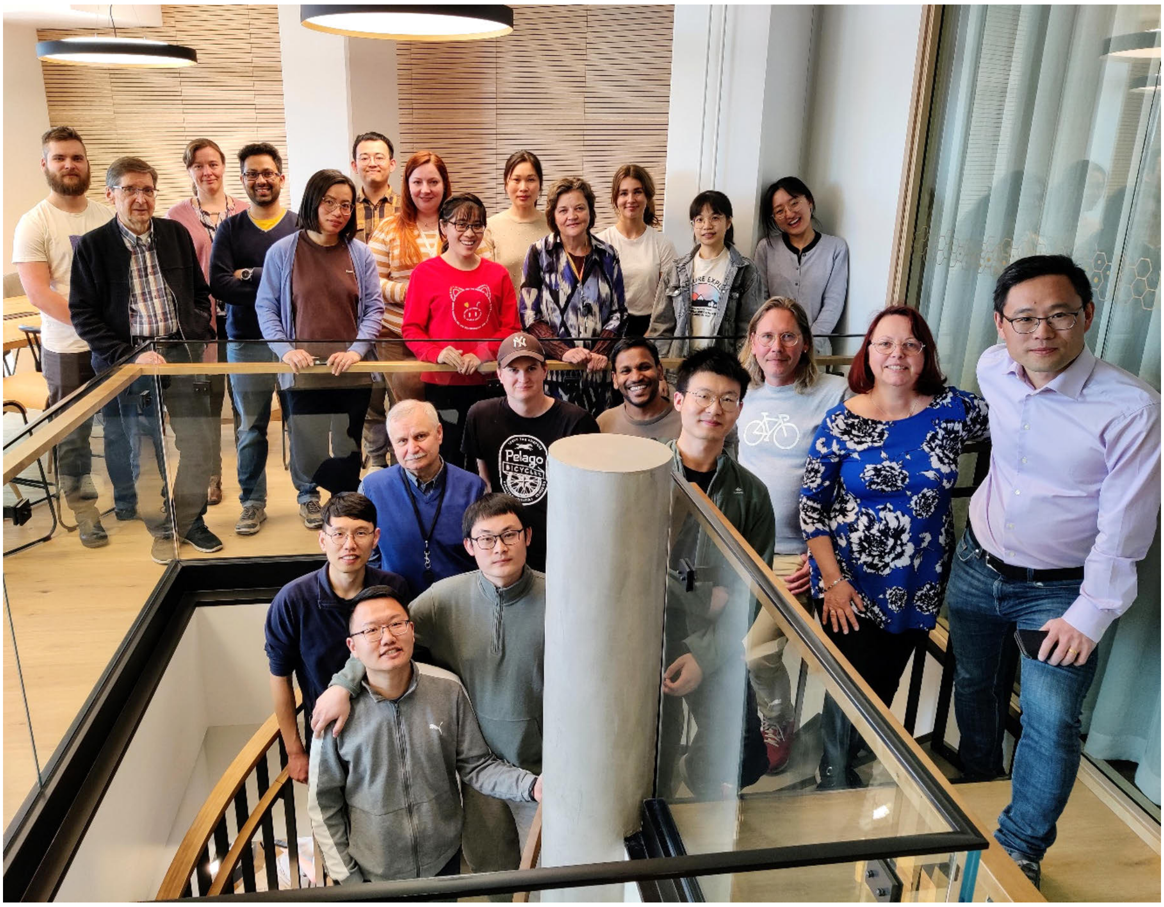
External research support 2020-2021 was obtained mainly from Academy of Finland, Business Finland and the industry, from Royal Swedish Academy of Agriculture and Forestry in the research program Tandem Forest Values, and from the China Scholarship Council in form of grants for PhD students. We also have 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 Aalto University, Tampere University, LUKE, and groups affiliated to the Biocity Turku Research Programmes 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.

- *'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.

- *'Novel Fiber Surfaces Functionalized by Lignins Refined and Engineered from Finnish Biorefinery Processes (LigninReSurf)' funded by Business Finland, 01.01.2021-31.12.2023.* Plastics with many society benefits are widely used for packaging and other applications in our daily life, however, much of these ends up as for single-use and have now accumulated in the landfills, oceans, waterways, and other natural environment and have further entered into animal and humans bodies, threatening our health. Lignin accounts for up to 30% of dry mass of plants, but so far, most of it is burnt for energy. The LigninReSurf consortium project plans to use the relevant lignin streams from Finnish biorefinery processes as raw materials to apply lignin-refining approaches to achieve well-defined fractions with well-characterized structures.




*Wood and Paper Chemistry personnel in spring 2022 in the new coffee room of Aurum, 4th floor.*

**Personnel**

*Professors*

Chunlin Xu
Stefan Willför (Vice Rector of Åbo Akademi 2019-2022)
Bjarne Holmbom (Emeritus)

*Docents*

Petri Kilpeläinen (LUKE)
Risto Korpinen (LUKE)
Andrey Pranovich
Annika Smeds
Anna Sundberg (Senior University Lecturer)

*Researchers*

Jarl Hemming
Ekaterina Korotkova
Xiaoju Wang (Academy Research Fellow)
Wenyang Xu
Hao Zhang

*Early-stage researchers*

Marie Alopaeus
Oskar Backman
Liqiu Hu
Minette Kvikant
Zhiqiang Li (SAPPI)
Rui Liu
Zonghong Lu
Veronica Matamala (Arauco)
Luyao Wang
Qingbo Wang
Weihua Zhang
Jiayun Xu
Gaoyuan Ye
Yidong Zhang
Lulu Zhu

*Secretary* Karita Åberg

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

# 2.2 Process Analytical Chemistry

Our research in analytical chemistry is focused on the development of novel electrochemical sensors based on advanced functional materials, new receptor molecules and new signal transduction methods. Our activities involve 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 in environmental analysis and personal health monitoring. Emerging analytical applications, such as distributed chemical analysis and on-body sensing, would benefit greatly from calibration-free and maintenance-free chemical sensors. This is an important driving force for our research. Our long-term development of solid-contact ion-selective electrodes and solid-state reference electrodes represent two important steps towards maintenance-free ion sensors. Our main research achievements during 2020–2021 can be summarized as follows:

A few years ago we introduced a coulometric method, which allows amplification of the analytical signal of solid-contact ion-selective electrodes. The coulometric transduction method was developed further, with support from the Academy of Finland, and this work has already obtained significant international recognition.

Our development of anion sensors based on new receptor molecules, synthesized by our collaborators at the University of Tartu, is progressing well. Some of the ion-sensors were successfully applied to determine benzoate in lingonberries and cranberries.

Thin-layer ion-selective membranes are commonly used in various types of ion-selective electrodes. In our work we found that such thin-layer membranes may cause an erroneous response in solid-contact ion-selective electrodes, which is important knowledge for future developments.

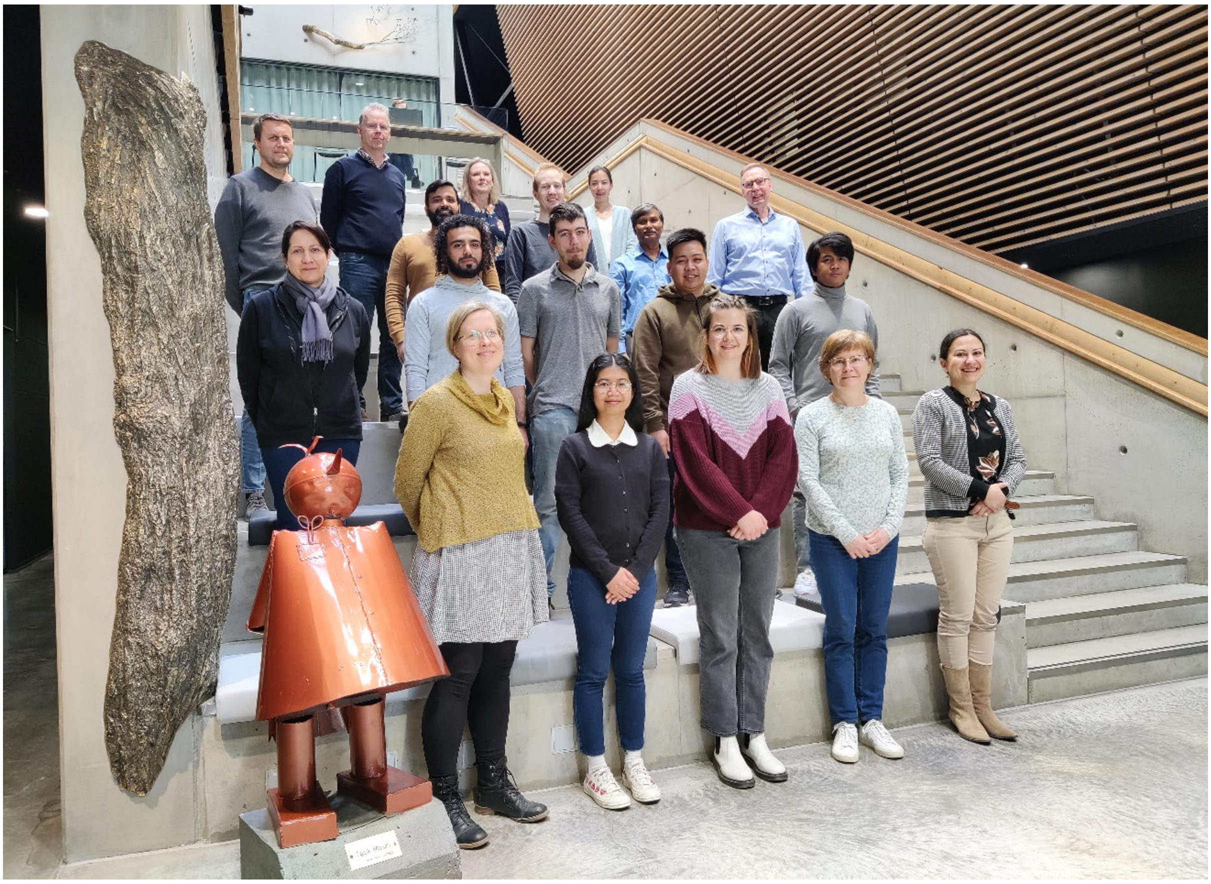
Paper-based microfluidic sampling systems were studied with a special focus on biofouling. We found that addition of gold nanoparticles slows down the transport of proteins in the paper substrate, which reduces the risk of biofouling at the sensor surface.

Our research on wearable biosensors for glucose contributed to the development of needle-free health diagnostics at GlucoModicum Oy. Special emphasis was placed on optimizing the skin-sensor interface.

Nanostructured catalytic materials were developed for electrocatalytic hydrogenation and oxidation of glucose and xylose. This work is an example of our collaboration with the Catalysis and Reaction Engineering team at PCC. In collaboration with the University of Turku and the Wood and Paper Chemistry team at PCC, we are developing electrode substrate materials to capture electricity from photosynthetic processes in cyanobacteria and microalgae. This is an interesting route towards sustainable generation of electrical energy.

A new research direction is our development on artificial noses, i.e. devices that mimic and enhance the biological olfactory mechanism using a sensor array, signal transduction, training and recognition. New types of electronic noses were developed by using different conducting polymer derivatives as sensors.

External research funding during 2020-2021 was obtained from the Academy of Finland, Business Finland, industrial partners and several 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 program *Excellence in Analytical Chemistry* (EACH), supported by EU, has dramatically increased the number of MSc theses in analytical chemistry from our group.



*Process Analytical Chemistry personnel in 2022 (missing from the photo: Ulriika Mattinen, Jay Pee Oña)*

## Personnel

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

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

### *Senior researchers*
Zhanna Boeva

### *Doctoral students*
Ashiq Ahamed
Narender Joon
Jay Pee Oña
Tingting Han
Sara Lund
Ville Yrjänä

### *Laboratory Engineer*
Tor Laurén

### *Secretary*
Mia Mäkinen

### *Economy secretary/Accountant*
Anna Lyubavina (–16.1.2021)
Benita Martiala (16.1.2021–)

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

# 2.3 Industrial Chemistry and Reaction Engineering

The birth date of Industrial Chemistry and Reaction Engineering (Teknisk kemi och reaktionsteknik, TKR) at Åbo Akademi is clearly defined: Faculty of Chemical Engineering (Kemisk-tekniska fakulteten, KTF) started its activities 1st of July 1920 and the first chair of the new faculty was the Borgström professorship in general chemical technology. In summer 2020 we had the pleasure to celebrate this historical landmark together with our strategic partner VTT. A scientific seminar was organized in Turku/Åbo archipelago on the topic Intensified Chemical Processes (ICP).

The core competence of today's TKR is in catalysis, kinetics, chemical reactor technology as well as exploring new reaction environments and development of green process technology. Process intensification, particularly intensification of chemical transformations by unconventional forms of energy and new reactor and catalyst structures is the hard core of our research activities. The main application area of this strongly methodological approach is the valorization of molecules originating from biomass to fine and specialty chemicals as well as new fuel components. Heterogeneous catalysis combined to very detailed kinetic studies and avant-garde reactor technologies are the keys for success in the revolutionary green transition 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 the long-term strategy of TKR. A new roadmap our research visions was prepared in spring 2020, in close collaboration with the strategic partner VTT.

Green chemistry is transformed to 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 materialized by using micro- and milliscale reactors, which provide a real technology jump in 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 down to 10% of the size of conventional reactor equipment, such as packed beds or tank reactors.

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 and hydrogenation of sugars originating from hemicelluloses, aqueous-phase reforming to produce bio-hydrogen as well as catalytic oxidation of alcohols. 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 was continued. This extensive research effort was 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. Intensive collaboration is flourishing with several universities and research centers. The main 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 were in progress, the biggest one of them being the Academy Professor T. Salmi's five-year project devoted to deep understanding of the mechanisms of three-phase oxidation and epoxidation processes on solid surfaces. Transient techniques and ATR spectroscopy are the main tools in the project.

The structure of TKR was improved by transforming the tenure track professorship of Henrik Grénman to a permanent position and appointing Adriana Freites Aguilera to a docentship in multiphase chemical reaction engineering. Professor Johan Wärnå was appointed a member in Svenska Tekniska Vetenskapsakademien i Finland thanks to his high scientific and pedagogic merits in chemical reaction engineering. The co-workers of TKR obtained several prizes for their research effort. Wilhelm Wikström got a national scholarship for his B.Sc. thesis devoted to semibatch technology in kinetic measurements, Rectora Magnifica of Åbo Akademi gave the best doctoral thesis award, Elfvings legat to Adriana Freites Aguilera for her doctoral thesis devoted to epoxidation of fatty acids by using microwave technology and catalysis. The award for best doctoral thesis in catalysis 2019-21 was given by Finnish Catalysis Society to Soudabeh Saeid for her ground-breaking research in the destruction of pharmaceuticals in waste waters. A novel method of combined ozonation and heterogeneous catalysis was very successfully applied on wastewater cleaning and a huge amount of fundamental knowledge on reaction mechanisms was collected in this pioneering work. Besides the numerous scientific publications on international arena, we are very happy that in total eight high-level doctoral theses were defended at TKR in 2020-21. Great news reached us from European Federation of Chemical Engineering (EFCE): we are going to host the oldest and most prestigious conference in chemical reaction engineering, International symposium on Chemical Reaction Engineering, ISCRE28 in June 2024 in Turku/Åbo – Cordially welcome!

*Personnel of the Laboratory of Industrial Chemistry and Reaction Engineering in 2021*

## Personnel

### *Professors*

Tapio Salmi (Academy professor 1.1.2019-31.12.2023)
Dmitry Murzin (Borgström professor in chemical technology)
Johan Wärnå (professor in chemical reaction engineering)
Jyri-Pekka Mikkola (joint professor with Umeå University, technical chemistry)
Henrik Grénman (professor in chemical process intensification)
Päivi Mäki-Arvela (docent, associate professor in industrial chemistry)
Heather Trajano (visiting professor 2019-2020, University of British Columbia, Vancouver)

### *Docents*

Atte Aho
Adriana Freites Aguilera
Narendra Kumar
Matti Reinikainen (VTT)
Fredrik Sandelin
Pasi Virtanen
Ikenna Anugwom (LUT University)
Sébastien Leveneur (INSA-Rouen)
Vincenzo Russo (Università di Napoli 'Federico I
Pasi Tolvanen (senior lecturer)
Zuzana Vajglová

### *Laboratory manager*

Kari Eränen

### *Senior researchers*

Erfan Behravesh
Sigmund Fugleberg
Javier Ibanez Abad
Jussi Rissanen
Wander Pérez Sena
Teuvo Kilpiö
Marisa Navas
Nataliya Shcherban
Ramakrishna Jogi
Ali Najarnezhadmashhadi
Irina Simakova
Nemanja Vucetic
Xiaojia Lu
Wander Pérez Sena

### *Doctoral students and researchers*

Alberto Goicoechea Torres
Alvaro Asensio
Ananias Medina Ferrer
Anna Barone
Bernadette Worgul
Carmen Rossano
Christoph Schmidt
Cristina Pizzolitto
Ekaterina Kholkina
Emiliano Salucci
Fabrizio Ciccarelli
Federica Orabona
Francesco Taddeo
German Araujo Barahona
Giuseppe Rossi
Jay Pee Oña
Jorge Mendez Fernández
José Delgado Liriano
Leolincoln Correia da Silva
Luca Mastroianni
Luca Riccio
Maria Herrero Manzano
Marie-Louis Reich
Mark Martinez Klimov
Marta Ramos Andrés
Maryam Hmoudah
Matias Alvear Cabezon
Michele Fortunato
Mouad Hachhach
Ole Reinsdorf
Pontus Lindroos
Ralf Sirén
Rossana Suerz
Sebastian Franz
Shekoufeh Adhami
Simon Engblom
Taimoor Kaka Khel
Tom Winkler
Tommaso Cogliano
Tyko Viertiö
Wilhelm Wikström

## 2.4 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: Technologies for a Sustainable Future; and Solutions for Health. 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 and conversion of biomass with particular focus on polyphenols 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 as well as development of analytical methods for renewable materials and industrial processes. We also closely collaborate with several national and international partners and actively participate in research networks.

*The laboratory of Organic Chemistry celebrating Lucas Lagerquist at his doctoral dinner in May 2022*

## Personnel

### *Professors*

Reko Leino
Jorma Mattinen (Emeritus)

### *Docents*

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

### *Teachers*

Dr. Jan-Erik Lönnqvist

### *Early stage researchers*

Lucas Lagerquist
Robert Lassfolk (Turku Centre for Chemical and Molecular Analytics)
Ida Mattsson (Optinova)
Patrik Runeberg
Atefeh Saadabadi
Anton Örn
Veronika Badazhkova

### *Laboratory engineer*

Teija Tirri

### *Secretaries*

Annika Fougstedt
Mia Mäkinen

### *Economy secretary*

Benita Martiala

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

## 2.5 Combustion and materials chemistry

Our research strategy is to provide expertise in detailed chemistry knowledge in high-temperature processes and high-temperature materials. Our primary research endeavours are foremost in bioenergy, inorganic materials and biomedicine, with a broader outreach to the green transition and circular economy. Management of material streams and emissions, treatment and recycling of various waste and side streams in an 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, combustion process modelling, emission measurements, and developing a detailed understanding of the interactions between the combustion device materials, fuels and their ashes. All of these support the increasing utilisation of $CO_2$-neutral fuels for energy generation.

We study recycling and recovering valuable materials from ashes, electronic waste and ceramic demolition waste in several projects. We utilise thermodynamic equilibrium calculations to describe high-temperature processes, especially in various ash, slag, metal 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, slags, metals, and ceramics. 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 model 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" but $CO_2$ neutral.

Our research includes laboratory-scale 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 containing, e.g., alkalis, chlorides, bromides, fluorides. Recently, we have developed new techniques to accurately measure and understand the corrosion and reaction mechanisms of the materials in their target environments.

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

Our research is in collaboration with groups and people from many universities, companies and research centres. It is financed by Åbo Akademi, Business Finland, the Academy of Finland, the EU, 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 of Combustion and Materials Chemistry in June 2022*

## Personnel

***Professors***
Leena Hupa
Mikko Hupa (Emeritus)

***Docents***
Anders Brink (*external*)
Niko DeMartini (*external*)
Markus Engblom
Sonja Enestam (*external*)
Oskar Karlström
Juho Lehmusto
Daniel Lindberg (*external*)
Bengt-Johan Skrifvars (*external*)
Fiseha Tesfaye(*external*)
Patrik Yrjas
Maria Zevenhoven

***Laboratory manager***
Tor Laurén

***Senior researchers***
Meheretu Dirbeba
Thomas Kronberg
Jonne Niemi
Emil Vainio
Johan Werkelin

## *Doctoral students and researchers*

Laura Aalto-Setälä
Roland Balint
Sarah Benalia (Johan Gadolin Scholar)
Nina Bruun
Jan-Erik Eriksson
Rasmus Fagerlund
Stefan Heberlein
Elisa Hupa
Farzad Jafarihonar
Arturo Keim
Alessandro Ruozzi
Maryam Sadegh Mousavi (Johan Gadolin Scholar)
Paulo Santochi
Daniel Schmid
Christoffer Sevonius
Minna Siekkinen
Polina Sinitsyna
Adrian Stiller
Sarah Yahi
Raju Viswamoorthy

**Laboratory technicians**

Peter Backman, Luis Bezerra, Jaana Paananen, Linus Silvander

**Secretary**

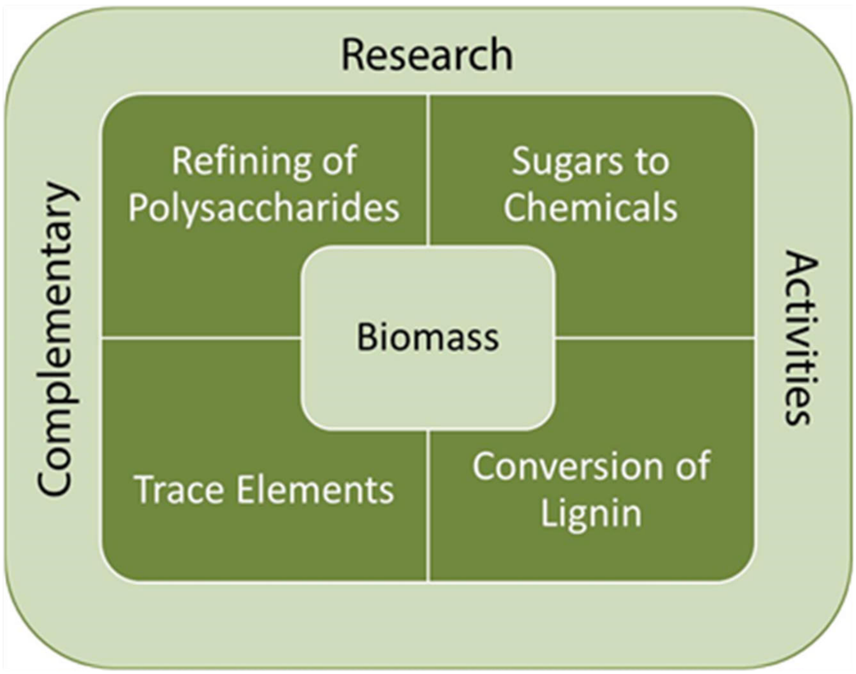
Benita Martiala (accountant), Mia Mäkinen

www.abo.fi/en/inorganic-chemistry-research-and-researchers

# 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.



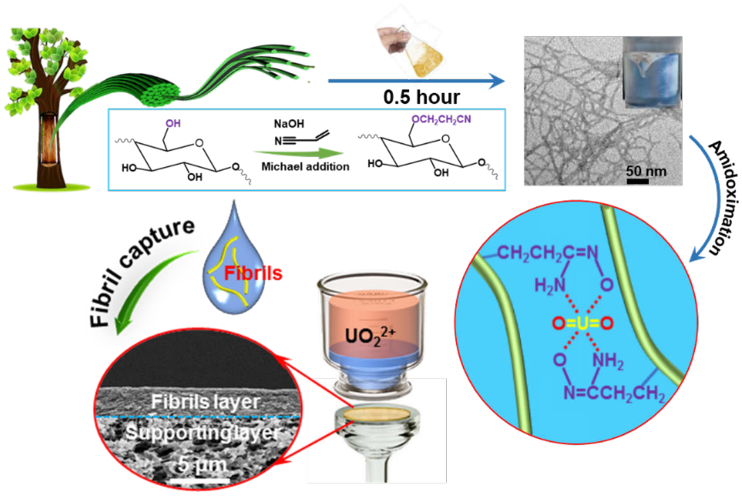

***PCC*** *research areas.*

# Exfoliation of Amidoximated Cellulose Nanofibrils for Large-capacity Filtration Capture of Uranium

Main funding: China Scholarship Council (CSC), Research mobility of Åbo Akademi University

*Weihua Zhang, Stefan Willför, and Chunlin Xu*

Extracting aquatic uranium element is of great significance for both green energy acquirement and water environmental remediation. On one hand, mining uranium from seawater has been long pursued for nuclear energy, and drawn growing research interest because approximately $10^3$ times available uranium resources are reserved in the ocean by contrast to the conventional exhaustible sources of terrestrial ores. On the other hand, uraniferous wastewater discharged from mineral deposits, nuclear industries, and military actions, poses a severe threat to human health and the ecological environment due to its dual impact of lethal toxicity and radioactivity. Compared with the traditional approaches of chemical precipitation, evaporative concentration and ion exchange, adsorption has been widely considered promising for the capture of uranium from aqueous solutions due to its high efficiency, easy operability, wide adaptability and low cost. Biopolymers, like cellulose, chitin and protein/polypeptide, have also aroused considerable attention when used as adsorbents for uranium removal from wastewater or extraction from seawater. Cellulose, as the most abundant polymer in nature, holds the greatest potential in the light of its sustainability, low cost, abundant chemical diversity and high mechanical properties.




*Scheme of the process for preparing amidoximated cellulose nanofibrils membrane and their applications for uranium ions capture by filtration.*

In this work, cyanoethyl substitution was found to enable rapid exfoliation of cyanoethyl cellulose nanofibrils by mild shear (e.g., manual shake and homogenization) within 30 min with a conversion up to ~90% and unique re-dispersibility in many organic solvents. After hydrolyzing cyanoethyl into amidoxime, the resultant amidoximated cellulose nanofibrils, serving as a novel type of green absorbent, exhibited a rapid kinetics (<5 min) and large reversible capacity (1327 mg $g^{-1}$) in aquatic uranium adsorption. Their rigid fibrous feature and super dispersibility facilitated the construction of fibrous porous films to capture uranium ions in high capacity in continuous filtration flow. Therefore, this cyanoethyl exfoliation may not only provide an unprecedently route for rapid and energy-efficiency production of cellulose fibrils, but also promise a green and sustainable alternative for high-efficiency extraction of aquatic uranium element.

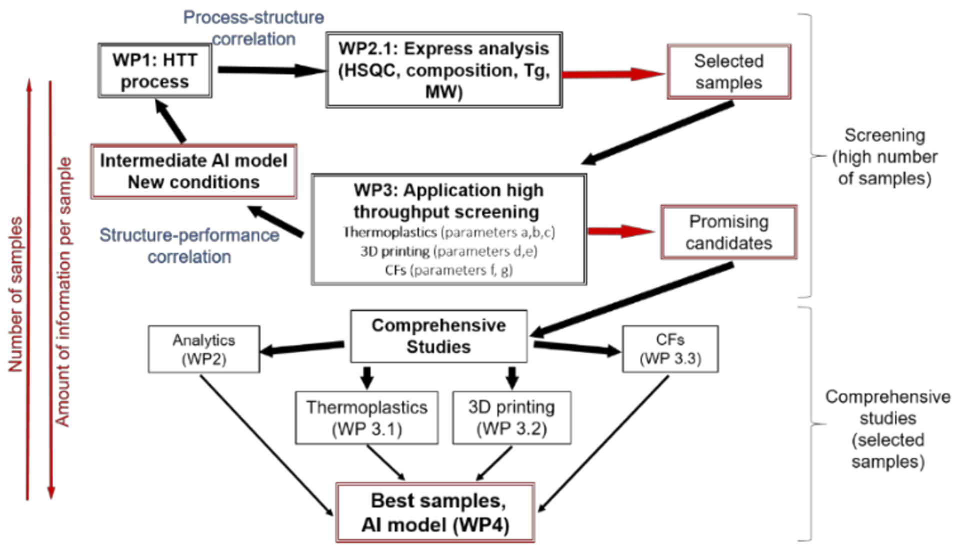
**Cooperation:**
Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences & Shandong Energy Institute (China)

## Exploiting Lignin-Carbohydrate Complex (LCC) through Artificial Intelligence (AI-4-LCC)

Main funding: Academy of Finland

*Marie Alopaeus, Luyao Wang, Andrey Pranovich, Chunlin Xu*

Hydrothermal treatment (HTT) of wood material is a biorefinery process that generates lignin as a by-product that can be used for low-value applications. Together with coworkers at Aalto University, we have presented an HTT process where all streams can be utilized for producing lignin as potential high-value products. Furthermore, under specific HTT conditions, lignin-carbohydrate complexes (LCCs) were generated with higher yields than reported earlier. LCCs are a promising material for producing high-value materials as it possesses properties of both lignin and carbohydrates. The objectives of the AI4LCC consortium are divided into four working packages. The HTT process followed by solvent extraction will be optimized for producing lignin, hemicelluloses and LCCs with the highest possible yields. After that, the products will be extensively analyzed, and selected samples will be chosen for application studies with the main focus on 3D printing. Simultaneously, an AI will be developed and optimized to engineer LCCs for high-value applications.




**An overview of the main objectives of the AI4LCC consortium**

The main HTT process conditions that have been monitored and optimized for the production of LCCs from birch wood were severity (P factor) and the liquid to solid ratio (L/S). The obtained LCCs were analyzed with, i.a. comprehensive NMR ($^{13}C$, $^{31}P$, and HSQC NMR), wet chemistry, and gel permeation chromatography. The highest yield of LCCs was obtained with a moderate P factor (~400-600) and L/S=1. With a low P factor, the carbohydrate content was high, and by increasing the P factor, the carbohydrate content decreased. Due to the high carbohydrate content at low P factor, the amount of hydroxyalkylated groups was substantial. The molecular weight and the glass transition temperature increased with the increased P factor. The S/G ratio in the LCCs was not affected by an increase in the P factor. Acid methanolysis followed by GC analysis showed that the main carbohydrate in the LCCs was xylan. Furthermore, the surface activity of LCCs was reduced with severe HTT conditions. LCC nanoparticles were produced directly from the solvent extract and showed a promising application in e.g. stabilizing THFMA emulsions.

**Cooperation:** Aalto University, BOKU (Austria), Univ. of Wollongong (Australia), St1 Oy, Kemira Oy

## Hybrid nanocomposite (bio)inks/(bio)resins based on woody nanomaterials and biopolymers in building biomedical hydrogels *via* light-based 3D printing

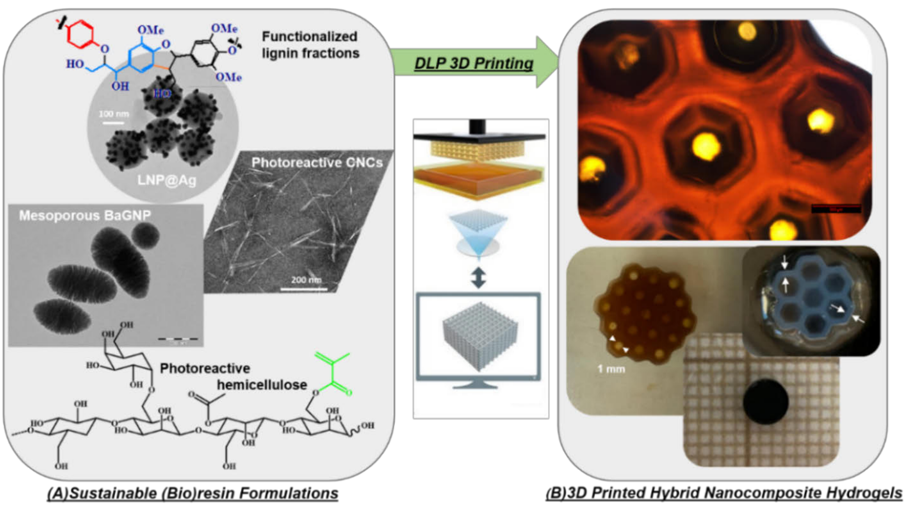
Main funding: Academy of Finland, Jane and Aatos Erkko Foundation, UPM Biomedical, Bayer

*Qingbo Wang, Xue Zhang, Wenyang Xu, Oskar Backman, Luyao Wang, Chunlin Xu and Xiaoju Wang (P.I.)*

Biomedical hydrogels are one intriguing profiling area for wood-derived lignocellulosic nanomaterials and biopolymers, where in lieu of their synthetic counterparts they offer not only sustainability but also many as-preferred characteristics as biomaterials. These competitive niches mainly refer to high mechanical strength of the nanofiber, broad modifying capacity in polysaccharide chemistry, and the most important, excellent biocompatibility of these biopolymers with respect to the most crucial cellular activities, etc. To produce biologically relevant hydrogels in high efficiency, additive manufacturing has been established as a mainstream approach. At present, light-based 3D printing techniques based on hydrogel extrusion of (bio)inks synchronizing with photocrosslinking or on layer-by-layer photocuring of (bio)resin in digital light processing (DLP) printing are applicable by offering adequate spatial resolution and pattern fidelity with rapid fabrication speed. When formulating the bioink/bioresin system, the nanocomposite approach is integrative to increase the bio-relevant functions of the hydrogel and even to embed biological cues in it in order to obtain direct cell response in a controlled manner.

The ongoing Academy of Finland Research Fellow project SusCellInk and the 'Healing the wounds with Finnish woods' project funded by Jane and Aatos Erkko Foundation (09.2019-12.2022) are operating in the field of developing renewable and sustainable nanocomposite bioinks/-resins for 3D bioprinting. The research activities are focused on tailoring chemistry to a few woody lignocellulosic nanomaterials and biopolymers, including both types of nanocellulose (CNF and CNC), lignin nanoparticles (LNP), and hemicelluloses to better integrate these in the bioink/-resin system. Meanwhile, hybrid strategies are extended in several ongoing research lines:

i) to construct hybrid hydrogel biomaterials with inorganic bionanoceramics such as bioactive glass nanoparticles (BaGNP) in delivery of therapeutic ions for bone tissue regeneration;
ii) to hybrid or composite with electroactive materials such as 2D inorganic MXene or conducting polymer (polypyrrole) for fabricating 3D conductive hydrogels as a biointerfacing matrix to more efficiently deliver endogenous electrical stimulation in accelerating wound healing;
iii) to hybrid lignin nanospheres with surface-embedded silver nanoparticles (LNP@Ags) as a high-performance nanoantibiotic in 3D fabricated antimicrobial woody biopolymer hydrogels.




*(A) natural polymers and nanostructured building blocks used for formulating bioresin and (B) nanocomposite hydrogels printed via DLP printing (DLP illustration in the middle is adapted from Schwab et al., (2020) Chem. Rev. 120, 11028).*

**Cooperation:** Leena Hupa, Rose-Marie Latonen (PCC) and Jessica Rosenholm (Pharmaceutical Sciences Laboratory, ÅAU); Susanna Miettinen (Tampere University); Gordon Wallace (University of Wollongong, Australia).

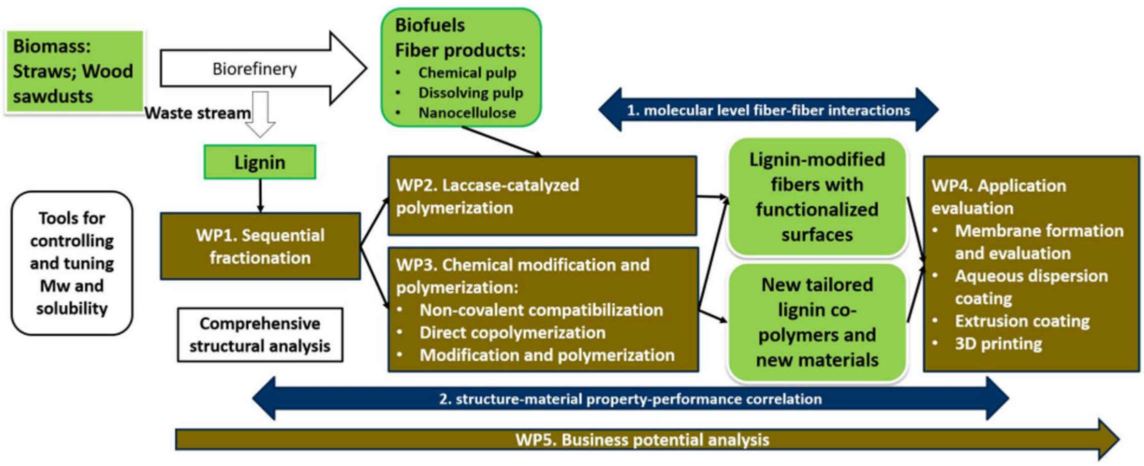
# Novel Fiber Surfaces Functionalized by Lignins Refined and Engineered from Finnish Biorefinery Processes (LigninReSurf)

Main funding: Business Finland

*Luyao Wang, Lucas Lagerquist, Minette Kvikant, Ellen Sundström, Denis Bouyer, Thomas Rosenau, Patrik Eklund, Chunlin Xu*

The forest biorefinery concept has recently been developed in Finnish society to provide upgraded pulping fibers, hemicelluloses, and lignin biopolymers that are renewable and sustainable alternatives to traditional fossil petrochemicals for novel products and applications. Lignin is the most abundant aromatic biopolymer and constitutes up to 30% of the dry mass of plants. So far, the valorization of lignin is still challenged by the inherent heterogeneity of lignin and the lack of innovative processing approaches.

To date, isolation of lignin with narrow structural complexity and molar mass dispersity through lignin fractionation is one of the primary strategies to engineer lignin into value-added materials. The LigninReSurf consortium project aims at understanding chemical structure versus material properties by studying well-defined fractions of lignin from Finnish biorefinery processes in order to utilize the fractions in their unmodified form, or as biochemical and chemical derivatives in high-performance copolymers and materials for membranes, functional coatings, packaging, and other bioplastic materials.




*The objectives of LigninReSurf consortium project and work tasks as well as the value chain.*

Different lignin fractionation methodologies (e.g., multi-alcohol fractionation, gradient ethanol/water extraction, successive acid precipitation, and membrane ultrafiltration) are used to fractionate the lignins (**WP1**). The properties of each lignin fraction, as chemical compositions, molar mass characteristics, functional group distributions, and physicochemical properties are determined by advanced analysis methods. The outcomes are highly significant for researchers and industries focusing on lignin and biomass utilization. Moreover, a biochemical method for *in situ* lignin polymerization using laccase in fiber suspension was developed, and the aqueous dispersion coating of fiber/lignin with tailored properties will be practiced for functional surface and packaging application (**WP2&WP4**). In addition, new non-covalently and covalently modified lignin derivatives as well as directly polymerized lignin copolymers are utilized in the fabrication of fiber-based porous membranes for water purification and thermoplastic composites based on the optimized lignin macromonomers from WP1 (**WP3&WP4**). The thermoplastic lignin derivatives will be utilized in extrusion coating and adhesive coating *via* 3D printing, which has promising market potentials.

The LigninReSurf project will result in a better understanding of the structure-material property-performance correlation, which is important for the development of feasible approaches to valorize lignin.

**Cooperation:** Université Montpellier (France), BOKU (Austria), Mirka Ltd, Metgen Oy, CH-bioforce Oy, St1 Oy, Kemira Oyj, 3D Tech Oy

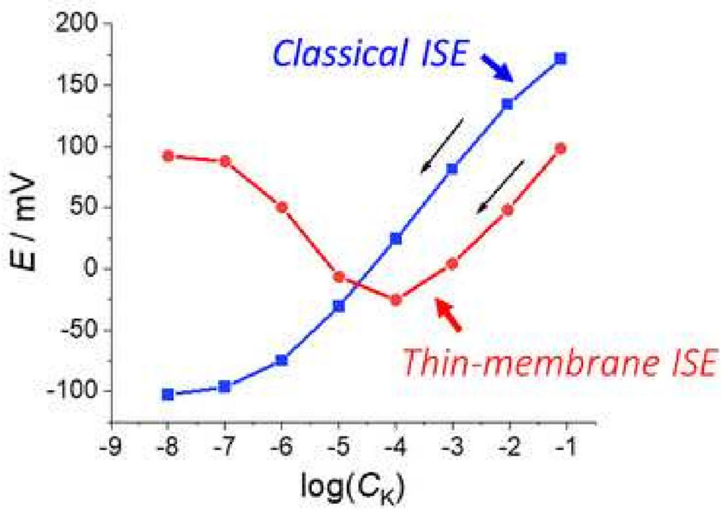
## Anomalous potentiometric response of solid-contact ion-selective electrodes with thin-layer membrane

Main funding: Academy of Finland

*Tingting Han, Andrey V. Kalinichev, Zekra Mousavi, Konstantin N. Mikhelson, Johan Bobacka*

In recent years it has become more common to use thin-layer membranes in various types of ion-selective electrodes. Thin-layer ion-selective membranes show a much lower resistance and therefore make it possible to utilize voltammetric transduction methods, in addition to potentiometry. However, the potentiometric performance of thin ion-selective membranes has not been studied in sufficient detail.

In this work, the potentiometric response of solid-contact ion-selective electrodes (SCISEs) with thin-layer ion-selective membranes (ISMs) was characterized. When calibrating potassium ion-selective solid-contact electrodes ($K^+$-SCISEs) with thin-layer membrane at a constant background concentration of 0.1 M NaCl, an anomalous increase in potential was observed at low concentrations of the primary potassium ion, as illustrated in the figure below.




*Anomalous potentiometric response of solid-contact ion-selective electrode with thin membrane*

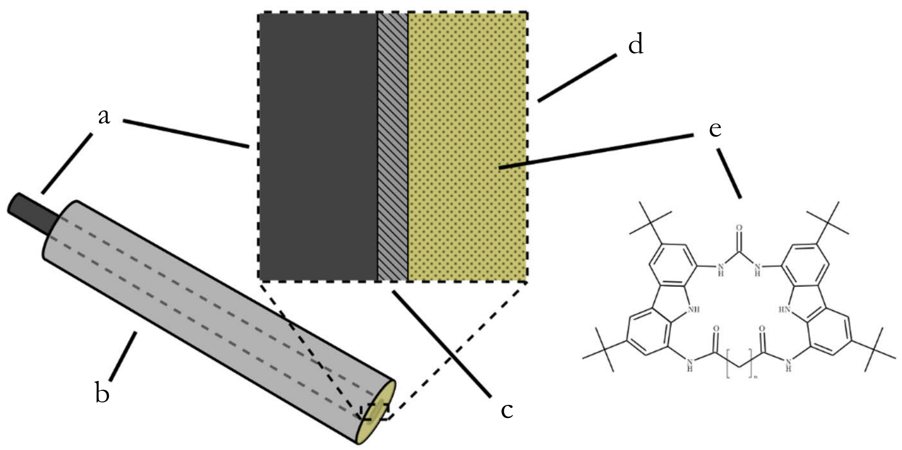
This unusual response was found to be strongly influenced by the thickness of the ISM, the lipophilicity of the solid-contact material, and the timescale of the potentiometric measurement, while the composition of the ISM had only a minor effect. It was concluded that the anomalous potentiometric response is a characteristic feature of SCISEs with thin-layer ISMs and originates from a relatively rapid change of the composition of the water layer between the ISM and the solid contact. Thus, the reported anomalous behavior of SCISEs with thin-layer ISMs, together with the established water layer test, can be used as a diagnostic tool indicating the presence of water between the ISM and the solid contact. The results emphasize the importance of using a sufficiently hydrophobic solid-contact material whenever a thin-layer ISM is employed.

# Development of potentiometric anion-selective electrodes

Funding: Magnus Ehrnrooth Foundation, Åbo Akademi, Svenska Litteratursällskapet i Finland

*Ville Yrjänä, Sajana Manandhar, Indrek Saar, Johan Bobacka*

Potentiometric ion-selective electrodes (ISEs) are used in applications requiring the ability to determine the activity of a particular type of ion. pH measurement, the determination of sodium levels in blood samples, and the determination of fluoride levels in aqueous samples are a few examples of such applications. Ion recognition is often handled by an ionophore, which is added to an ion-selective membrane (ISM) to selectively bind certain ions. Organic anions have proven themselves to be particularly challenging analytes. For example, in many cases a large variety of other species with significant structural similarities exist and may also form stable complexes with the ionophore. Also, the association/dissociation of the ionophore, the analyte, or both may drastically affect the stability of the complex. pH adjustment of the sample solution may be necessary, but this may in turn increase the concentration of strongly interfering species in the sample due to the shift in equilibria or the addition of new species. Water also acts as a competitor to the ionophore due to strong solvation of the analyte.




*Overview of a solid-contact ion-selective electrode: a) an electronically conducting substrate, b) an insulating shell, c) an ion-to-electron transducer, d) an ion-selective membrane, and e) an ionophore incorporated into the membrane.*

Our collaborative research project has focused on the development and application of ISEs for carboxylates. The work covers the design, synthesis, and characterization of ionophores to the development, characterization, optimization, and application of ISEs that incorporate those ionophores. The synthesis of several novel acyclic and macrocyclic ionophores has been performed and followed by binding studies. Solid-contact ISEs with different membrane compositions and electrode shell materials have been prepared and characterized. Disruption of the anion recognition process, possibly due to the diffusion of a component in one of the shell materials, was observed. Some of the ISEs were used to determine benzoate concentrations in complex sample matrices prepared from frozen berries. The potentiometric method was compared with one based on ion chromatographic separation and conductometric detection, and similar concentrations were attained with both methods. However, the potentiometric method required less extensive sample preparation and all of the required equipment is more portable.

**Cooperation:** University of Tartu (Estonia)

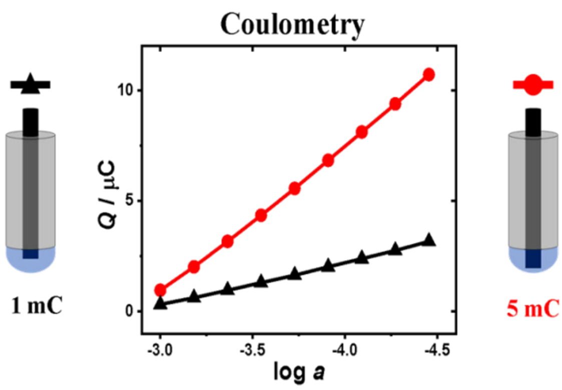
# Novel signal transduction principle enabling high-precision ion sensing

Main funding: Academy of Finland

*Tingting Han, Rustem Rustem, Ulriika Mattinen, Zekra Mousavi, Johan Bobacka*

A new coulometric transduction method for solid-contact ion-selective electrodes (SCISEs) was proposed by our group. In comparison with traditional potentiometry, an advantage of the coulometric method is that the analytical signal can be amplified by increasing the capacitance of the solid-contact. The figure below shows an example of the coulometric response for SCISEs with 1 mC and 5 mC solid contact of PEDOT(PSS), i.e. poly(3,4-ethylenedioxythiophene) doped with polystyrene sulfonate.

*Increasing the capacitance of the solid contact improves the sensitivity of solid-contact ion-selective electrodes.*




Interesting features were observed when comparing the coulometric response of SCISEs for two divalent cations ($Pb^{2+}$ and $Ca^{2+}$). The coulometric response of the $Pb^{2+}$-SCISEs was mainly limited by ion transport in the PEDOT(PSS) solid-contact layer, while the coulometric response of $Ca^{2+}$-SCISEs was mainly dependent on the ion transport through the ion-selective membrane. Furthermore, anion sensors based on PEDOT doped with different counterions were studied using the coulometric transduction method and cyclic voltammetry. All the results indicate that the coulometric method is appropriate and feasible for SCISEs. The high sensitivity of the coulometric method is particularly important for applications in clinical analysis and in wearable sensors for personal health monitoring, where the relevant concentration range is narrow.

The coulometric signal transduction method was compared with the traditional potentiometric method in studying the functionality of SCISEs with physically damaged ion-selective membrane (ISM). The aim was to determine which of these methods (coulometry vs. potentiometry) could be more suitable to evaluate the condition of a SCISE. It was shown that the type of electrode used and the background electrolyte present are determining factors. For example, chloride ion-selective electrodes with poly(3,4-ethylenedioxythiophene) (PEDOT) doped with chloride anions ($Cl^-$), i.e. PEDOT(Cl), as solid-contact showed near-Nernstian potentiometric response even after damaging the ISM. This is due to the fact that PEDOT(Cl) itself is sensitive to $Cl^-$ even without an ISM. However, in the case of potassium ion-selective electrode (K-ISE) based on PEDOT doped with poly(styrene sulfonate) (PSS), i.e. PEDOT(PSS), the malfunction of the electrode response with damaged ISM was noticeable in both methods. Hence, the coulometric transduction method was able to identify a malfunctioning SCISE under situations where potentiometry did not indicate any malfunction.

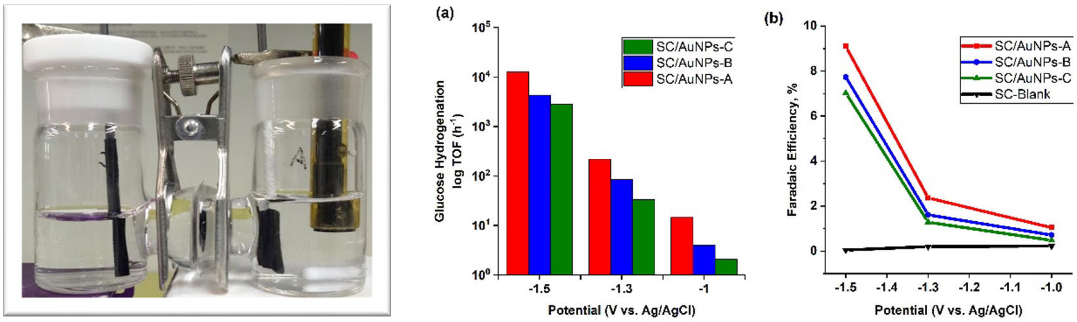
**Cooperation:** University of Geneva (Switzerland), University of Memphis (USA), Thermo Fisher Scientific (Finland)

# From fossil to biohydrogen in Finnish (bio)industry - utilizing electrocatalysis in aqueous phase reforming of hemicelluloses (FosToBioH2)

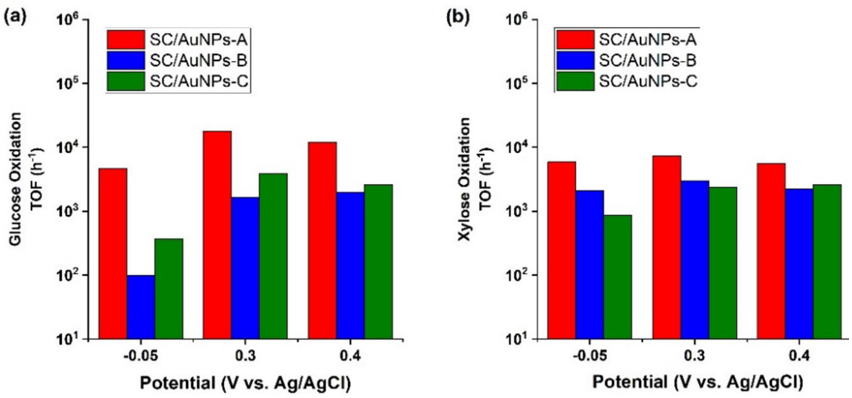
Main funding: Tiina and Antti Herlin Foundation

*Jay Pee Oña, Rose-Marie Latonen, Narendra Kumar, Henrik Grénman*

Catalytic conversion of biomass into fuels and value-added chemicals is a viable technology that can reduce our dependence on fossil fuels and mitigate global warming. In order to generate energy-dense chemicals and fuels, biomass-derived feedstocks need to be catalytically hydrogenated to achieve a high H:C ratio. This research focuses on the hydrogenation of glucose and xylose - two main components of wood hemicellulose - through an electrocatalytic route. Electrocatalytic hydrogenation (ECH) was carried out in ambient conditions and utilized water as source of hydrogen, thereby eliminating the use of high purity hydrogen gas. Gold was chosen as catalyst for ECH in this study due to its high selectivity and appreciable activity towards glucose hydrogenation. The conversion of glucose into sorbitol and xylose into xylitol was performed over different Au nanocatalysts to investigate the influence of the metal cluster size and surface area on the overall rate of conversion. The hydrogenation products - sorbitol and xylitol - can undergo aqueous phase reforming (APR) to produce (bio)hydrogen. Furthermore, recognizing the high activity of the fabricated carbon-supported Au nanocatalysts toward sugar electro-oxidation, catalyst structure-activity relationships were also explored. Results obtained so far contribute to the growing body of knowledge on the valorization of biomass through electrocatalysis which fit well within the context of wood-based biorefining.




*Electrocatalytic conversion of sugars carried out in an H-type electrochemical cell (left). Figures on the right show the activity and selectivity (Faradaic Efficiency) of three types of catalysts with different Au nanoparticle sizes (SC/AuNPs-A: 4.4nm, SC/AuNPs-B: 5.9 nm, SC/AuNPs-C: 88nm) towards glucose hydrogenation to sorbitol (TOF = Turnover frequency).*




*Catalytic activities of different Sibunit Carbon-supported Au nanoparticles (SC/AuNPs) towards oxidation of glucose to gluconic acid (a) and xylose to xylonic acid (b) (TOF = Turnover frequency)*

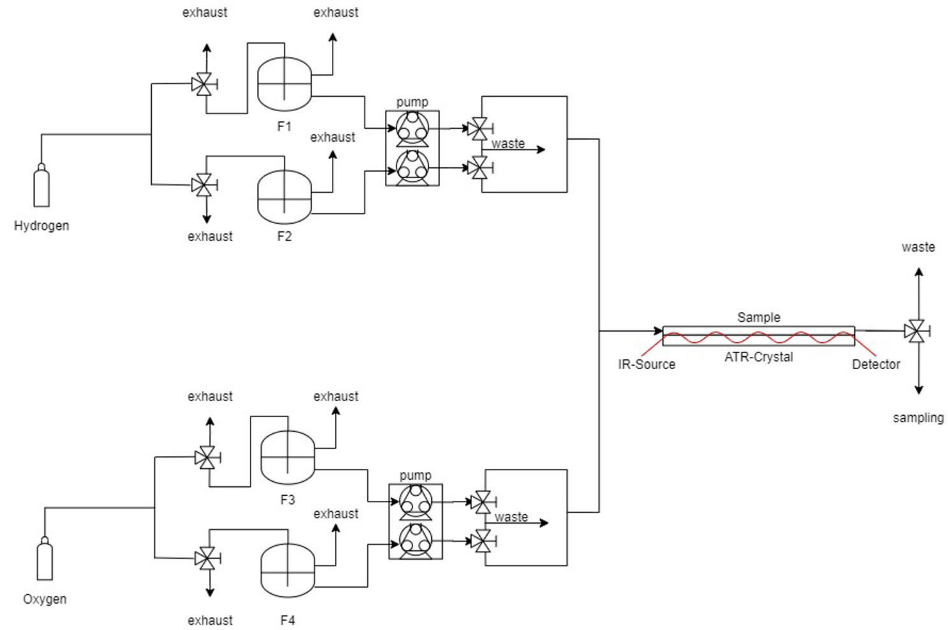
**Cooperation:**
Delft University of Technology

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

Main funding: Academy of Finland (Academy Professor's project 2019-2024), Åbo Akademi, Normandie Université INSA-Rouen, Università di Napoli, Università di Padova, Universidad de Valladolid, Helmholtz-Zentrum Dresden Rossendorf

*Tapio Salmi, Kari Eränen, Pasi Tolvanen, Adriana Freites Aguilera, Wander Perez Sena , Ole Reinsdorf, Matias Alvear, Christoph Schmidt, German Araujo Barahona, Michele Fortunato, Federica Orabona, Francesco Sandri, Tommaso Cogliano, Pontus Lindroos, Wilhelm Wikström, Marie-Louis Reich, Jani Rahkila, Dmitry Murzin, Johan Wärnå, Liisa Kanerva, Vincenzo Russo, Sébastien Leveneur, Rüdiger Lange, Stefan Haase, Mario Zecca, Paolo Centomo, Uwe Hampel, Markus Schubert*

The main focus of this large project financed by Academy of Finland is the investigation of reaction mechanisms with the aid of in situ and transient techniques. The project is the biggest one in the 100 year history of Industrial chemistry and reaction engineering at Åbo Akademi, providing a strong bridge between fundamental mechanistic investigations and new reactor technology. Conventional methods for investigating chemical kinetics arebased on the measurement of concentration changes as a function of reaction times in batch and semibatch reactors. 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 to get a better understanding on reaction mechanisms and to establish adequate kinetic model and mass transfer models for future 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. A globally pioneering work is going on.

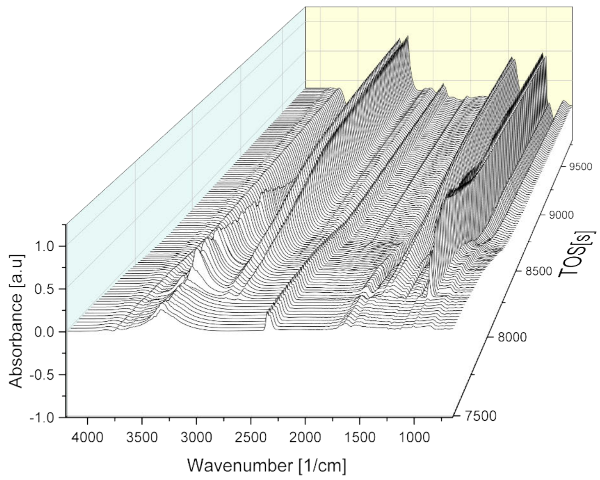



*In situ ATR reactor setup (K. Eränen and O. Reinsdorf).*

The molecules which are studied are biodegradable and originate from biomass. 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. Without a deep-going understanding of the underlying reaction mechanisms, a rational process design is not possible. The project is going on with studies of the reaction mechanisms of hydrogen peroxide direct synthesis, epoxidation of alkenes and fatty acids as well as catalytic oxidation of sugars. Molecular oxygen is used as the oxidant, whereas hydrogen peroxide is s the epoxidation agent. Three laboratory-scale trickle-bed reactors for step and pulse experiments are used in the transient studies of reaction mechanisms and an ATR spectroscopic device is a strong tool in hands to reveal intermediate chemical species on solid surfaces.

### *Direct synthesis of hydrogen peroxide*

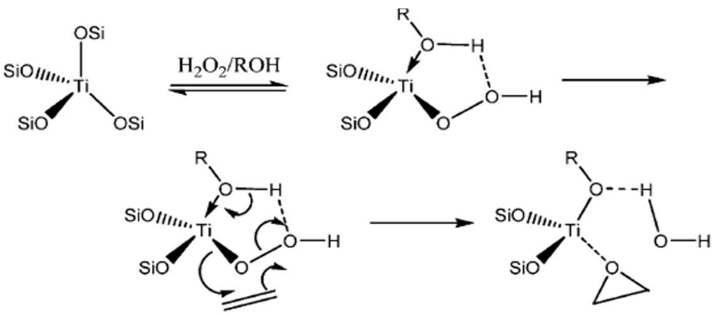
The direct synthesis of hydrogen peroxide from hydrogen and oxygen is an attractive reaction pathway, because the process is clean, green and simple compared to the established indirect anthraquinone process. The experimental set up for the direct synthesis consists of a concurrent downflow tubular trickle bed reactor. Transient and stationary experiments are conducted out at using both commercial and laboratory-prepared Pd and Pd/Au catalysts on inorganic and polymer carriers. Switching the solvent from water to an alcohol (methanol, ethanol or isopropanol) has revealed the active role of the solvent in the reaction mechanism – this is a completely new discovery. Oscillatory phenomena were detected in the transient experiments. After the switch from water to alcohol, the concentration profile of hydrogen peroxide started to undergo a pattern of four maxima. A similar oscillatory behavior was detected in the presence of ethanol and iso-propanol. The oscillations were confirmed by ATR experiments. A reaction mechanism was proposed based on these observations.



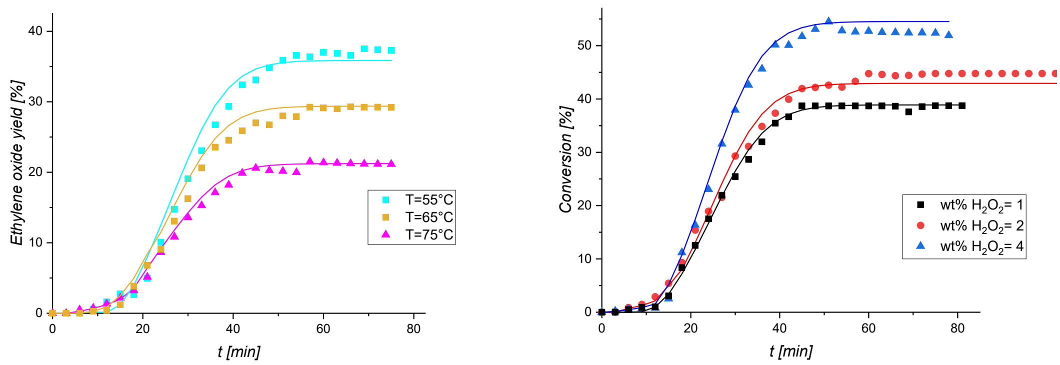

*Transient response from the FTIR-ATR set-up (O. Reinsdorf).*

### *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 with transient experiments in trickle bed reactors as well with ATR spectroscopy. Titanium silicalite (TS-1) is used as the heterogeneous catalyst and methanol is a typical solvent. The heterogeneous catalyst is placed 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 ethane, 1-propene, 1-butene, iso-butene and hydrogen peroxide are used in the experiments. The water-to-methanol ratio, the hydrogen peroxide-to-alkene ratio and the reaction temperature and pressure as well as the gas and liquid flow rates are studied to observe the changes in the reactant conversion and the product distribution.




*Mechanism of ethylene epoxidation via TS-1 and $H_2O_2$.*




*Experiments and modelling of transient behavior of ethylene epoxidation on TS-1 (M. Alvear and M. Fortunato).*

The alkene oxides were always the main products, but minor amounts of ring-opening products formed from the epoxide and the alcohol solvent were detected. In case of 2-butene epoxidation, a broader product distribution was obtained, leading to a complex consecutive and parallel reaction network. The reaction temperature had an important effect on selectivity. The increase of the excess of $H_2O_2$ in the feed improved the yield of the epoxide. Detailed modelling was carried out.

### *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.

Epoxidation of oleic acid, tall oil fatty acids (TOFA) and distilled tall oil (DTO) has been 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 and Novozym435 were s used as the solid heterogeneous catalysts. Novozym435 is an immobilized enzyme, which enables direct epoxidation of fatty acids, without the presence of a reaction carrier. The catalyst loading effect, the reactant ratios, the reaction temperature (40-70°C) and the influence of microwave and acoustic 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. Ultrasound irradiation had a clearly positive effect on the direct epoxidation process and considerable rate enhancement was achieve with this technique. Detailed kinetic and mass transfer modelling was conducted, and a completely new and very demanding multiphase reaction and reactor model was published.

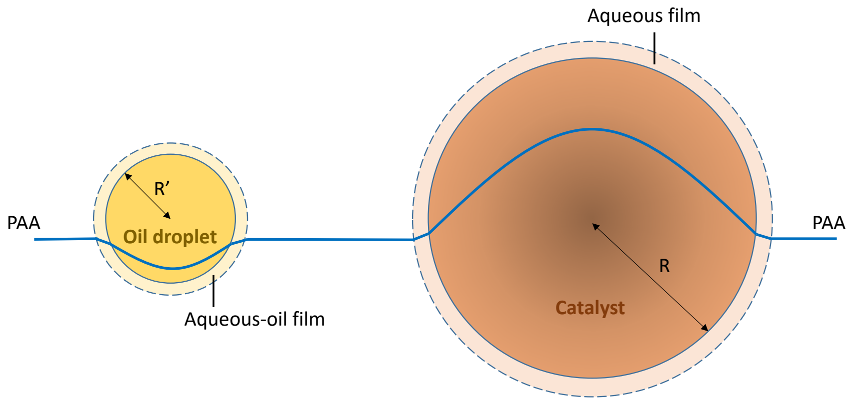
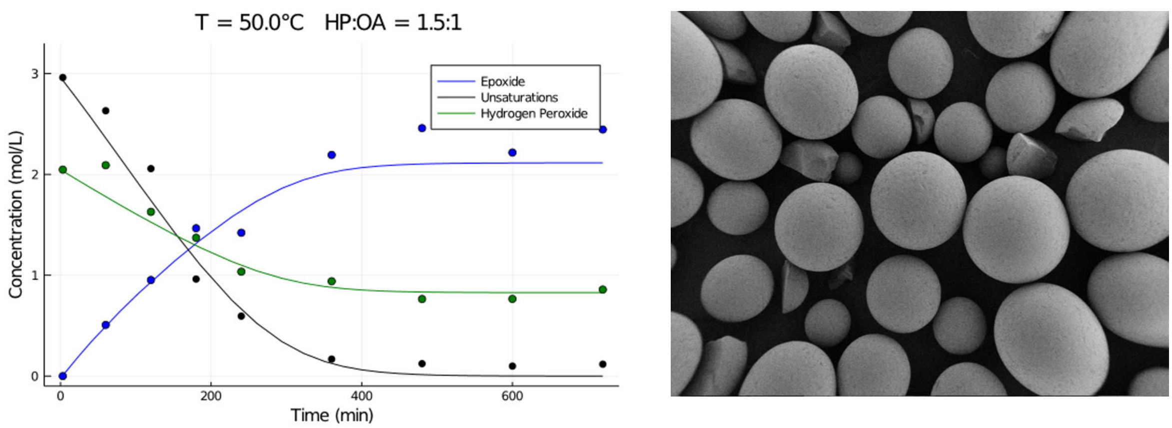



*Illustration of kinetics and mass transfer in fatty acid epoxidation (T. Salmi, V. Russo, A. Freites Aguilera).*

The doctoral thesis of Adriana Freites Aguilera got the very prestigious award, Elfving's legat' as the best doctoral thesis at Åbo Akademi for the academic year 2020-2021. The award was granted by *Rectora Magnifica* of our university and it got a large publicity. The monumental doctoral work was based on 8 journal articles and 14 conference presentations. It was granted the highest mark, with distinction by the Faculty of science and engineering (FNT) at Åbo Akademi University.




*Experimental and modelled oleic acid epoxidation kinetics on Novozym435 (A. Freites Aguilera, P. Lindroos, L. Kanerva, T. Salmi)*

**Cooperation**: Normandie Université INSA-Rouen, Università di Napoli 'Federico II', Università di Padova, Technische Universität Dresden (TUD), Universidad de Valladolid, University of Wisconsin, University of Turku

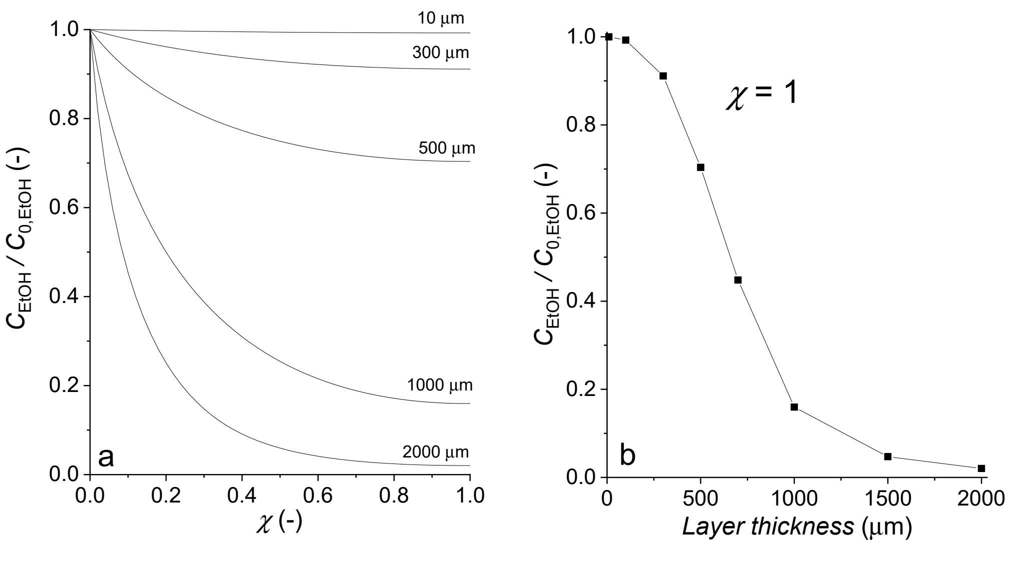
# Process intensification I: Microreactor technology

Main funding: Academy of Finland, Università di Napoli

*Kari Eränen, Rossana Suerz, Luca Mastroianni, Zuzana Vajglová, Narendra Kumar, Teuvo Kilpiö, Vincenzo Russo, Yaseen Khan, Juha Lehtonen, J.-P. Mikkola, Johan Wärnå, Dmitry Murzin, Tapio Salmi*

Microreactor technology is one of the revolutions of chemical reaction engineering. 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 comprise 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. In recent years, we have studied dehydration and oxidation of alcohols.

Partial oxidation of primary alcohols to produce aldehydes is one of the key reactions in organic chemistry. Molecular oxygen as an oxidant represents a clean alternative to the traditionally employed chromium-based stoichiometric reagents, which are harmful for both human beings and environment. Selective oxidation of methanol, ethanol, 1-propanol and 1-butanol was conducted in a microreactor with Au/$\gamma$-$Al_2O_3$ coated catalyst. Nanoparticle size distribution, acidity, specific surface area and the average pore size as well as uniformity and thickness of the coating layer were evaluated with relevant characterization techniques. The experiments were designed to reveal the effect of temperature, residence time and oxygen-to-alcohol ratio on both alcohol conversion and product distribution. Stability and repeatability of the coating procedure was successfully demonstrated. To describe the reaction kinetics, plausible kinetic equations were implemented in a pseudo-homogeneous plug flow model, which is an adequate approximation to describe the flow pattern in microreactors. Non-linear regression analysis enabled the determination of kinetic and adsorption parameters. An advanced kinetic and mass transfer model was developed to reveal the impact of the diffusion inside the catalytic washcoat layer, demonstrating that molecular diffusion is not a limiting factor for alcohol oxidation in the microreactor.




*Intrawashcoat concentrations profile of ethanol at different catalytic layer thicknesses b) dimensionless concentration vs layer thickness at $\chi$ = 1. (L. Mastroianni, V. Russo, T. Salmi)*

**Cooperation**: Università di Napoli 'Federico II', Italy

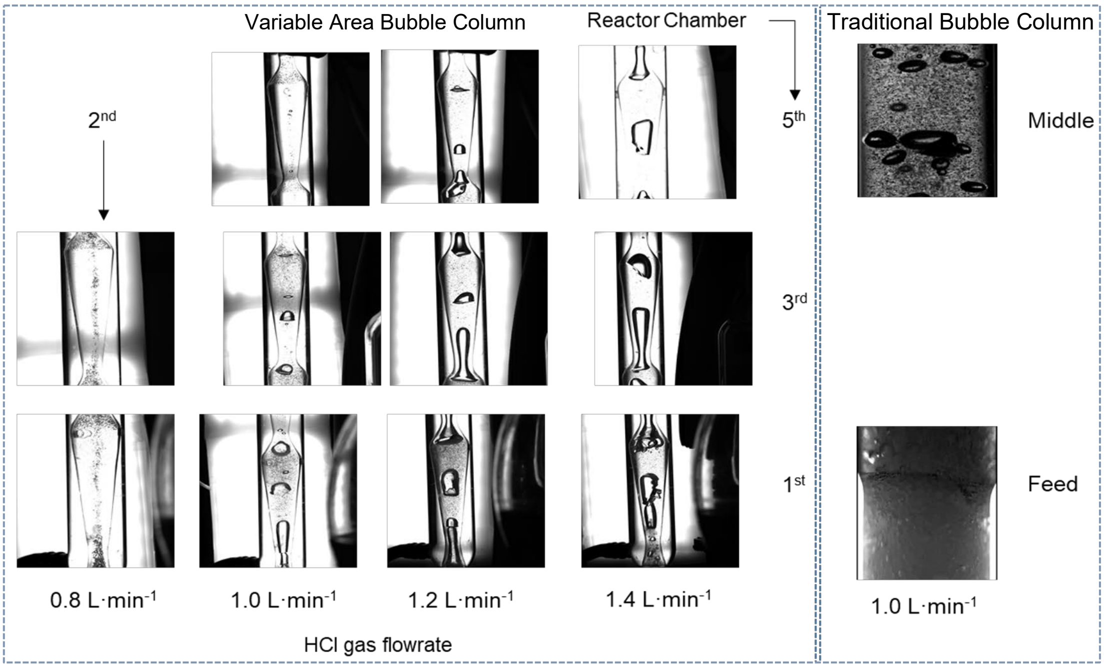
## Process intensification II: Novel multiphase reactor structures

Main funding: PCC, Graduate School in Chemical Engineering (GSCE), Academy of Finland, Magnus Ehrnrooth Foundation, Finnish Cultural Foundation, Svenska kulturfonden, Svenska litteratursällskapet i Finland, Åbo Akademi

*Johan Wärnå, Teuvo Kilpiö, Pasi Tolvanen, Cesar de Araujo Filho, Adriana Freites Aguilera, Atte Aho, Wander Perez Sena, Javier Ibanez Abad, Catarina Braz, Ananias Medina, German Araujo Barahona, Debanga Mondal, Vladimir Shumilov, Ali Najarnezhadmashhadi, Maria Herrero Manzano, Mouad Hachhach, Markus Schubert, Uwe Hampel, Sébastien Leveneur, Juan Garcia Serna, Henri Matos, Jyri-Pekka Mikkola, Dmitry Murzin, Tapio Salmi*

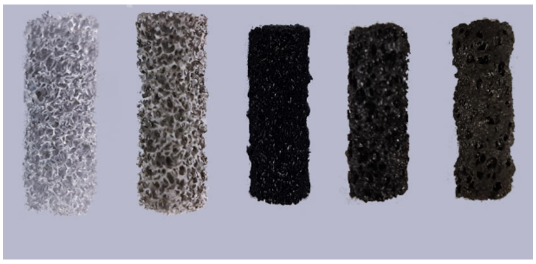
Development and advanced modelling of multiphase reactors and structured catalysts, such as solid foams is the topic of the project, involving various flow models in the bulk phases of the reactor as well as modelling of simultaneous reaction and diffusion in porous catalyst structures. The main applications are catalytic three-phase hydrogenation, oxidation, epoxidation, carbonation 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.

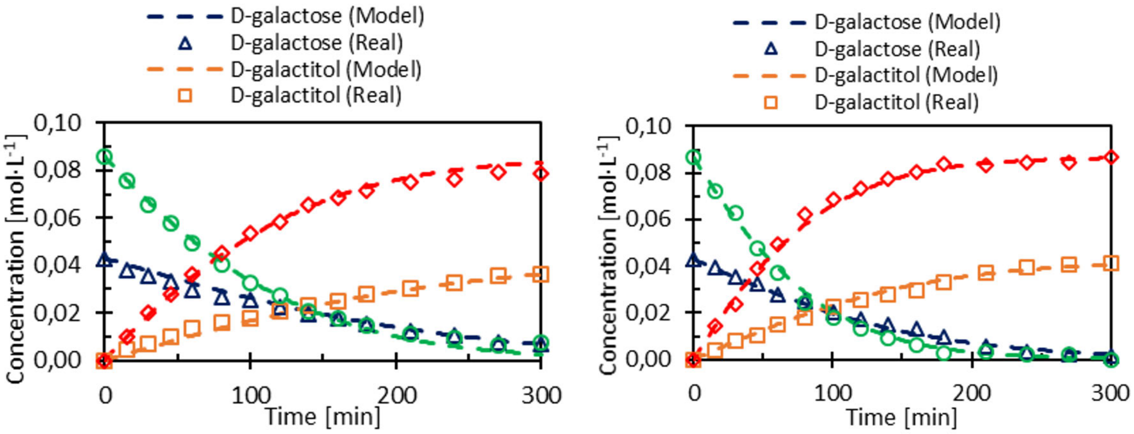



*Glycerol hydrogenation in the presence of homogeneous catalyst.*
*HCl flowrates: 0.8 – 1.4 L·min$^{-1}$, 6 mL·min$^{-1}$ of glycerol, 80 °C At the right the corresponding images of the traditional bubble column (J. Ibanez Abad, A. Medina, D. Mondal, P. Tolvanen, T. Salmi)*

Solid foams are trendy materials as catalyst structures. They haves have two great benefits: thin catalyst layers guaranteeing a high effectiveness factor and a low pressure drop in continuous operation. Solid foam catalysts were prepared on an aluminium matrix, which was coated with active carbon. The carbon-coated foam was immersed in a Ru salt solution to obtain active Ru nanoparticles for hydrogenation processes. The ability of ruthenium-based solid foam catalysts in the hydrogenation of monomeric sugars was illustrated with extensive experiments of L-arabinose and D-galactose hydrogenation. Kinetic experiments were carried out with individual sugars and binary sugar mixtures at different D-galactose-to-L-arabinose molar ratios to reveal the molecular interactions in the presence of the solid foam catalyst. The feasibility of the process was illustrated in a continuous fixed bed reactor and a batch reactor. The sugar hydrogenation process was considered from a viewpoint of elementary steps on the catalyst surface. The kinetic model based on the non-competitive adsorption of sugars and hydrogen on the ruthenium surface gave a very good description of the hydrogenation kinetics and product distribution on the solid foam catalysts. The work opens a perspective to the selective and very effective hydrogenation of several sugars to valuable sugar alcohols on solid foams, both in batch and continuous operation modes.



*Preparation stages of Ru/C open--cell foam catalyst(from left to right): untreated Al foam, anodized Al foam, Al foam coated with PFA, pyrolyzed/oxygen treated carbon-coated foam, carbon-coated, Ru impregnated and reduced catalyst (A. Najarnezhadmashhadi, G. Araujo Barahona, k. Eränen).*




*Modelling of sugar mixture hydrogenation, G:A ratio=0.5: 90 °C (left) and 100 °C (right). Modelling of sugar mixture hydrogenation data, G:A ratio=0.5: 90 °C and 100 °C.*

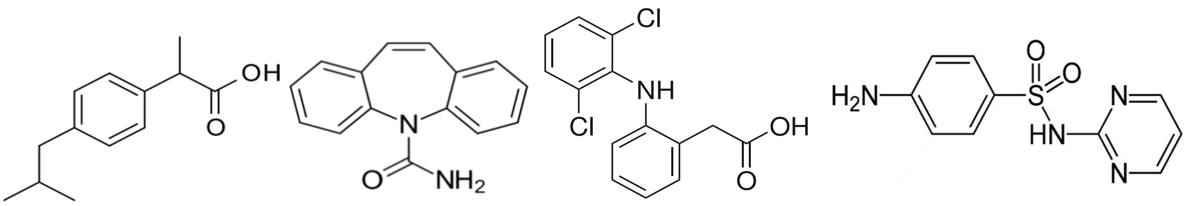
**Cooperation:** Università di Napoli 'Federico II', Normandie Université INSA Rouen, Universidad de Valladolid, Technische Universität Dresden, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Umeå University, Instituto Superior Técnico Lisboa.

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

Main funding: Åbo Akademi University, Graduate School in Chemical Engineering (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*

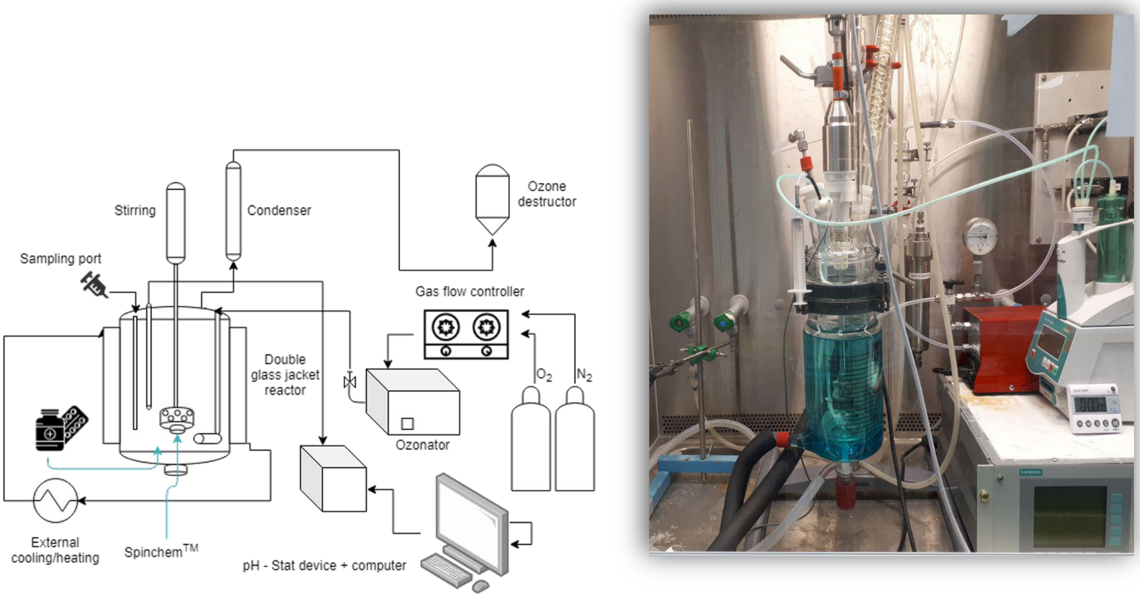
The slip of pharmaceuticals from wastewaters to aquatic environment is a serious and growing environmental problem. In spite of the very advanced wastewater treatment technologies of today, many pharmaceutical components remain in the cleaned water and end up in rivers, lakes and seas. The crowded and 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 were studied in detail in the project: ibuprofen (IBU), carbamazepine (CBZ), diclofenac (DCF) and sulfadiazine (SDZ).



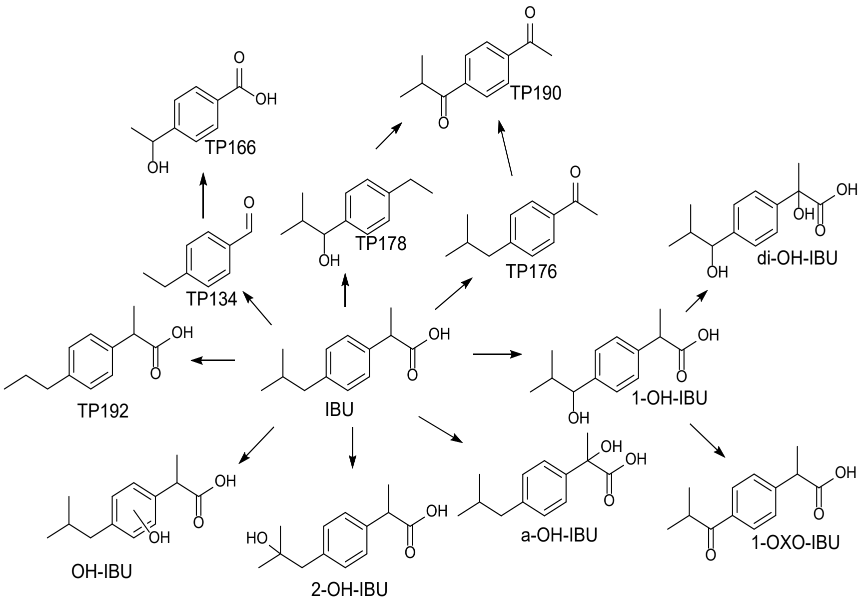
IBU CBZ DCF SDZ

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.

Compared to previous research in the subject, this 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 ibuprofene (IBU).




*Experimental device for pharmaceuticals destruction: principally and in reality ((S. Saeid, P.Tolvanen, k. Eränen).*




*Suggested transformation pathway for IBU (M. Kråkström).*

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 and confirmed in most cases. Catalyst characterization was carried out in a very fruitful 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). The doctoral thesis of Soudabeh Saeid obtained a highly ranked national prize: the award of best doctoral thesis in catalysis in Finland during the years 2019-2021. The award was given to the happy winner at the Young Scientist Forum (YSF2022) organized by Finnish Catalysis Society. She gave an excellent Award lecture at the event.

**Cooperation**: Università di Napoli, University of Turku

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

Main funding: Academy of Finland

*Zuzana Vajglová, Irina Simakova, Narendra Kumar, Päivi Mäki-Arvela, Kari Eränen, 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. 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. 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. As an example, one-pot continuous synthesis of menthols both from citronellal and citral was investigated over 5 wt% Ni supported on H-Beta-38 (or MCM-41 mesoporous alumosilicate) sepiolite composite catalysts. The reaction network of this complex reaction is shown in Figure 1.

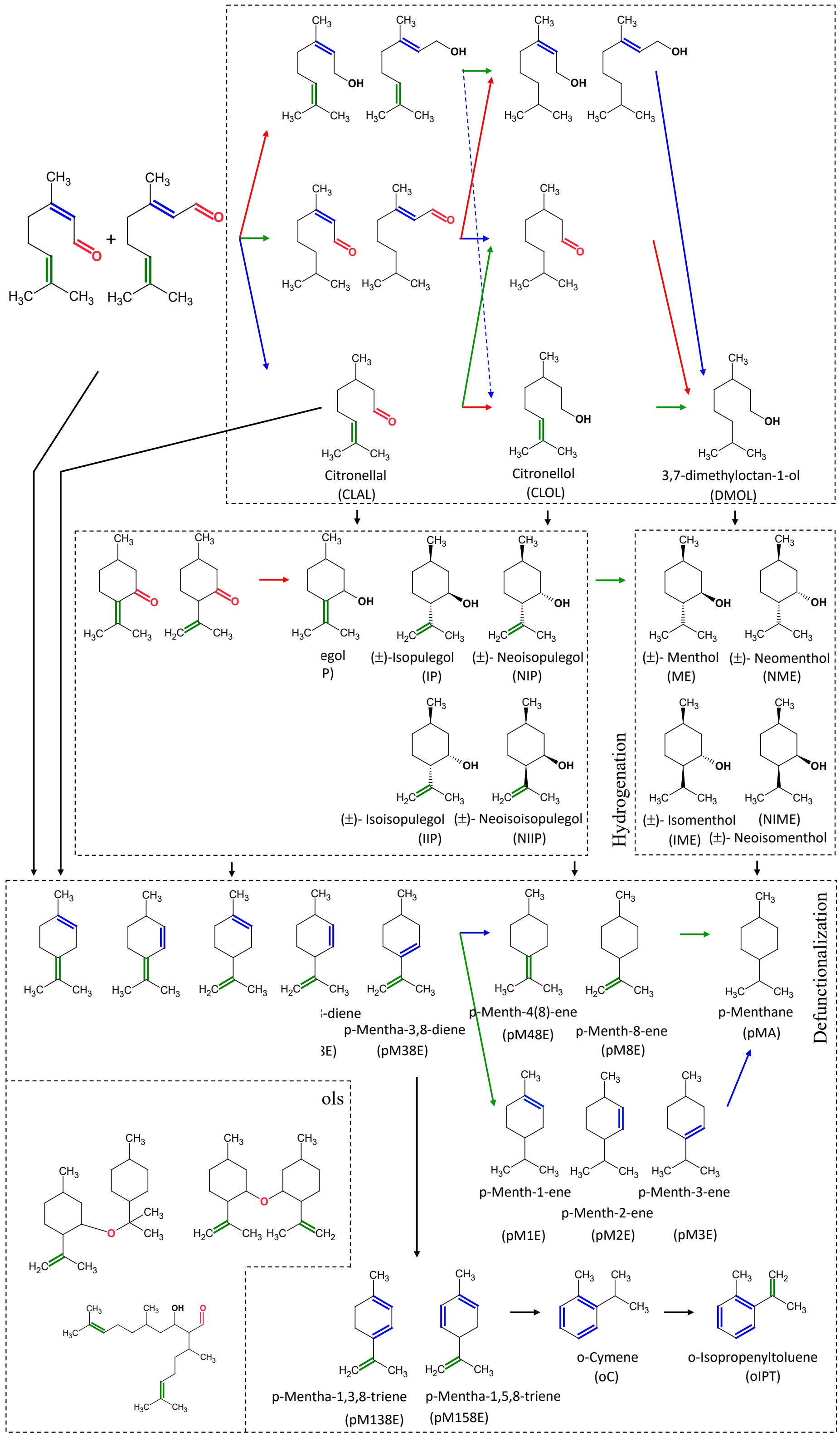



**Figure 1.** Scheme of menthol synthesis from citral with potential side reactions.

A relatively high menthols yield of 53% and 49% and stereoselectivity to menthol of 71-76% and 72-74% were obtained from citronellal and citral respectively at the contact time 4.2 min, 70ºC and 20 bar for the zeolite based composite.

With time on stream conversion of citral declined which was associated with catalyst deactivation. Kinetic analysis for citral transformations to menthol for both batch and continuous operation modes is absent in the open literature, thus in the current work a kinetic model capable of describing experimental data for transformations of citral to menthol in a continuous mode was developed for the first time. The model, including formation of the main reaction as well as side products, takes into account catalyst deactivation on two types of sites of the bifunctional catalyst. Numerical data fitting performed for the whole experimental data set confirmed applicability of the advanced kinetic model (figure 2)

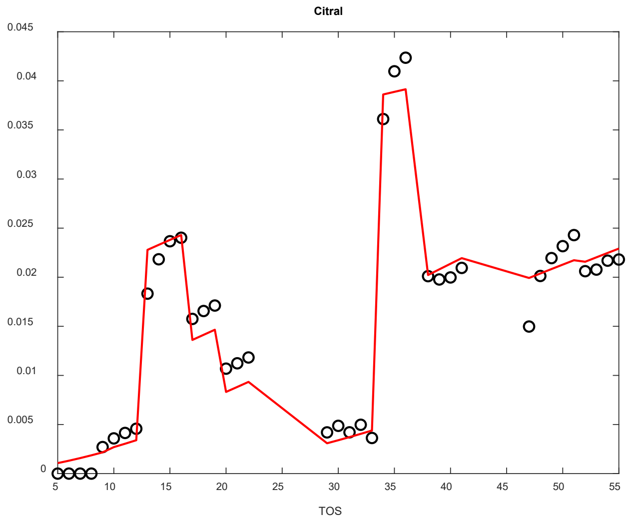



**Figure 2.** Comparison between experimental and calculated data. Time-on stream (TOS) dependence of citral.

# Mathematical modelling of hydrogen reduction of iron oxides

Main funding: Business Finland project (FFS)

*Emiliano Salucci, Nathalie Lillkaas, Henrik Grénman, Henrik Saxén*

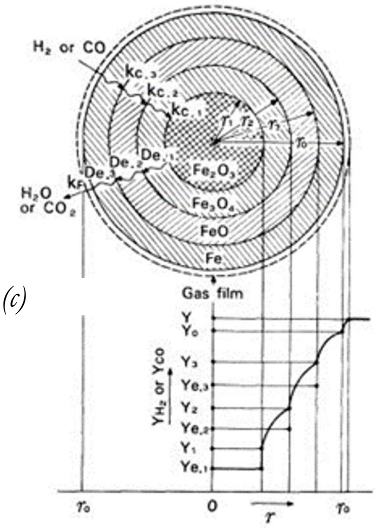
Modern steel production processes (over 1800 million tons per year) are burdened by large $CO_2$ emissions, which give rise to 7% of global anthropogenic production. The clearly biggest challenge for this industrial sector is decarbonisation which will have to be implemented in the near future. A major source of $CO_2$ emissions is when the iron oxides in iron ores are reduced to metallic iron, using coal, partially oxidized to carbon monoxide (CO), as the main reducing agent. The only valid reducing alternative to carbon is hydrogen, but for this purpose it is necessary to deeply modify the operating system by replacing the blast furnace with a suspension or direct reduction unit (DR) promoting the production of direct reduced iron (DRI).

$$\begin{cases} 3\underbrace{Fe_2O_3}_{Hematite} + H_2 \Leftrightarrow 2\underbrace{Fe_3O_4}_{Magnetite} + H_2O \\ \underbrace{Fe_3O_4}_{Magnetite} + H_2 \Leftrightarrow 3\underbrace{FeO}_{Wüstite} + H_2O \\ \underbrace{FeO}_{Wüstite} + H_2 \Leftrightarrow \underbrace{Fe}_{Iron} + H_2O \end{cases}$$

(a)

$$\begin{cases} 3\underbrace{Fe_2O_3}_{Hematite} + CO \Leftrightarrow 2\underbrace{Fe_3O_4}_{Magnetite} + CO_2 \\ \underbrace{Fe_3O_4}_{Magnetite} + CO \Leftrightarrow 3\underbrace{FeO}_{Wüstite} + CO_2 \\ \underbrace{FeO}_{Wüstite} + CO \Leftrightarrow \underbrace{Fe}_{Iron} + CO_2 \end{cases}$$

(b)



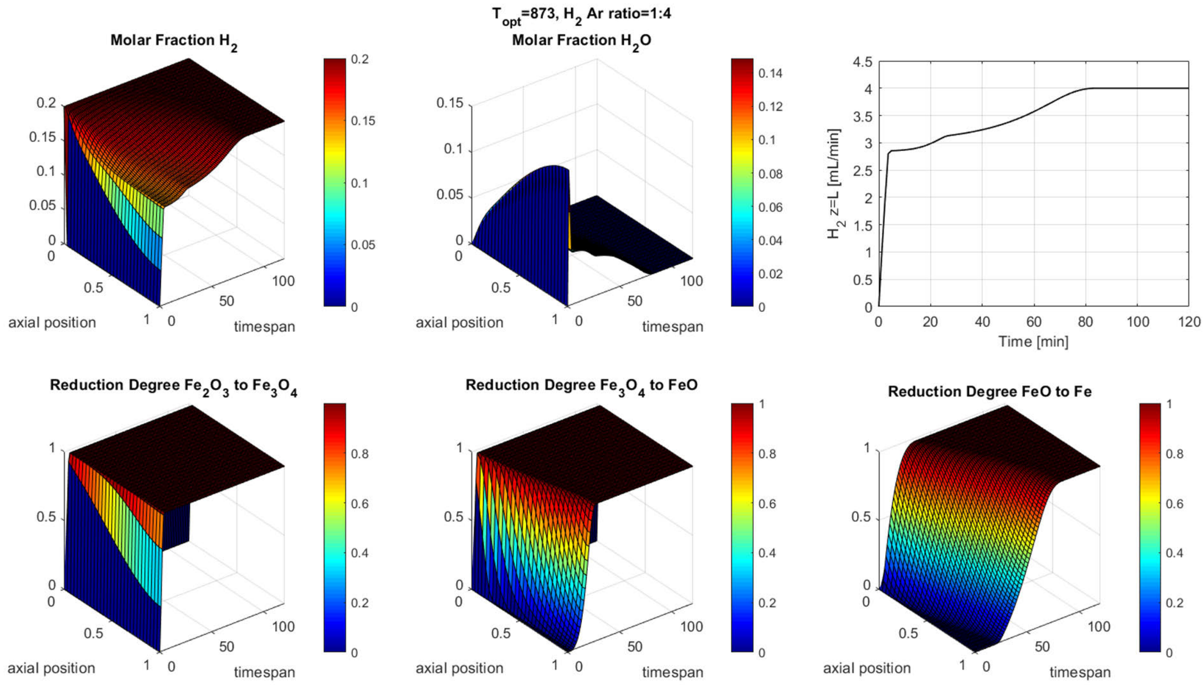

(c)

*Reduction reactive networks with reducing agent carbon monoxide (a) and hydrogen (b). Scheme of the triple front reaction in the particle (c).*

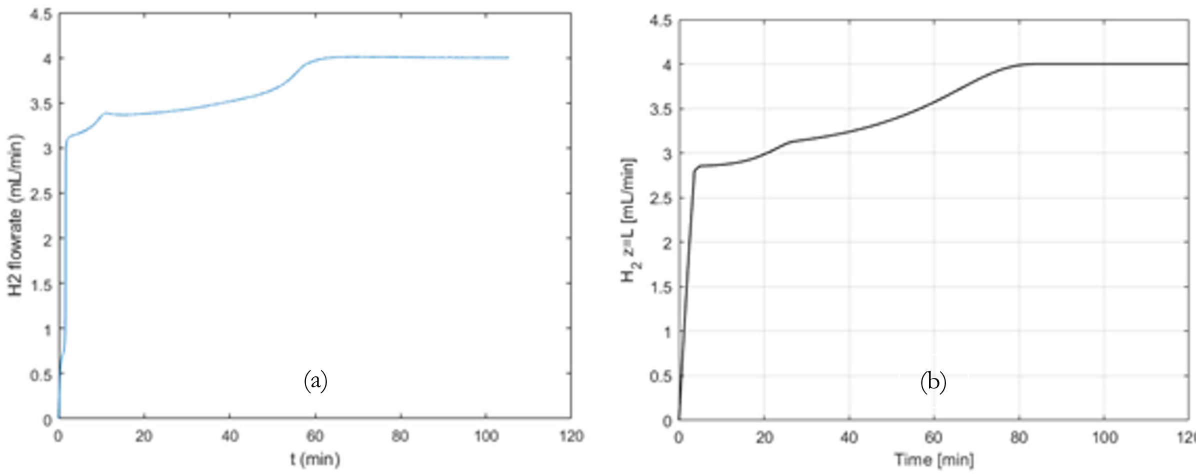
This research focuses on the development of accurate models of the reduction kinetics of iron oxides for application in process-model studies of (mainly) hydrogen-based DRI production. The modeling is partly based on results of kinetic experiments reported in the literature and partly on own reduction experiments.

First reduction experiments with fine particles were conducted, where intraparticle mass transfer resistance is considered negligible, in order to obtain information necessary for kinetic modeling. The experimental apparatus consists of a bed containing iron ore fines (previously treated) to which it is initially sent inert gas (Ar) to a defined flow rate. As soon as the system reaches the operating temperature, the composition of the gas is changed according to the percentage of hydrogen to which the system is to be subjected. Through the TCD and MS analyzes it is possible to observe the hydrogen and water content of the gas leaving the reactive bed and calculate, indirectly, the degree of reduction of iron oxides.

Starting from an in-depth study of the key assumptions of the shrinking core model and of the characteristics of the experimental apparatus, a mathematical model was developed in MATLAB in order to simulate the three different reductions that occur in the reactive system. For this purpose, mass balances have been defined for the gaseous species ($H_2$ and $H_2O$), described by partial differential equations (PDE). Ordinary differential equations (ODE) have been developed for the evaluation of the conversion degree of the three different iron oxides. The mathematical model uses the Methods or Lines for the resolution of PDEs. Using kinetic, thermodynamic, and diffusive parameters obtained or borrowed from the literature, it was possible to conduct the first simulations that seem to correctly describe the reactive network.




*Simulation obtained from the mathematical model developed starting from the assumptions of the shrinking core model. In the first line of the plot are reported: the molar fraction of hydrogen and water with respect to the axial coordinate of the reactor over time and finally the volume flow rate of hydrogen leaving the reactor over time. The second line of the plot shows: the conversions of the reductions of the three different iron oxides with respect to the axial coordinate of the reactor and to the time.*




*Scaled $H_2$ flowrate (TCD) at 873 K hematite reduction with 4mL/min $H_2$ flowrate and 16 mL/min Ar flow rate (a), simulated $H_2$ flowrate with the same experimental operating conditions.*

The very first simulated results are encouraging if compared with the experimental ones and further experiments will allow the formulation of assumptions useful for an improvement of the description of the real system and its understanding.

The study is currently focusing on the need to make the model more solid as the operating conditions change. Furthermore, an intense parametric study is under development in order to evaluate the sensitivity of the system to the variation of each structural parameter of the model. This is a very useful approach before proceeding with a potential calibration of the mathematical model parameters.

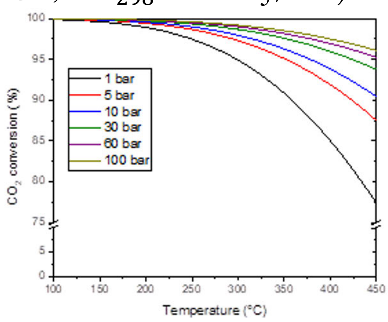
**Cooperation:** Università di Napoli

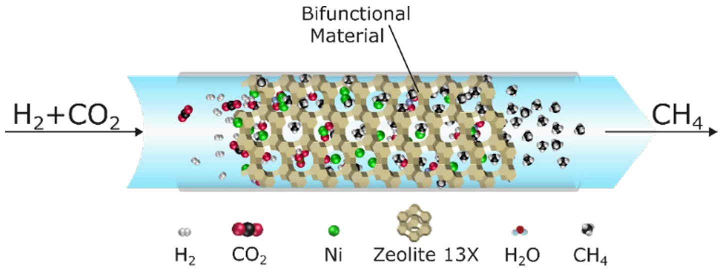
# Pure methane from $CO_2$ hydrogenation using a sorption enhanced process with catalyst/zeolite bi-functional materials

Main funding: China Scholarship Council, Academy of Finland (via TSF research profiling area)

*Liangyuan Wei, Wim Haije, Wiebren de Jong, Henrik Grénman*

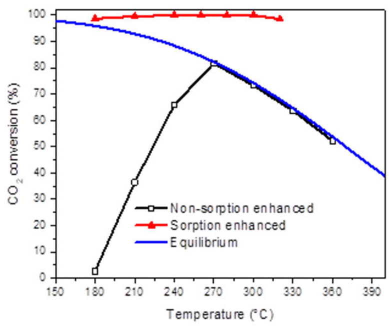
Methanation i.e. the Sabatier reaction is a potential large-scale option for $CO_2$ utilization, and it is one of the solutions for decreasing carbon emission and production of synthetic green fuels. One of the advantages is that the needed infrastructure and large utilization of methane already exists, which makes market implementation of the product easy. However, the $CO_2$ conversion is limited by thermodynamics at high temperature and kinetics at low temperature. ($CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O$; $\Delta H^0_{298}$= -165 kJ/mol)

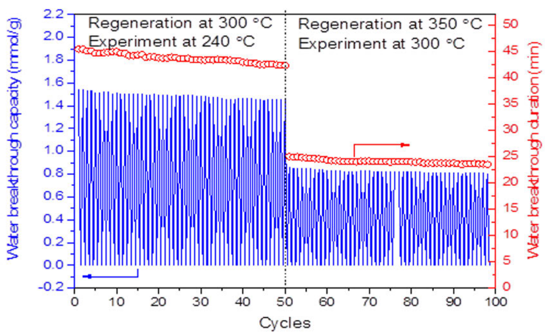



*Thermodynamic equilibrium conversion for the stoichiometric feed gas composition of $CO_2$ methanation (left) and conceptual representation of sorption enhanced $CO_2$methanation (right)*

In order to increase the conversion, high catalytic activity at rather low temperature combined with the removal of one of the reaction products, namely water, would be required according to Le Chatelier's principle. The aim of the current work was to combine these two functions into one material instead of designing a sequentially process (Figure 1.). Several materials with both catalytic and water adsorption properties were tested in a fixed bed reactor and a sub-nanometer zeolite 13X-supported Ni-ceria proved to be an exceptionally efficient catalyst/sorbent combination. Ce loading affected the catalysts metal dispersion, reducibility, basicity and acidity, and thence the activity and selectivity. STEM-EDX elemental mappings showed that Ce and Ni are predominantly highly dispersed. Both the **conversion and $CH_4$ selectivity were close to 100 %** with stoichiometric feeds of $CO_2$ and $H_2$ even at 200°C, which is one of the **highest activities reported in literature**. During prolonged stability testing in a **100 reactive adsorption – desorption cycles** (with a total experimental time of about 223 hours) the activity **remained stable** and only a slight decrease in the water uptake capacity was observed.




*Representation of process improvement with sorption enhanced $CO_2$ methanation (red, left) and 100 cycles (223 hours) stability test of activity and adsorption/desorption (right).*

**Cooperation:** Delft University of Technology, the Netherlands

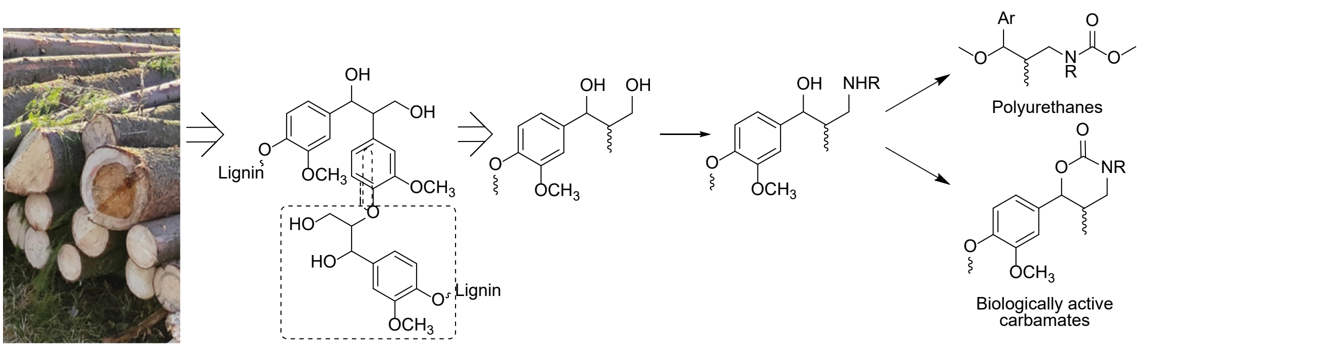
# From forest industry waste streams to new chemicals and materials: Value from lignin degradation

Main funding: Suomen Luonnonvarain Tutkimussäätiö – Finnish Natural Resource Research Foundation 2020-22

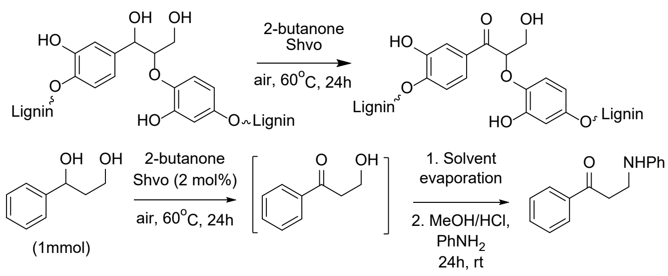
*Veronika D. Badazhkova, Risto Savela and Reko Leino*

Lignin - the nature's aromatic polymer is one of the potential sustainable feedstocks for fuels and material manufacturing processes. Direct use of lignin for new bio-based materials is, however, limited due to its low thermal and mechanical stability. For improving the stability and imparting desirable properties, lignin can be chemically modified by utilizing the functional groups in its structure. In various earlier studies, it has been demonstrated that the hydroxyl groups in lignin can be selectively oxidized by catalytic methods. Compared to many other approaches, catalytic hydrogen transfer is a highly selective, safe and eco-friendly process, taking place in the presence of a wide range of metal catalysts.

In this project, ruthenium-catalyzed amination of lignin hydroxyl groups has beem selected as the main pathway of modification, since it can be considered as a value-added reaction process for further synthesis of biologically active compounds and advanced materials from lignin-derived starting materials.




**Key results:**




At the current state of the project, selective ruthenium-catalyzed oxidation procedure of lignin diol model compounds and native lignin by transfer hydrogenation methodology has been developed (Badazhkova, V.; Savela, R.; Leino, R. Dalton Transactions 2022, 51, 6587-6596).

Ketoalcohols obtained by Ru-catalyzed transfer hydrogenation of the model compounds were further involved in reactions with aniline, resulting in the formation of β-aminoketones. Detailed kinetic studies, two-step lignin amination processes and the use of the aminated products in the synthesis new compounds and materials are currently pursued.

**Cooperation:** Professor Dr. Timo Repo, Department of Chemistry, University of Helsinki, Finland; Professor Dr. Dieter Vogt, Faculty of Bio and Chemical Engineering, Technical University of Dortmund, Germany.

## Synthesis of rare sugars through site-selective epimerization

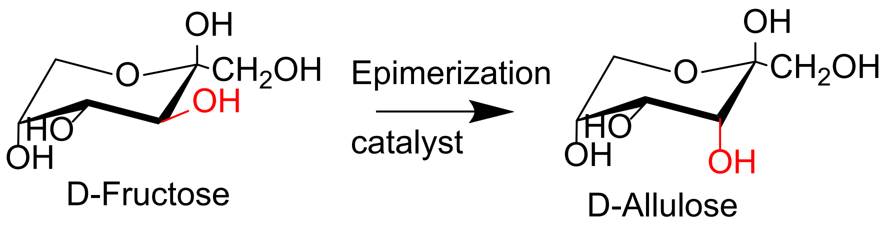
Main funding: Raisio plc's Research Foundation

*Anton Örn, Tiina Saloranta-Simell, Reko Leino, Dmitry Yu. Murzin,*

Rare sugars are types of carbohydrates that are not very common in nature. They can, however, be of value for their health benefits, such as anti-diabetic and anti-obesity. Because of these properties, rare sugars offer promising alternatives for replacing sucrose in various food and drink applications. For example, D-allulose, which is the C3-epimer of D-fructose, is an excellent substitute since its sweetness profile is very similar to that of sucrose.

Syntheses of these rare sugars, including D-allulose, typically utilize an enzyme as a catalyst. Enzymes in general have relatively short half-lives and therefore need to be added constantly, making the manufacturing processes often expensive. As a result, the products will be more expensive and alternative, cheaper methods for producing rare sugars are of great industrial interest.

The aim of this work is to develop non-enzymatic, yet economically viable catalytic methods for producing rare sugars, particularly D-allulose. Mainly heterogeneous catalysts will be tested, offering benefits also in terms of scale-up of the manufacturing processed. Discovery of a suitable catalyst could result in more widespread use of allulose in the food industry and not only in expensive luxury cuisine.




*Catalytic C3 epimerization of D-fructose into D-Allulose.*

Our primary method for solving this problem is based on initially screening several different catalysts for epimerization of D-fructose, followed by analysis of the reaction products by HPLC for rapid estimate of the product distribution. Several different epimers and isomers are expected to be formed in most cases. When a potential catalyst is found, optimization of the reaction conditions will then be attempted for shifting the equilibrium towards the desired D-allulose.

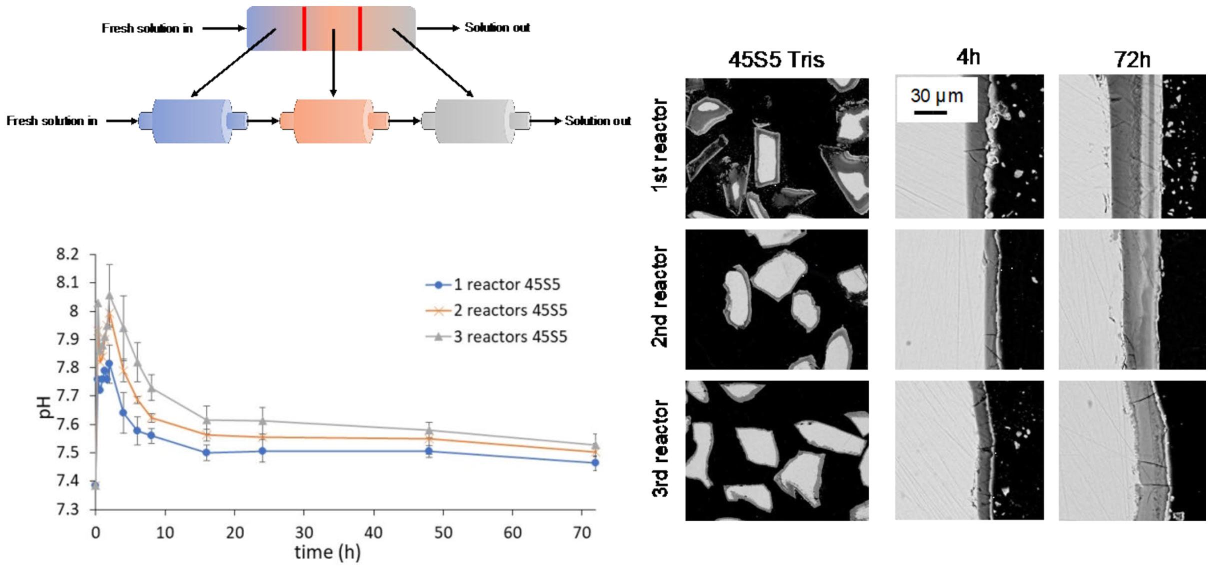
The secondary aim of this project is to gain more insight into the mechanisms of these epimerization reactions, as there is substantial interest also for other rare sugars in different applications. Epimerization can also be achieved through traditional oxidation/reduction reaction sequence of the hydroxyl group in question, and the selectivity of these reactions will also be investigated. A key challenge here is to obtain the desired product without the use of protecting groups, avoiding additional reaction steps and the generation of excess waste. The use of catalysts will be employed in this process as well.

## Bioactive glasses for biomedical applications

Main funding: Graduate School of Chemical Engineering, Business Finland, Academy of Finland, Companies, Svenska Kulturfonden, Victoriastiftelsen, Maud Kuistila Memory Foundation

*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 glasses' hot-working properties 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 to understand better the local environment's impact on the reactions of bioactive glass particles in a particle bed exposed to continuous flow conditions mimicking the body conditions.




*The continuous flow-through reactor concept is used to mimic the conditions the implanted bioactive glass-based implant experiences in the dynamic body environment. Using a cascade reactor gives additional information on the impact of bioactive glass particle location in the implantation site on its surface reactions.*

Controlled, predetermined ion release and the gradual total dissolution of the glass are critical characteristics for 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 experts in medicine and cell and molecular biology. Our research strives to achieve 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.

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

# Chemical challenges in gasification of biomass and waste

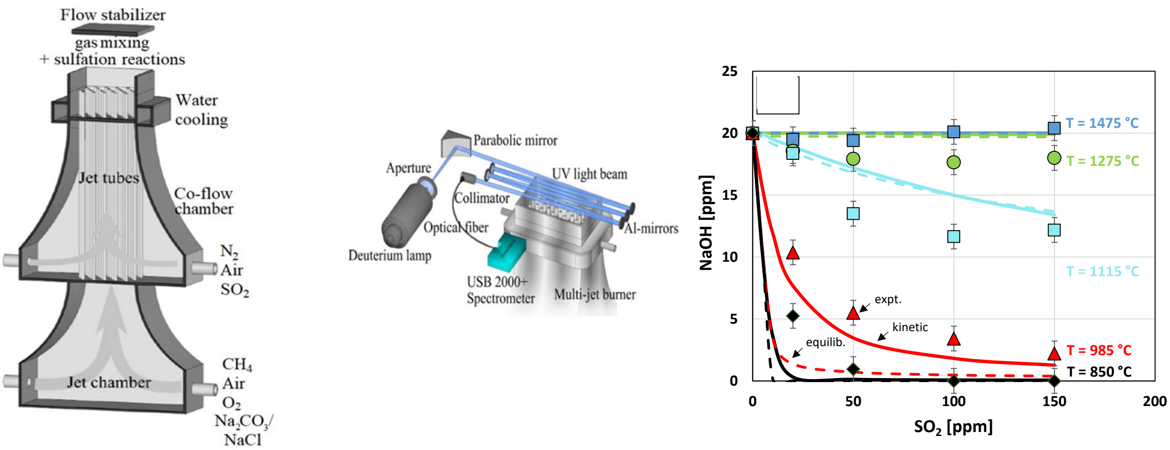
Main funding: Academy of Finland, Companies

*Oskar Karlström (PI), Daniel Schmid, Mikko Hupa*

Gasification of waste and biomass can be used to produce valuable chemicals, recover the fuel-bound energy and produce ash residues from which valuable elements can be recovered. Several challenges in gasification are related to the release of elements such as N, K, S, Cl, P, Zn and Pb. In the project, several topics related to the high-temperature chemistry and release of these elements have been investigated in collaboration with Lund University and the Technical University of Denmark (DTU).

Lund University (combustion physics) have access to nonintrusive laser and optical measurements to investigate the fate of various elements under harsh gasification conditions. In the project, gas phase sulfation of NaOH and NaCl was investigated at temperatures up to 1500 °C using broadband UV absorption spectroscopy.

The figures below show the novel reactor setup providing a separate feed of NaCl/NaOH and $SO_2$ and the experimental and modelling results of the sulfation reactions. The kinetic model was developed at DTU and the University of Northern Texas. Equilibrium modelling was done at ÅA in collaboration with DTU, Lund University and Aalto University. These results advance our understanding of gas phase sulfation reaction kinetics and are of crucial importance for understanding sulfation reactions under gasification conditions.




*Schematic picture of the Multi-Jet Burner at Lund University, setup for broadband UV absorption spectroscopy system, and example of experimental and both kinetic and equilibrium modelling data.*

**Cooperation:** Lund University, Technical University of Denmark

## Clean and efficient utilisation of demanding fuels (CLUE$^2$)

Main funding: ANDRITZ, UPM-Kymmene, Metsä Fibre, International Paper, Valmet Technologies, Graduate School at Åbo Akademi, PostDocs in Companies Programme, Finnish Recovery Boiler Committee, Svenska Kulturfonden, Johan Gadolin Scholarship Programme

*Sara Benalia, Nina Bruun, Meheretu Dirbeba, Markus Engblom, Jan-Erik Eriksson, Rasmus Fagerlund, Leena Hupa, Mikko Hupa, Oskar Karlström, Thomas Kronqvist, Tor Laurén, Juho Lehmusto, Maryam Mousavi, Viswamoorthy Raju, Alessandro Ruozzi, Paulo Santochi, Daniel Schmid, Christoffer Sevonius, Fiseha Tesfaye, Emil Vainio, Johan Werkelin, Sarah Yahi, Patrik Yrjas, Maria Zevenhoven*

CLUE$^2$ is an industry-academia consortium project that covers several research topics connected to converting renewable and challenging fuels to energy (Figure 1). The research within the project is industrially relevant and based on a fundamental understanding of detailed chemistry. Low-grade biomasses and waste-derived fuels bring challenges to process design and operation. The work aims to provide the industry with better tools to handle the impacts of fuel impurities, minimise fouling and corrosion, meet tightening emission limits, and find new approaches to utilising ashes and other waste streams. Research methods include laboratory experiments and analyses, full-scale boiler measurements, and mathematical modelling. The work is carried out in close collaboration with the industry. Figures 2 and 3 present examples of recent results.

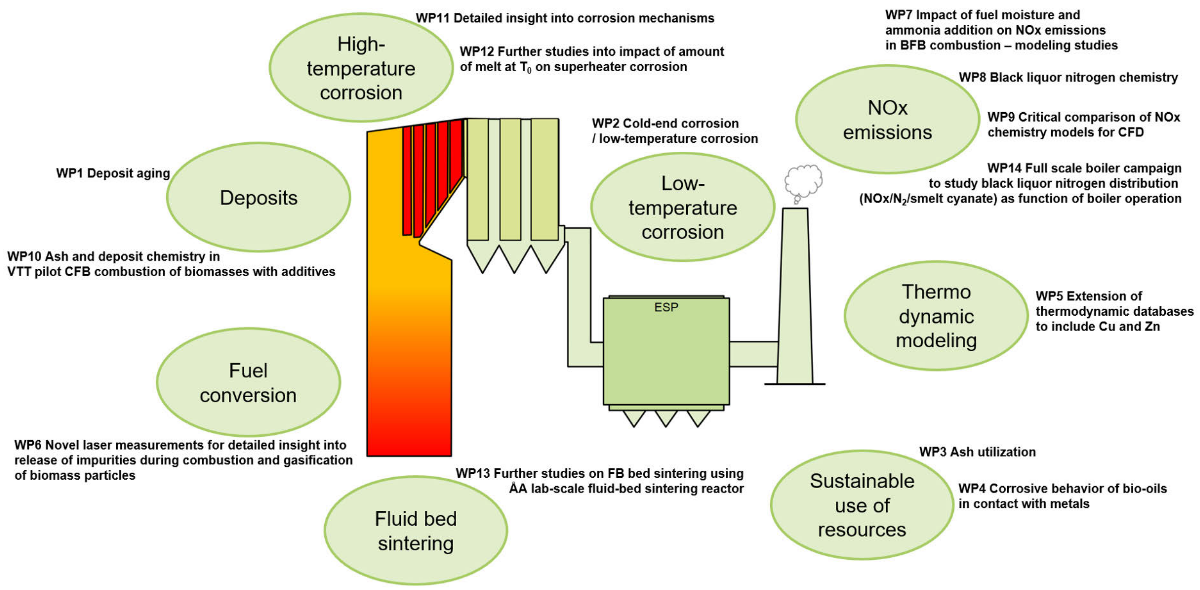



*Figure 1. CLUE$^2$ research topics and work packages*

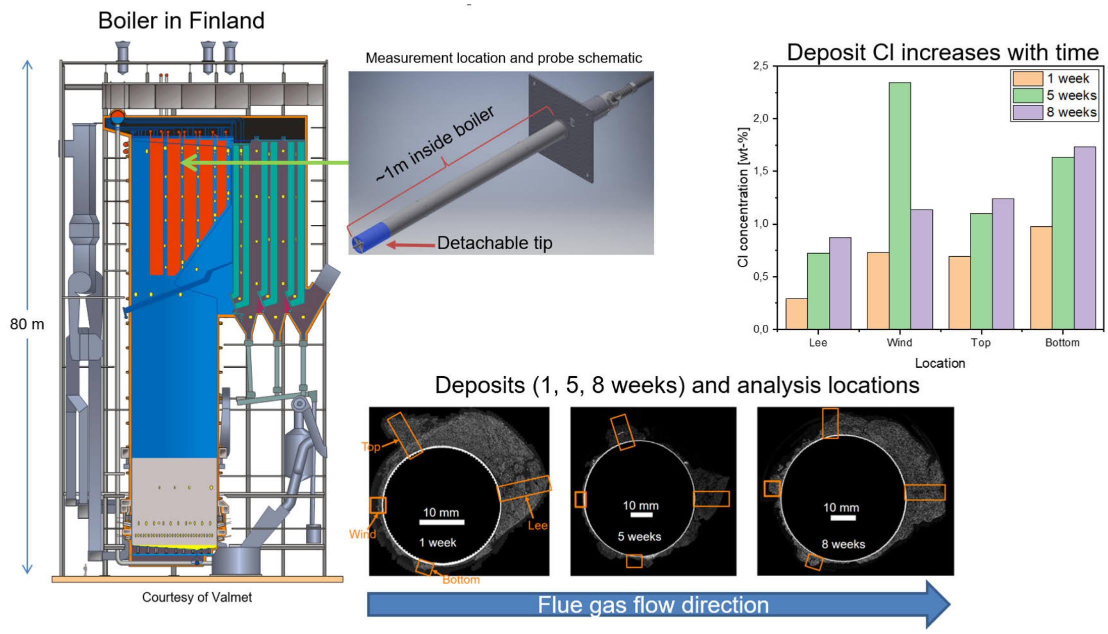



*Figure 2. Black liquor recovery boiler probe measurements show the increase in deposit chlorine concentration and indicate the boiler superheater deposits become more corrosive with time.*

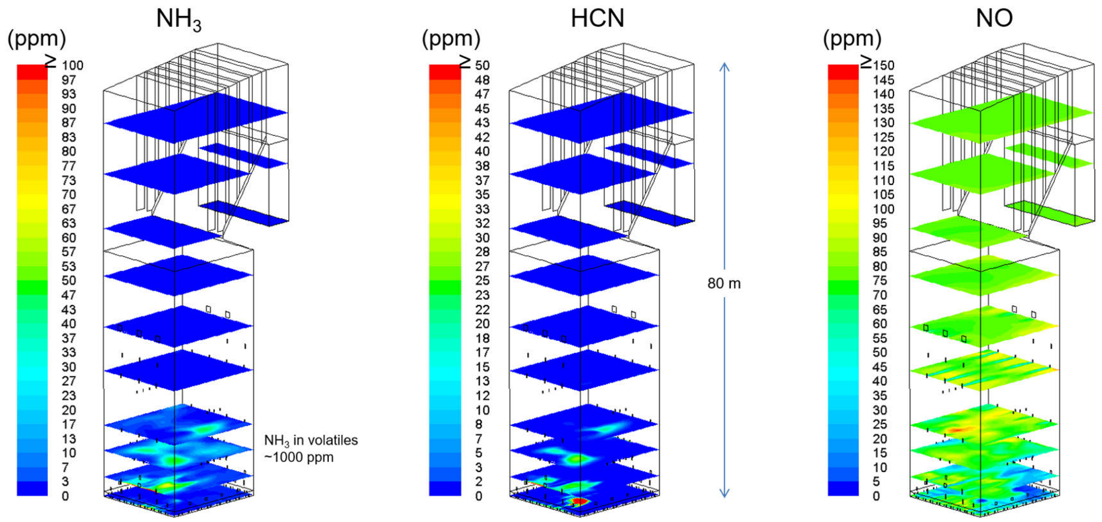



*Figure 3. CFD model predictions of nitrogen species concentration in the boiler furnace: $NH_3$ released from fuel is converted into the final NO emission, with HCN as an intermediate species. Using the model, engineering calculations of boiler design and operation can be carried out to minimise NO emissions.*

**Collaboration**: Aalto University, University of Toronto

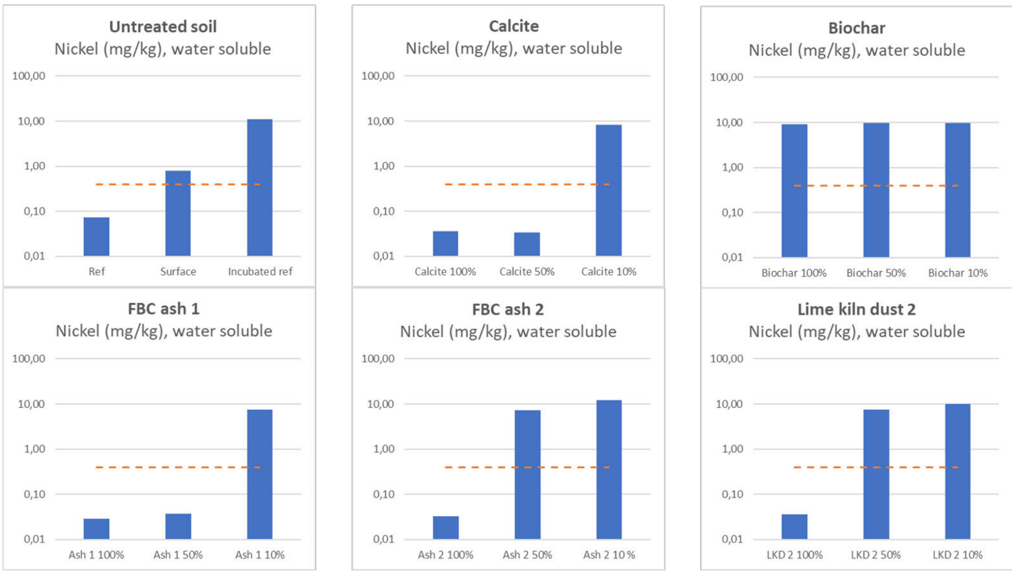
## Circular economy – Utilisation of industrial waste streams

Main funding: European Regional Development Fund (ERDF), Uudenmaan liitto, 6 Aika, Turku Urban Research Programme, Companies

*Thomas Kronberg, Jan-Erik Eriksson, Oskar Karlström, Johan Werkelin, Peter Österholm (ÅA Geology), Miriam Nystrand (ÅA Geology), Walter Strandell (ÅA Geology), Leena Hupa*

Utilising waste streams is a way to promote a circular economy. The research aims at finding new ways to utilise large-scale waste streams sustainably.

**CircVol2** project generates added information for companies and cities to bring solutions for utilising large volume masses. The project aims to support a systemic change toward a circular economy and reduce the carbon footprint of infrastructure construction, thus mitigating climate change. For this, industrial side streams were used instead of cement to neutralise acid sulfate clays to stabilise the soil. The figure below shows laboratory test results of Ni leached from dredged clay harvested from the area of Naantali Housing Fair 2022.




*Leaching of Ni from dredged soil stabilized with different industrial side streams.*

**TUKEMA** project provides the City of Turku and its urban environment with new knowledge that promotes the resource-wise utilisation of large-volume industrial side streams, mainly ash, in stabilising challenging soils such as dredging masses and sulfide clays. The research aims to find stabilisation methods that promote Turku's goal of becoming a carbon-neutral city.

**KERPUR** project explores new efficient ways to sort, recycle and reuse ceramic demolition waste. Usually, most of the heterogenous demolition waste ends up in landfills. However, ceramic materials are highly processed compounds that could find new recycling applications. Traditional ceramics used in construction consist of compounds produced in high-temperature reactions; thus, these energy-intensive materials are feasible as secondary raw materials to several products.

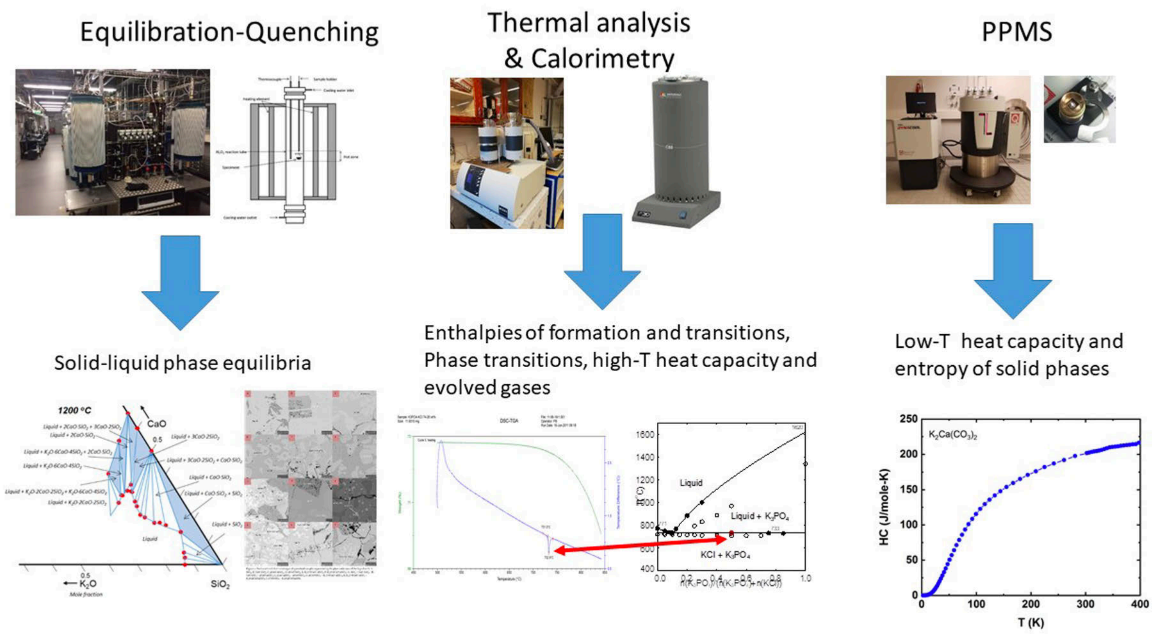
**Cooperation:** Geological Survey of Finland GTK, City of Turku, Finnish Environment Institute SYKE, Turku University of Applied Sciences, Turku Business Region

# High-temperature chemistry of phosphorus – pathways to more effective recycling and utilization

Main funding: Academy of Finland, Companies

*Markus Engblom, Oskar Karlström, Adrian Stiller, Emil Vainio, Patrik Yrjas, Leena Hupa*

The consortium project with Aalto University (Prof. Daniel Lindberg) strives to increase the knowledge of phosphorus chemistry in various high-temperature processes. The goal is better to understand the effective utilisation and recycling of phosphorus. This is done by studying phosphate-containing melts' thermodynamic properties, phase equilibria, and molecular structure with compositions corresponding to biomass ashes and bioactive glasses. Equilibration-quenching technique and differential scanning calorimetry are utilised to measure phase equilibria at temperatures up to 1500 °C. Thermodynamic properties will be measured using various techniques (see figure below). These data will be used as input for thermodynamic optimisations of the chemical systems. These data will be used as input for thermodynamic optimisations of the chemical systems $Na_2O$-$K_2O$-$MgO$-$CaO$-$SiO_2$-$P_2O_5$ and the Na,K/$PO_3$, $PO_4$, $SO_4$, Cl systems. The developed databases are used to predict the behaviour of phosphorus in biomass and waste combustion, thermal treatment of ash, and in producing bioactive glasses. The results are also relevant to phosphorus recycling and recovery strategies and finding new ways of extracting phosphorus from various industrial streams. This may lead to a lower carbon footprint and better phosphorus extraction from primary and secondary sources.




*Techniques used to measure high-temperature properties of phosphorus melts.*

**Cooperation:** Aalto University, University of Toronto (Canada), Umeå University (Sweden), University of Borås (Sweden), Ecole Polytechnique de Montreal (Canada), Friedrich Schiller University of Jena (Germany), Friedrich-Alexander University of Erlangen-Nuremberg (Germany), Valmet Technolgies, Metso Outotec, Bonalive Biomaterials

# Highly-efficient and flexible integration of biomass and renewable hydrogen for low-cost combined heat and power generation to the energy system

Acronym: Bio-FlexGen

Funding: European Union   https://www.linkedin.com/company/bio-flexgen/

*Patrik Yrjas, Emil Vainio, Markus Engblom, Leena Hupa*

Bio-FlexGen (2021-2024) is an EU-funded Research and Innovation Action (RIA) project. 14 partners from five countries (Sweden, Finland, Hungary, Spain and Germany) will collaboratively work for a decarbonised future. The Swedish research organization RISE coordinates the 36 months project.

The global demand for energy is constantly increasing. That´s why renewable sources are crucial for a decarbonised future. Bio-FlexGen will develop an optimised combination of bioenergy with green hydrogen providing secure and plannable sources for power and heat. This will complement intermittent renewable sources such as wind and sun. Bio-FlexGen will also increase the efficiency and flexibility of renewable combined heat and power (CHP), playing a key role in the energy system integration. Moreover, Bio-FlexGen will combine gasification and gas turbine technology.

Due to the high efficiency, more power can be generated from biomass for the same heat load. Starting and operating on 100% green hydrogen, the CHP-plant can quickly achieve full load. To meet fluctuations in seasonal energy demands and prices, there will be a variant of the plant. It adapts to long periods of low electricity prices or heat demand by producing climate-positive green hydrogen.

The Bio-FlexGen approach is highly efficient – both energetically and economically. A power plant with a unique combination of gasification and gas turbine technology that allows the plant to utilise hydrogen for fast dispatch and biomass for low operating costs over time will be developed. Green hydrogen is an energy carrier to stabilise electrical grids. It is generated through solar or wind energy.

Åbo Akademi University is mostly involved in WP1 (Biomass hybrid gasification technology for heat and power with increased efficiency and flexibility) with focus on biomass pyrolysis and reaction kinetics under pressurised conditions. Atmospheric experiments will be done with "the single particle furnace" and both atmospheric and pressurised runs will be done with the recently aquired pressurised thermogravimetric analyzer which is shown in the figure below.

- 25 – 1 200 °C
- Heating rate 5°C/sec
- 1 – 150 bar
- Sample mass up to 5 g
    - Resolution 0.1 µg
- Steam generator
- Three gas lines (more can be added)

## New insights on the effects of temperature gradients on high-temperature corrosion

Main funding: Academy of Finland, Graduate School at Åbo Akademi

*Jonne Niemi (PI), Roland Balint, Juho Lehmusto, Markus Engblom*

Heat and power boilers utilizing low-grade fuels (e.g., biomass and waste) often experience high amounts of fouling and slagging of the heat exchanger surfaces. Ash deposits within the boilers can contain high amounts of alkali and heavy metal salts, which can induce fast corrosion kinetics and be detrimental to the heat exchanger material. The effects of temperature gradients on ash deposit chemistry and high-temperature corrosion have been studied before. However, the results have been indicative so far, and no comprehensive, comparable corrosion results between isothermal and temperature gradient conditions are available. The detailed effects of the temperature gradients on high-temperature corrosion are still elusive. The research aims to provide a detailed understanding of the effects of temperature gradients on high-temperature corrosion and ash deposit chemistry. High-temperature corrosion is systematically studied in isothermal and temperature gradient conditions. Different mathematical modelling principles are utilized to understand better the ash deposit, corrosion product, and alloy interactions. The laboratory experiments and the modelling will result in a quantitative understanding of the effects of temperature gradients on high-temperature corrosion in boilers and a qualitative understanding of the underlying fundamental chemical and physical phenomena for high-temperature corrosion and ash deposit ageing.

The detailed objectives of the research project are to 1) identify the detailed deposition routes of various species of the K-Pb-Cl-$SO_4$ system, 2) study and quantify the effects of temperature gradients on high-temperature corrosion of heat exchanger materials through comparison tests with isothermal and temperature gradient exposure, 3) study and qualitatively identify temperature gradient driven mechanisms within an ash deposit-corrosion product interface with solid and liquid phases present, and 4) develop a mathematical model utilizing thermodynamics and computational fluid dynamics capable of predicting temperature gradient induced liquid-phase migration within mainly solid ash deposits and corrosion layers. The research will result in knowledge that can be utilized by heat exchanger material, boiler manufacturers, and boiler operators to manage corrosion in high temperatures and better optimize the production parameters and availability of boilers.

**Cooperation:** Aalto University, VTT, Chalmers University of Technology, Umeå University, Valmet Technologies Oy

# Properties and behavior of deliquescent salts and deposits in biomass and waste thermal conversion – Towards improved efficiency and reliability

Main funding: Academy of Finland, Graduate School at Åbo Akademi

*Emil Vainio (PI), Alessandro Ruozzi, Farzad Jafaribonar, Leena Hupa*

Clean and efficient utilization of biomass and waste fuels as energy sources for producing heat and electricity is of great importance. Utilizing biomass and waste for energy production is one alternative for reducing fossil fuel use and increasing energy self-sufficiency. Biomass-based fuels are the most important renewable fuels in Finland. In 2020, 71% of the renewable energy and 28% of the total energy consumption in Finland originated from biomass (stat.fi). Biomass conversion for the production of heat and electricity is conducted in large industrial combustors, such as fluidized bed boilers, black liquor recovery boilers, biomass gasifiers, and grate-fired boilers. Research and development of these technologies have been of great importance for the Finnish industry since many boiler manufacturers and developers have activities in Finland.

The qualities and properties of different biomasses vary a lot, and the ash-forming elements may lead to several challenges in their use (Figure 1). The ash-forming elements can form hygroscopic and corrosive deposits in the cold-end of power boilers. Recently, it has been shown that challenges related to corrosion and operational issues in the cold-end, e.g., deposit build-up, decrease in heat transfer, corrosion in various parts, and plugging of flue gas cleaning equipment, are mainly caused by hygroscopic salts and deposits. Ammonium chloride (NH4Cl) is one example of a hygroscopic and corrosive salt that may form in the cold-end of boilers (Figure 2).

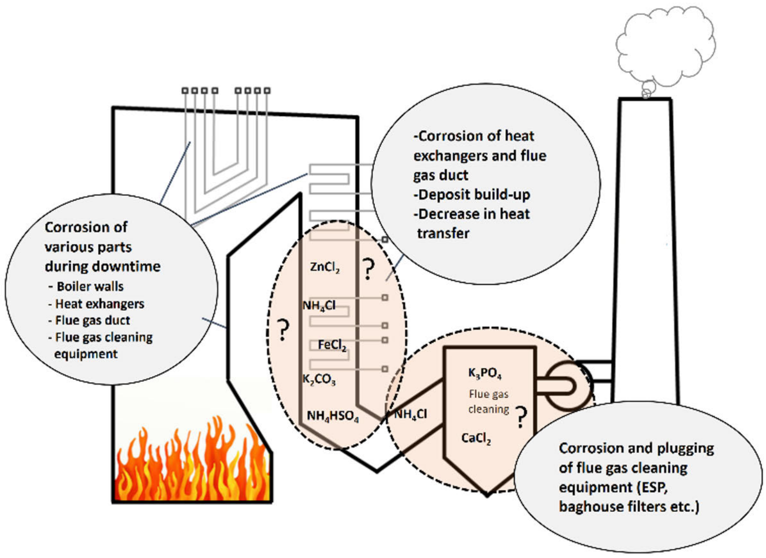



*Figure 1. Challenges caused by hygroscopic and deliquescent salts/deposits.*

This research aims to develop innovative solutions to improve energy efficiency while avoiding operational challenges and corrosion in the thermal conversion of sustainable biomass and waste fuels. This research will explain the properties, formation, and behaviour of hygroscopic salts and deposits and determine their influence on corrosion and operational performance. Based on this, a new understanding of the formation of hygroscopic salts will be gained, the lower limits of heat exchangers for various fuels can be mapped, and new strategies for preventing corrosion and deposit build-up can be developed. Understanding the root cause is key when devising viable strategies to avoid corrosion and deposit build-up problems while improving efficiency.

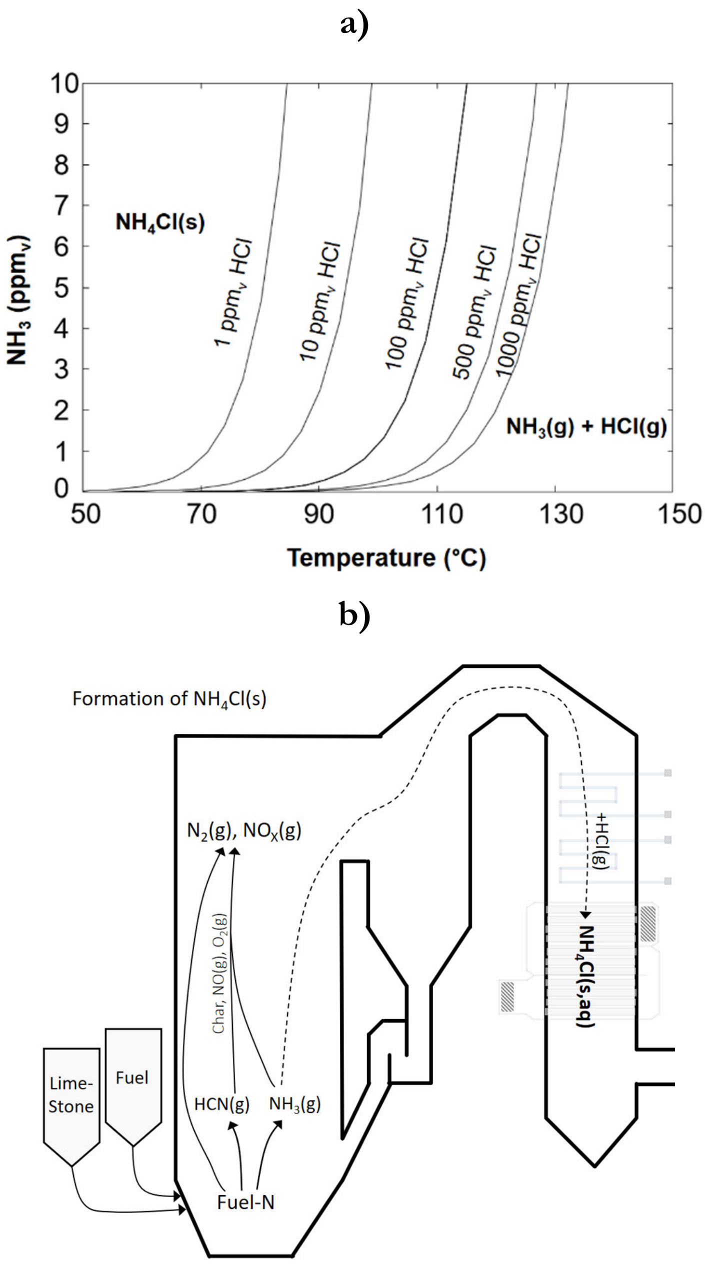



*Figure 2. a) Formation route for $NH_4Cl$ in a CFB boiler. b) Stability of $NH_4Cl$ (Vainio et al. FUEL 2021)*

**Cooperation:** Valmet Technologies Oy, Andritz Oy, Sumitomo FW SHI Energia Oy, University of Toronto

## Role of feedstock impurities in novel pyrolysis-based technologies for low-grade biomass and waste feedstocks

Main funding: Svenska Kulturfonden (via PoDoCo, Post Docs in Companies) and Valmet Technologies Oy

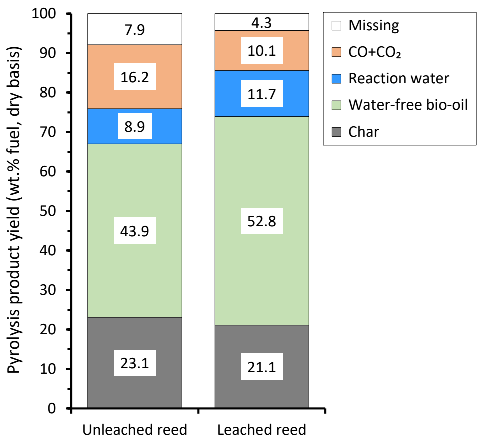
*Meheretu Jaleta Dirbeba, Oskar Karlström, Atte Aho, Mikko Hupa, Dmitry Murzin, Leena Hupa*

The fast pyrolysis process is a potential technology to refine low-grade biomass and waste streams into more valuable products. Crude bio-oil is the main product of the process, while biochar and non-condensable gases are the by-products. The bio-oil has versatile applications, including the production of heat, electricity, chemicals, and transportation fuel. The by-products (biochar and gas) from the process are mainly used for heat and power production. However, there is high market demand to produce value-added chemicals from the by-products, especially from the biochars. The biochars can be used as soil fertilizer/conditioner. At the same time, returning the biochars to the soil serves as carbon sequestration. In addition, biochars have the potential to substitute fossil-based industrial carbons (e.g., activated carbon, calcined coke, and graphite).

Low-grade biomass and waste feedstocks such as agricultural residues, industrial by-products, and municipal solid wastes have been considered to be sustainable feedstocks for bio-oil production. Besides bio-oil production, the use of such feedstocks in fast pyrolysis processes reduces the burden on the environment and improves market competitiveness and feedstock supply, making the process an alternative option for a circular economy. However, compared to wood, several challenges are associated with them for utilizing in thermal conversion processes. The challenges are primarily due to the high levels of impurities in the feedstocks. The impurities are mainly ash-forming elements (e.g., Na, K, Ca, Si, P, S, and Cl) and nitrogen (N), and they are known to strongly influence the yield and quality of bio-oils from fast pyrolysis processes and pose serious problems in upgrading the bio-oils.

The objective of this project work is to clarify to what extent low-grade biomass and waste feedstocks are suitable for the fast pyrolysis process. The focus will be on the role of the various impurities in these so far un-utilized feedstocks. The aim is to provide the necessary information for designing and developing fast pyrolysis processes with high bio-oil yield and quality. Moreover, this work characterizes the biochars for their physicochemical properties, such as surface area, porosity, and reactivity, which are important for upgrading the biochars for industrial and soil applications.

The figure below shows the influence of impurities on the fast pyrolysis product yields for reed. The reed was pyrolyzed at 400 °C in Åbo Akademi's lab-scale fluidized bed pyrolysis reactor before and after removing the ash-forming elements of the reed by leaching, i.e., washing away the ash-forming elements from the reed with dilute nitric acid.




*Influence of impurities on fast pyrolysis product yields*

**Cooperation:**
Valmet Technologies Oy

# Understanding the interactions of refractory materials with volatile non-processing elements in metal production

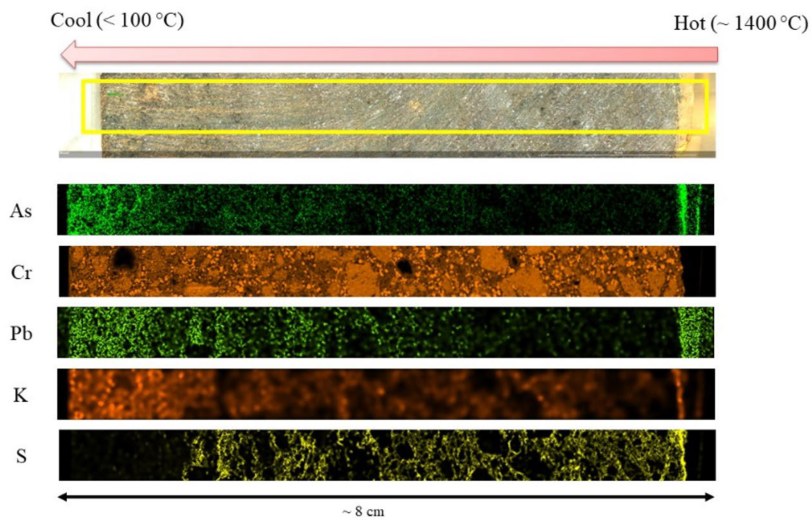
Åbo Akademi sub-project of the consortium project TOCANEM

Main funding: Business Finland

*Markus Engblom, Leena Hupa, Juho Lehmusto*

Achieving carbon neutrality in metal production means not only replacing fossil fuels and coke with renewable fuels and biochar but also increasing the utilization of recycled metals instead of primary raw materials such as ores. These recycled material streams contain valuable metals but often also unwanted impurities not present in the primary raw materials. In pyrometallurgical processing, the infiltration of certain elements into refractories may trigger new refractory failure mechanisms. These foreign elements may chemically react with the refractory components or otherwise change their properties. However, the impact of these non-processing elements on the properties of the refractory materials is not well understood. Furthermore, the role of the temperature gradient over the refractory material in the diffusion of species has not been previously addressed. The overall goal of this study is to achieve a better understanding of the impact of non-processing elements originating from recycled materials and sidestreams on the fate of the refractories in carbon-neutral metal production.

The infiltration of the volatile elements will be analyzed from refractory samples tested in the laboratory- and pilot-scale experiments as well as from smelter samples. The focus is on samples exposed to the non-processing elements at or above the slag/gas interface in the smelter. In addition, the effect of the temperature gradient on diffusion as well as the catalytic role of the refractory material in $SO_2$-to-$SO_3$ conversion will be addressed.




The effect of a temperature gradient on diffusion within a refractory exposed to flash smelter furnace conditions for several years.

**Cooperation**: This work is a part of a consortium project called *Towards Carbon Neutral Metals* (TOCANEM). The overall aim of the project is to address the different steps needed for turning the metal production into a carbon-neutral process and that way aid Finland to become a carbon-neutral society by 2035. The research partners of this work are Aalto University, Boliden Harjavalta, Metso Outotec, Oulu University, VTT Technical Research Centre of Finland.

# 5. PCC publications and reports 1.1.2020-31.12.2020

## 5.1 Theses 2020

### 5.1.1 Doctoral Theses (6)

*Behravesh, Erfan,* Development of microreactor technology for partial oxidation of ethanol, 6.3.2020

*Dirbeba, Meheretu Jaleta,* Thermochemical Conversion Characteristics of Vinasse, 28.08.2020

*Freites, Adriana,* Epoxidation of vegetable oils- process intensification for biomass conversion, 15.1.2020

*Kronberg, Thomas,* Properties of raw glazes – The impact of composition, firing and functional coatings, 18.09.2020

*Saeid, Soudabeh*, Destruction of selected pharmaceuticals by ozonation and heterogeneous catalysis, 16.3.2020

*Zhang, Yongchao*, Formic acid fractionation of bamboo and valorization of isolated lignin, 14.2.2020

### 5.1.2 Masters's theses (10)

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

*Fortunato, Michele,* Transient investigation in heterogeneous catalysis (collaboration with Università di Napoli 'Federico II')

*Franz, Sebastian,* Aerobic oxidation of arabinose-glucose mixtures over gold nanoparticles

*Herrero Manzano, Maria,* Oxidation of sugar mixtures on gold nanoparticle extrudates

*Kesäläinen, Sara,* Improving plasticity and film-forming quality of xylans through chemical modification in aqueous phase

*Kirm, Helmi Ulrika*, Characterization of Na-selective solid-contact ion-selective electrodes using coulometric signal transduction

*Laurén, Isabella,* Bio-based stabilizers for hydrophobic nanoparticle dispersions

*Monteiro, João Marcos*, Thin-layer composite reference electrodes

*Rosnell, Jenni Julia*, Redskapen i experimentellt arbete: Utredning av skollaboratoriets utrustning ur kemilärarens synvinkel

*Rautelin, Wolter*, Evaluation of calculative tools for viscosity: Prediction of hydrocarbon mixtures

# 5.2 Publications 2020

### 5.2.1 Articles in refereed international scientific journals and series (145)

1. Abiev, R,. Sladkovskiy, D., Semikin, K., Murzin, D., Rebrov, E., **Non thermal plasma for process and energy intensification in dry reforming of methane**, *Catalysts MDPI* 10 (2020) 11, 1358.

2. Abushahba, F., Tuukkanen, J., Aalto-Setälä, L., Miinalainen, I., Hupa, L., Närhi, T.O., **Effect of bioactive glass air-abrasion on the wettability and osteoblast proliferation on sandblasted and acid-etched titanium surfaces**, *European Journal of Oral Sciences* 128 (2020) 2, 160–169.

3. Agarwal, V., Halli, P., Helin, S., Tesfaye, F., Lundström, M., **Electrohydraulic fragmentation of aluminum and polymer fractions from waste pharmaceutical blisters**, *ACS Sustainable Chemistry and Engineering* 8 (2020) 10, 4137–4145.

4. Agudelo, A. F. G., Pérez-Sena, W. Y., Kebir, N., Salmi, T., Ríos, L. A., Leveneur, S., **Influence of steric effects on the kinetics of cyclic-carbonate vegetable oils aminolysis**, *Chemical Engineering Science* 228 (2020) 115954.

5. Aho, A., Rosales, C., Eränen, K., Salmi, T., Murzin, D. Yu., Grénman, H., **Biohydrogen from dilute side streams-Influence of reaction conditions on the conversion and selectivity in aqueous phase reforming of xylitol**, *Biomass and Bioenergy* 138 (2020) 105590.

6. Ain Syed Hashim, S.N., Az-Zahraa Norizan, B., Baharin, K.W., Zakaria, S., Chia, C.H., Potthast, A., Schiehser, S., Bacher, M., Rosenau, T., Syed Jaafar, S.N., **In-depth characterization of cellulosic pulps from oil palm empty fruit bunches and kenaf core, dissolution and preparation of cellulose membranes**, *Cellulose Chemistry and Technology* 54 (2020) 7–8, 643–652.

7. Alvear, M., Aho, A., Simakova, I. L., Grénman, H., Salmi, T., Murzin, D. Yu., **Aqueous phase reforming of alcohols over a bimetallic Pt-Pd catalyst in the presence of formic acid**, *Chemical Engineering Journal* (2020) 125541.

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11. Azkaar, M., Vajglová, Z., Mäki-Arvela, P., Aho, A., Kumar, N., Palonen, H., Perez-Ramirez, J. P., Mondelli, C., Murzin, D. Yu., **Hydrocracking of hexadecane to jet fuel components over hierarchical Ru-modified faujasite zeolite**, *Fuel* 278 (2020), 118193.

12. Bankiewicz, D., Vainio, E., Yrjas, P., Hupa, L., Lisak, G., A**pplication of bipolar electrochemistry to accelerate dew point corrosion for screening of steel materials for power boilers**, *Fuel* 265 (2020), 116886.

13. Beaumont, M., Winklehner, S., Veigel, S., Mundigler, N., Gindl-Altmutter, W., Potthast, A., Rosenau, T., **Wet esterification of never-dried cellulose: a simple process to surface-acetylated cellulose nanofibers**, *Green Chemistry* 22 (2021) 17, 5605– 5609.

14. Bobacka, J., **Electrochemical sensors for real-world applications**, *Journal of Solid State Electrochemistry* 24 (2020) 2039–2040.

15. Bui, T. Q., Konwar, L. J., Samikannu, A., Nikjoo, D., Mikkola, J. P., **Mesoporous melamine-formaldehyde resins as efficient heterogeneous catalysts for continuous synthesis of cyclic carbonates from epoxides and gaseous $CO_2$**, *ACS Sustainable Chemistry & Engineering* 8 (2020) 34, 12852–12869.

16. Burger, D., Winter, A., Subbiahdoss, G., Oberlerchner, J.T., Beaumont, M., Tamada, Y., Rosenau, T., **Partial amorphization of cellulose through zinc chloride treatment: A facile and sustainable pathway to functional cellulose nanofibers with flame-retardant and catalytic properties**, *ACS Sustainable Chemistry and Engineering* 8 (2021) 36, 13576 –13582.

17. Danilevska, N.B., Moroz, M.V., Nechyporuk, B.D., Haievska, S.H., Novoseletskyi, M.Yu., Prokhorenko, M.V., Yarema, N.P., Yukhymchuk, V.O., Tesfaye, F., Reshetnyak, O.V., **The effect of chemical composition and electrolyte temperature on the size and structure of cadmium sulfide nanocrystals obtained by the electrolytic method**, *Journal of Nano- and Electronic Physics* 12 (2020) 4, 04035-1 – 04035-6.

18. Demidova, Yu. S., Mozhaitsev, E. S., Suslov, E. V., Saraev, A. A., Volcho, K. P., Salakhutdinov, N. F., Simakova, I. L., Murzin, D. Yu., **Monoterpenoid oximes hydrogenation over platinum catalysts**, *Topics in Catalysis* 63 (2020) 187–195.

19. Demidova, Yu. S., Mozhaitsev, E. S., Suslov, E. V., Nefedov, A. A., Saraev, A. A., Volcho, K. P., Salakhutdinov, N. F., Simakov, A., Simakova, I. L., Murzin, D. Yu., **Menthylamine synthesis via gold-catalyzed hydrogenation of menthone oxime**, *Applied Catalysis A. General* 605 (2020) 117799, 1–10.

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**5.2.4 Book chapters (5)**

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**5.2.4 Articles in refereed international edited volumes and conference proceedings (3)**

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### 5.2.5 Other publications (7)

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## 5.3 Edited conference proceedings and reports

Tolvanen, P., Bobacka, J., Eklund, P., Latonen, R.-M., Mäki-Arvela, P., Sundberg, A., Werkelin, J. (editors) **Johan Gadolin Process Chemistry Centre at Åbo Akademi University : annual report 2018-2019,** Åbo Akademi University, 2020, ISSN: 1459-8213

## 5.4 Patents and invention disclosures

Mikkola, J.-P., Samikannu A., Van Klint K., Siljebo, W., Konwar J., L., **Hydrothermal method for producing renewable paraffinic hydrocarbons,** WO2020/039031 A1.

Xu, C., Wang, X., Willför, S., **Photo-crosslinkable 3D printing inks of lowly-charged and non-charged nanocellulose**. U/03/2019, Åbo Akademi University

## 5.5 Awards granted

*Freites, Adriana,* Colleague of the Year Award 2020

*Freites, Adriana,* Elvings legat for the best doctoral thesis at Åbo Akademi 2020

*Wikström, Wilhelm*, Suomalaisten Kemistien Seuran award for best Bachelor thesis 2020

*Xu, Wenyang,* Forest Products Engineers' (www.puunjalostusinsinoorit.fi) C.J.Jansson prize 2020.

*Xu, Wenyang*, Det Alfthanska priset 2020.

# 6. PCC publications and Reports 1.1.2021-31.12.2021

## 6.1 Theses 2021

### 6.1.1 Doctoral Theses (8)

*Hameed Sultan Akbar Ali, Ashiq Ahamed*, Life Cycle Assessment of Plastic Waste, its Treatment, and Application of the Upcycled Product: A Comprehensive Circular Approach, 23.06.2021

*Han, Tingting*, Coulometric Transduction Method for Solid-Contact Ion-Selective Electrode, 11.06.2021

*Jogi, Ramakrishna,* Green aviation fuel hydrocarbons from lignocellulosic biomass via hydrothermal liquefaction, 21.5.2021

*Kråkström, Matilda,* Application of LC-MS for the identification and quantification of pharmaceuticals and their transformation products during catalytic ozonation, 19.2.2021

*Lu, Xiaojia,* Reductive catalytic depolymerization of industrial lignin and hemicellulose – process development and intensification (*Cotutelle* with INSA-Rouen), 1.10.2021

*Najarnezhadmashhadi, Ali,* Development of structured catalyst and reactor technologies for biomass conversion: Continuous production of sugar alcohols, 19.5.2021

*Pérez Sena, Wander Y.,* Monomers from vegetable oil feedstock: kinetics, catalysis and thermal risk (*Cotutelle* with INSA-Rouen), 9.7.2021

*Vucetic, Nemanja,* Mizoroki-Heck cross-coupling-palladium based catalysts and operation modes, 16.12.2021

### 6.1.2 Masters's theses (33)

*Araujo Barahona, German,* Hydrogenation of selected carbohydrate molecules in the presence of solid foam catalysts in a stirred tank reactor (collaboration with Universidad de Valladolid)

*Björklind, Robert*, Framställning av högbarriärpapper med reversgravyr

*Björnvik, Elisabeth,* Exfoliering av grafit i cellulosa nanokristaller (CNC) och framställning av elektriskt ledande grafen-CNC-kompositfilmer

*Båssar, André,* Challenges in flame retardant wood coatings

*Engblom Simon,* A study of glucose transformaiton to lactic acid and methyl lactate

*Engström, Emma,* Printing and spectrometric detection of active pharmaceutical ingredients on different surfaces

*Gauli, Bibesh,* Hydrodeoxygenation of lignin-derived model compound isoeugenol over Fe-, Ni-, and Fe-Ni supported zeolites

*Ghimire, Hamal,* Biobased and biodegradable barrier coatings on paper with slot die technolog

*Guagneli, Luca*, Novel design of a flow-through potentiometric sensing device

*Holmberg, Charlotte*, Method development for the analysis of polydimethylsiloxane in bio-oil

*Holmqvist, Alfred*, Formulation of a composite with a binder system using microfibrillated cellulose

*Högnabba, Emil,* Catalysts for slurry-phase hydrotreating of bio-oil

*Jansson, Oskar*, Study of the washing efficeincy of hydrolysed kraft pulp with a washing simulator

*Karppanen, Suvi,* Development of a microfluidic bead-based immunoassay

*Lehtimäki, Watti*, The role of extensional viscosity in curtain coating

*Lillrank, Pinja*, Extractives in unbleached birch kraft pulp and filtrate: Focus on analytical method development

*Lindroos, Pontus,* Lipase catalyzed chemo-enzymatic epoxidation of fatty acids using ultrasound as a process intensification method

*Lindqvist Wilma,* Non-halogenated fire retardant additives for an opaque exterior wood paint

*Malm, Ebba,* Alkali chloride induced superheater corrosion – Impact of percentage of molten phase

*Manandhar, Sajana*, Determination of benzoate in cranberry and lingonberry using solid-contact ion-selective electrode; comparison with ion chromatography

*Mastroianni, Luca,* Oxidation of alcohols promoted by gold in a microreactor: kinetic and modeling study (collaboration with Università di Napoli 'Federico II')

*Nick, Tapani,* The effects of high solids content on coating color rheology and runnability

*Nurmi, Linda,* Inventory and management of process wastewater streams in a pharmaceutical production plant in Finland

*Nyman, Isac*, Barriärbestrykning för specialpapper

*Nyman, Oskar,* Degradation of polydimethylsiloxane in simulated industrial process environments, 2021

*Osazuwa, Peter Odion*, Synthesis of an Electroconductive Hydrogel in 3D Printing Formulation for Tissue Engineering

*Rustem, Rustem*, Functionality of solid-contact ISEs with physically damaged ion-selective membranes: a comparison between potentiometric, coulometric and amperometric methods

*Selaković, Miloš,* Development of a novel artificial nose with conductive polymers of 3,4-ethylenedioxythiophene and its functionalised derivatives

*Sjöblom, Malin,* Characterization of Industrial Filter Materials for Improved Filter Medium Selection

*Sundberg, Richard,* Redutio n of iron oxides with hydrogen

*Visuri, Aino,* Analys av växtsteroler med gaskromatografi och FT-NIR-spektroskopi

*Volobujeva, Jelena,* Polymer and electrocatalytic membranes for improved selectivity of glucose biosensor

*Wilson, Viola*, Analysis of major ions, stable water isotopes and black carbon in the upper part of Belucha ice core, Siberian Altai

## 6.2 Publications 1.1-31.12.2021

### 6.2.1 Articles in refereed international scientific journals and series (147)

1. Aalto-Setälä, L., Uppstu, P., Sinitsyna, P., Lindfors, N.C., Hupa, L., **Dissolution of amorphous S53P4 glass scaffolds in dynamic in vitro conditions**, *Materials* 14 (2021) 17, 4834; https://doi.org/10.3390/ma14174834.

2. Abushahba, F., Gürsoy, M., Hupa, L., Närhi, T.O., E**ffect of bioactive glass air-abrasion on Fusobacterium nucleatum and Porphyromonas gingivalis biofilm formed on moderately rough titanium surface**, *European Journal of Oral Sciences* 129 (2021) 3, e12783.

3. Ahamed, A., Liang, L., Lee, M. Y., Bobacka, J., Lisak, G., **Too small to matter? Physicochemical transformation and toxicity of engineered n$TiO_2$, n$SiO_2$, nZnO, carbon nanotubes, and nAg**, *Journal of Hazardous Materials* 404 (2021) 124107–124128.

4. Ahamed, A., Vallam, P., Iyer, N. S., Veksha, A., Bobacka, J., Lisak, G., **Life cycle assessment of plastic grocery bags and their alternatives in cities with confined waste management structure: A Singapore case study**, *Journal of Cleaner Production* 278 (2021) 123956–123967.

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6. Ahamed, A., Liang, L., Chan, W. P., Tan, P. C. K., Yip, N. T. X., Bobacka, J., Veksha, A., Yin, K., Lisak, G., **In situ catalytic reforming of plastic pyrolysis vapors using MSW incineration ashes**, *Environmental Pollution* 276 (2021) 116681–116693.

7. Aho, A., Engblom, S., Eränen, K., Russo, V., Mäki-Arvela, P., Kumar, N., Wärnå, J., Salmi, T., Murzin, D. Yu., **Glucose transformation over a mechanical mixture of ZnO and Ru/C catalysts: Product distribution, thermodynamics and kinetics**, *Chemical Engineering Journal*, 405 (2021) 126945 (1–14).

8. Alipoormazandarani N., Benselfelt T., Wang L., Wang X., Xu C., Wågberg L., Willför S. and Fatehi P., **Functional lignin nanoparticles with tunable size and surface properties: fabrication, characterization, and use in layer-by-layer assembly**, *ACS Applied Materials & Interfaces* 13 (2021) 22, 26308–26317.

9. Alvear, M., Fortunato, M. E., Russo, V., Eränen, K., Di Serio, M., Lehtonen, J., Rautiainen, S., Murzin, D. Yu., Salmi, T., **Continuous liquid-phase epoxidation of ethylene with hydrogen peroxide on a titanium-silicate catalyst**, *Industrial & Engineering Chemistry Research* 60 (2021) 26, 9429–9436.

10. Alvear, M., Eränen, K., Murzin, D. Y., Salmi, T., **Study of the product distribution in the epoxidation of propylene over TS-1 catalyst in a trickle-bed reactor**, *Industrial & Engineering Chemistry Research* 60 (2021) 6, 2430–2438.

11. Balakshin, M.Y., Capanema, E.A., Sulaeva, I., Schlee, P., Huang, Z., Feng, M., Borghei, M., Rojas, O.J., Potthast, A., Rosenau, T., **New opportunities in the valorization of technical lignins**, *ChemSusChem* 14 (2021) 4, 1016–1036.

12. Balint, R., Engblom, M., Niemi, J., Silva da Costa, D., Lindberg, D., Yrjas, P., Hupa, L. & Hupa, M., **Temperature gradient induced changes within superheater ash deposits high in chlorine**, *Energy* 226 (2021) 120439.

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**6.2.2 Review articles in refereed international scientific journals and series (9)**

148. Jusner, P., Schwaiger, E., Potthast, A., Rosenau, T., **Thermal stability of cellulose insulation in electrical power transformers – A review**, *Carbohydrate Polymers* 252 (2021), art. no. 117196.

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150. Mäki-Arvela, P., Martinez-Klimov, M., Murzin, D. Yu., **Hydroconversion of fatty acids and vegetable oils for production of jet fuels**, *Fuel* 306 (2021) 121637.

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152. Mäki-Arvela, P., Ruiz, D., Murzin, D. Yu., **Catalytic hydrogenation/ hydrogenolysis of 5-hydroxymethylfurfural to 2,5-dimethylfuran**, *ChemSusChem* 14 (2021) 1, 150–168.

153. Mäki-Arvela, P., Simakova, I. L., Murzin, D. Y., **One-pot amination of aldehydes and ketones over heterogeneous catalysts for production of secondary amines**, *Catalysis Reviews* (2021) 1–68.

154. Savela, R., Méndez-Gálvez, C., **Isoindolinone synthesis via one-pot type transition metal catalyzed C-C bond forming reactions,** *Chemistry: A European Journal* 27 (2021) 17, 5344-5378.

155. Shen, L., Tesfaye, F., Li, X., Lindberg, D., & Taskinen, P., **Review of rhenium extraction and recycling technologies from primary and secondary resources**, *Minerals Engineering* 161 (2021) 106719.

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### 6.2.3 Books (2)

157. Anderson, C., Goodall, G., Gostu, S., Gregurek, D., Lundström, M., Meskers, C., Nicol, S., Peuraniemi, E., Tesfaye, F., Tripathy, P., Wang, S., Zhang, Y. (Eds.) (2021). Ni-Co 2021: **The 5th International Symposium on Nickel and Cobalt.** (1 ed.) (The Minerals, Metals & Materials Series). Springer, Cham, XXIX, 351. DOI: 10.1007/978-3-030-65647-8.

158. Lee, J., Wagstaff, S., Anderson, A., Tesfaye, F., Lambotte, G., & Allanore, A. (Eds.) (2021). **Materials Processing Fundamentals 2021.** (1 ed.) (The Minerals, Metals & Materials Series). Springer. DOI: 10.1007/978-3-030-65253-1.

### 6.2.4 Book chapters (4)

159. Jogi, R., Mäki-Arvela, P., Virtanen, P.  Mikkola, J-P., **A sustainable bio-jet fuel: An alternative energy source for aviation sector**, In *Biorefineries: A Step Towards Renewable and Clean Energy,* Verma, P. (ed.). 1 ed. Singapore: Springer, (Clean Energy Production Technologies), 18, 465–497.

160. Martínez-Klimov, M. E., Mäki-Arvela, P., Murzin, D. Yu., **Catalysis for production of jet fuel from renewable sources by hydrodeoxygenation and hydrocracking,** *Catalysis*, 33, ed. J. Spicey, Y.-Y., Han, D. Shekhawat, The Royal Society of Chemistry, UK, 2021, ch. 6, 00. 181–213.

161. Moroz, M., Tesfaye, F., Demchenko, P., Prokhorenko, M., Rudyk, B., Soliak, L., Lindberg, D., Reshetnyak, O., Hupa, L., **Thermodynamic examination of quaternary compounds in the Ag–Fe–(Ge, Sn)–Se systems by the solid-state EMF method**. In: Lee, J. et al. (Eds.) Materials Processing Fundamentals 2021. The Minerals, Metals & Materials Series. Springer, Cham. DOI: 10.1007/978-3-030-65253-1_24 .

162. Si, C., Xu, J., Dai, L., Xu C. (2021), **Novel and efficient lignin fractionation processes for tailing lignin-based materials**. In Liu Z.-H. and Ragauskas A., eds. Emerging Technologies for Biorefineries, Biofuels, and Value-Added Commodities. Springer International Publishing, 363–387. http://dx.doi.org/10.1007/978-3-030-65584-6_15

### 6.2.5 Articles in refereed international edited volumes and conference proceedings (1)

163. Vainio, E., Yrjas, P., Hupa, L., Hupa, M., **Formation of $NH_4Cl$ and its role on cold-end corrosion in CFB combustion**, *CFB 2021 - Proceedings of the 13th International Conference on Fluidized Bed Technology*, 2021, pp. 521–526.

### 6.2.6 Other publications (5)

164. Iloeje, C.O., Tesfaye, F., Anderson, A.E., **Editorial: Thermodynamic Optimization of Critical Metals Processing and Recovery: Part I**, *JOM* 73(2) (2021), 665–667.

165. Iloeje, C.O., Tesfaye, F., Anderson, A.E., **Editorial: Thermodynamic Optimization of Critical Metals Processing and Recovery: Part II**, *JOM* 73(3) (2021), 1-3.

166. Tesfaye, F., Iloeje, C.O., **Editorial: Thermodynamic Considerations for Improved Renewable Energy**, *JOM* 73(5) (2021), 1484–1486.

167. Tesfaye, F., Peng, H., & Zhang, M., **Editorial: Advances in the Circular Economy of Lanthanides**, *JOM* 73(1) (2021), 16–18.

168. Vainio, E., Yrjas, P., Hupa, L., Hupa, M. **Formation of $NH_4Cl$ and its role on cold-end corrosion in CFB combustion,** CFB 2021 - Proceedings of the 13th International Conference on Fluidized Bed Technology, 2021, 521–526.

## 6.3 Awards granted

*Saeid, Soudabeh,* The best doctoral thesis award of the Finnish Catalysis Society of years 2019-2021

*Wang, Q., Xu, W., Xu, C., Wang, X.,* (2021) First prize in TAPPI Nano 2021 Virtual conference poster competition, A Strategy of Wood-based UV-cross-linkable Hydrogel Fabrication.

# 7. External interactions 2020

## 7.1 Organization of conferences/courses/meetings 2020

Computer-Aided Chemical Reaction Engineering (CACRE2020), two-week intensive course for postgraduate students, October 2020

International Recycling and Recovery Congress, Vienna, Austria, web-congress, October, 2020, steering committee member, *Patrik Yrjas*

International Recycling and Recovery Congress, Vienna, Austria, web-congress, October, 2020, session moderator, *Patrik Yrjas*

International Chemical Recovery Conference, Sao Paolo, Brazil, May, member of the Technical Program Committee, *Patrik Yrjas*

## 7.2 Visits and visitors

### Visits

*Weihua Zhang,* Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, China, 20.07.2020-31.12.2020

### Visitors

*Barone, Anna*, University of Naples Federico II, Italy, 4.2-15.5.2020

*Delgado, Jose*, INSA Rouen, France, 1.1.-30.9.2020

*Dou, Jinze*, visiting doctoral student, Aalto University, Finland, 09.03.2020-13.03.2020 and 06.10.2020-09.10.2020

*El Hajam, Maryam*, visiting doctoral student, University of Sidi Mohamed Ben Abdelah, Morocco, 01.01.2020-25.07.2020

*Fortunato, Michele*, University of Naples Federico II, Italy, 28.2-15.6.2020

*Hamel, Gregory*, ECAN Lyon, France, 28.1-31.3.2020

*Herrero Manzano, Maria*, University of Valladolid, Spain, 1.1.-30.9.2020

*Kong, Yi,* visiting master student, Qingdao University of Science and Technology, China, 01.01.2020-31.1.2020

*Link, Siim*, Tallinn University of Tecnhology, Tallinn, Estonia, 7-18.9.2020

*Mendez, Fernandez, Jorge,* Universidad Complutense de Madrid, Spain, 7.1.2020-15.6.2020

*Hachhach, Mouad*, Abdelmalek Essaâdi University, Morocco 1.1-15.3.2020

*Navas, Marisa*, University of La Plata, Argentina 3.2-31.8.2020

*Ramos Andres, Marta*, visiting doctoral student, University of Valladolid, Spain, 06.10.2020-31.12.2020

*Rossano, Carmelina*, University of Naples Federico II, Italy, 2.3-15.7.2020

*Scherban, Nataliya*, L. V. Pisarzhevsky Institute of Physical Chemistry, Kiev, Ukraine, 4.2-15.5.2020

*Souza de Oliveira, Adriana*, University of Madrid, Spain, 1.1-15.1.2020

*Taddeo, Francesco*, University of Naples Federico II, Italy, 2.3.-15.7.2020

*Tan, Liping,* visiting researcher, Lecturer, Qilu University of Technology, China, 01.01.2020-28.06.2020

*Trajano, Heather*, University of British Columbia, Canada, 1.1.-30.6.2020

*Winkler, Tom,* Germany, TU Dresden, Germany, 1.10-31.12.2020

*Yang, Xiaodeng*, visiting researcher, Associate Professor, Qilu University of Technology, China, 01.01.2020-09.06.2020

*Yilmaz, Bilge,* visiting doctoral student, Karadeniz Teknik Üniversitesi, Turkey, 30.01.2020-20.03.2020

*Yong, Qiwen,* visiting researcher, Lecturer, China West Normal University, China, 12.12.2020-31.12.2020

*Zergane, Hichem*, visiting doctoral student, USTHB university, Algeria, 01.01.2020-30.09.2020

## 7.3 Evaluation of candidates

Committé member for evaluation of tenure track professor Henrik Grénman, *Johan Bobacka*

Committé member for PhD defences at Åbo Akademi University: Adriana Freites Aguilera and Muhammad Talha Masood, *Johan Bobacka*

Committé member for PhD defences at Åbo Akademi University: Thomas Kronberg, *Rose-Marie Latonen*

Committé member for PhD defences at Åbo Akademi University: Carl Haikarainen, *Anders Brink (chair), Magnus Hellström, Pasi Tolvanen*

Committé member for PhD defences at Åbo Akademi University: Soudabeh Saeid and Mauricio Roche Tabata, *Patrik Yrjas*

Committeé member for docent lecture by Sonja Enestam, *Patrik Yrjas*

## 7.4 External evaluations and reviews

### External evaluations

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

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

Evaluation of proposals, EU HORIZON EUROPE (2021-2027), *Narendra Kumar*

Evaluation of proposals, EU HORIZON EUROPE, *Narendra Kumar*

Evaluation of proposals, M-ERA NET, *Narendra Kumar*

Evaluation of proposals, European Science Foundation, *Narendra Kumar*

Evaluation of proposals, EU H2020-FETOPEN, *Rose-Marie Latonen*

Evaluation of proposals, Latvian Council of Science, *Rose-Marie Latonen*

Evaluation of Humboldt-Stiftung guest professorship, *Tapio Salmi*

Evaluation of research proposals for Swiss Research Agency, *Tapio Salmi*

Evaluation of promotion of H. Heeres to full professor at University of Groningen, *Tapio Salmi*

Expert assessment (external reviewer) for promotion to Associate Professor (Gaston Crespo), KTH, Sweden, *Tom Lindfors*

### Doctoral thesis evaluations

*Adibi Larijani, Amir,* University of Jyväskylä, pre-examiner, *Xu, Chunlin*

*Albrand, Pierre*, ENSIACET- Toulouse, jury member, *Tapio Salmi*

*Bremer, Jens*, Otto-von-Guericke-Universität Magdeburg, jury member, *Tapio Salmi*

*Chen, Yifeng*, Luleå University of Technology, pre-examiner, *Päivi Mäki-Arvela*

*Garcia Hernandez, Elisabeth*, INSA-Rouen, jury member, *Tapio Salmi*

*Granestrand, Jonas*, KTH Stockholm, jury member, *Tapio Salmi*

*Grigonyté-Lopez Rodriguez, Julija,* University of Eastern Finland, pre-examiner, *Patrik Yrjas*

*Iashin, Vladimir,* University of Helsinki, reviewer, *Reko Leino*

*Khan, Yaseen*, Aalto University, pre-examiner, *Henrik Grénman*

*Müller, Pia*, Eindhoven University of Technology, jury member, *Tapio Salmi*

*Varini, Maria,* KTH, Sweden, examiner in the grading committee, *Johan Bobacka*

*Wang, Yanhun*, INSA Rouen Normandie, opponents *Henrik Grénman* and *Tapio Salmi*

## 7.5 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*

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

Electroanalysis, editorial 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*

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

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

Industrial Crops and Products, editorial board member, *Chunlin Xu*

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*

Oil Shale, editorial board member, *Tapio Salmi*

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

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

Russian Journal of Physical Chemistry, editorial board member, *Tapio Salmi*

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

Sensors, editorial advisory board member, *Andrzej Lewenstam*

Sensors and Actuators B: Chemical, 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 of scientific committees and boards

Baltic University Programme (BUP), 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*

Biocity Turku Research Programme: Advanced Bioresources and Smart Bioproducts Programme, *Rose-Marie Latonen*

Catalysis in Multiphase Reactors & International Symposium on Multifunctional Reactors (CAMURE 11), Milan, 2020, Member of scientific committee, *Tapio Salmi*

Clic Innovation Ltd (innovation cluster in bioeconomy, energy, and cleantech), ÅAU representative, *Chunlin Xu*

Climate Leadership Coalition Forest Group (https://clc.fi/), *Stefan Willför*

COST Action CA17128 "Establishment of a Pan-European Network on the Sustainable 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 Polysaccharides Network of Excellence (EPNOE), ÅAU representative, *Chunlin Xu*

Expand Fibre Ecosystem, ÅAU representative, *Chunlin Xu*

Finnish Catalysis Society, member of the board, *Pasi Tolvanen*

Finnish Catalysis Society, Chairman, *Henrik Grénman,* member of the board, *Pasi Tolvanen*

Finnish Chemical Society, Representative of the Division of Analytical Chemistry (DAC) of the European Chemical Society (EuChemS), *Johan Bobacka*

GlucoModicum Oy, member of the board, *Johan Bobacka*

GlucoModicum Oy, sensor lead, *Zhanna Boeva*

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

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

8th International Conference on Engineering for Waste and Biomass Valorisation, Guelph, Canada, 2020, Member of Scientific Committee, *Narendra Kumar*

International Academy of Wood Science / IAWS, Fellow**,** *Andrey Pranovich*

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

International Energy Agency – Fluidised Bed Conversion (IEA-FBC), executive committee member, *Patrik Yrjas*

International Energy Agency - Fluidized Bed Conversion (IEA-FBC) executive committee alternative member, *Emil Vainio*

Scandinavian-Nordic Section of the Combustion Institute, president, *Patrik Yrjas*

IFRF-FFRC (International Flame Research Foundation - Finnish Flame Research Committee), board member, *Patrik Yrjas*

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*

Multicomponent Materials Centre of Expertise for Additive Manufacturing (MMAM), Member of the Steering Committee, *Chunlin Xu*

Nordic Catalysis Society, board member, *Henrik Grénman*

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

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*

Subject cluster: Chemistry and Chemical Technology at the Faculty of Science and Engineering, head of the subject cluster, *Johan Bobacka*

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*

University of Valladolid, international advisory board, *Tapio Salmi*

Åbo Akademi strategic research profile: Molecular Process and Material Technology, chairman of the steering group, *Johan Bobacka,* member of the steering group, *Henrik Grénman*

# 8. External interactions 2021

## 8.1 Organization of conferences/courses/meetings 2021

Young Scientist Forum of Finnish Catalysis Society (YSF), April 2021
Reaction kinetics, intensive course for postgraduate students, December 2021

Member of the Scientific Committee of the "1st International Meeting for Young Analytical Chemists (IMYAC)", On-line meeting, 27–28.9.2021.

## 8.2 Visits and visitors

### Visits

*Salmi, Tapio*, Russian Academy of Sciences, Zelinsky Institute of Organic Reactions, 20.11-31.12.2021

*Zhang, Weihua*, Chinese Academy of Sciences, China, 01.01.2021-31.12.2021

### Visitors

*Araujo Barahona, German*, University of Valladolid, Spain, 1.1-31.12.2021

*Asensio, Alvaro,* University of Vallidolid, Spain, 18.10.2021-30.3.2022

*Baccot, Fabien*, ENSICAEN, France, 26.4-13.8.2021

*Bi, Hongjie,* Northeast Forestry Uniersity, China, 20.3.2021-31.12.2021

*Cabaud, Helene,* ENSICAEN, France, 26.4-13.8.2021

*Cogliani, Tommaso,* University of Naples, Italy , 4.10.2021-3.10.2022

*Calimli, Mehmet,* Iğdır Üniversitesi, Igdir, Turkey, 1.2-31.7.2021

*Goioechea Torres, Alberto*, University of Vallidolid, Spain, 27.8.21-26.8.22

*Korábková, Eva*, Tomas Bata University in Zlín, Czech Republic, 1.10.-30.11.2021

*Lasne, Basile*, ENSICAEN, France, 26.4-13.8.2021

*Lebendig, Florian*, Forschungszentrum Jülich, Germany, 20.9-30.10.2021

*Lyu*, *Yan*, Guangzhou, China, 1.11.2020 - 03.11.2021.

*Mastroianni, Luca*, University of Naples Federico II, Italy, 20.1-15.8.2021

*Muller, Joseph*, ENSICAEN, France, 26.4-13.8.2021

*Orabona, Federica*, University of Naples, Federico II, Italy, 20.01-15.08.2021

*Ramos, Andres Marta*, University of Vallidolid, Spain, 1.1-28.4.2021

*Reich, Marie-Louis*, TU Dresden, Germany, 30.8.21-28.2.22

*Sandri, Francesco*, University of Padova, Italy, 16.11.21-15.6.22

*Simakova, Irina*, Boreskov Institute of Catalysis, Novosibirsk, Russia, 15.4-20.5.2021, 15.6-15.7.2021; 1.08.-18.08.2021

*Snidaro, Rémi*, ENSICAEN, France, 26.4-13.8.2021

*Sokolsky, Pavel*, Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, Moscow, Russia, 1.11.21-31.11.21

*Taghavi, Somayeh*, Ca' Foscari University of Venice, Venice, Italy, 01.04.2021-30.06.2021

*Tanguy, Flory*, ENSICAEN, France, 26.4-13.8.2021

*Than, Jennifer*, INSA Rouen, France, 26.4-13.8.2021

*Ye, Gaoyuan*, Northeast Forestry University, China, 20.3.2021-31.12.2021

*Yong, Qiwen,* China West Normal University, China, 1.1.2021-16.12.2021

*Vergat-Lemercier, Camille*, INSA Rouen, France, 26.4-13.8.2021

*Vikanova, Ksenia*, Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia 1.11.21-31.11.21

*Winkler, Tom*, TU Dresden, Germany, 1.1.-31.05.2021

*Worgul, Bernadette*, Friedrich-Alexander-Universität (FAU) Erlangen-Nürnberg, Germany 11.1.2021-15.8.2021

## 8.3 Evaluation of candidates

Committé member for PhD defences at Åbo Akademi University: Matilda Kråkström, *Johan Bobacka, Anna Sundberg*

Committé member for PhD defences at Åbo Akademi University: Ali Najarnezhadmashhadi, *Henrik Saxen (chair), Pasi Tolvanen, Pasi Virtanen*

Committé member for PhD defences at Åbo Akademi University: Maedeh Arvani, *Rose-Marie Latonen*

Committé member for recruitment of postdoctoral researcher to the research profile Technologies for a Sustainable Future: Javier Farfan, *Johan Bobacka*

## 8.4 External evaluations and reviews

### External evaluations

Appointment Committee member for the vacant Professorship in Analytical Chemistry, University of Helsinki, *Tom Lindfors*

Belgian Research Agency (FNRS) 2020-22, *Reko Leino*

European Research Council (ERC) 2021, *Reko Leino*

Expert, Haldor Topsoe PhD scholarship program, *Dmitry Murzin, 2021*

Evaluation of proposals, EU Horizon Europe Programme, *Päivi Mäki-Arvela*

Evaluation of proposals, FNRS, Belgium, *Päivi Mäki-Arvela*

Evaluation of proposals, Catalonia, Spain, *Päivi Mäki-Arvela*

Evaluation of proposals, European Science Foundation, *Päivi Mäki-Arvela*

Evaluation of proposals, EU Horizon Europe Programme, *Narendra Kumar*

Evaluation of proposals, M-ERA NET, *Narendra Kumar*

Evaluation of proposals, European Science Foundation, *Narendra Kumar*

Evaluation of proposals, HORIZON-EIC-2021-PATHFINDEROPEN-01, *Rose-Marie Latonen*

Evaluation of candidates, doctoral program in chemical engineering, regional funding Normandie, France, *Henrik Grénman*

External expert assisting the European Commission Research Executive Agency (REA) in H2020 and Horizon Europe framework programmes 2020-22, *Reko Leino*

Latvian Council of Science 2021-22, *Reko Leino*

Slovenian Research Agency 2021, *Reko Leino*

## Doctoral thesis evaluation

*Arshanitsa, Alexandr*, University of Latvia, Latvia, Official opponent, *Andrey Pranovich*

*Coronado, Irene,* Aalto University, Opponent, *Henrik Grénman,*

*Estevez, J. Reynose,* University of Bilbao, opponent, *Dmitry Murzin*

*Fenes, Endre,* NTNU, Trondheim, opponent, *Dmitry Murzin*

*Kantarelis, Efthymios (*associate professor), KTH Stockholm, evalution of promotion, *Tapio salmi*

*Kupila, Riikka*, University of Oulu, Opponent, *Henrik Grénman*

*Liangsupree, Thanaporn*, University of Helsinki, pre-examiner, *Johan Bobacka*

*Lu, Xiaojia*, INSA-Rouen and Åbo Akademi (cotutelle), president of the jury, *Tapio Salmi*

*Ma, Chunyan,* Luleå University of Technology, opponent, *Päivi Mäki-Arvela*

*Ma, Hongfo*, NTNU Trondheim, Opponent, *Tapio Salmi*

*Perez Sena, Wander*, INSA-Rouen & Åbo Akademi (cotutelle), member of the jury, *Tapio Salmi*

*Roopchund, Rishen*, University of KwaZulu-Natal, South Africa, Pre-examiner, *Chunlin Xu*

*Rusanen, Annu,* University of Oulu, reviewer, *Päivi Mäki-Arvela*

*Schandel, Christian,* DTU, Lyngby, opponent, *Dmitry Murzin*

*Suhonen, Heikki,* University of Eastern Finland, reviewer, *Patrik Yrjas*

*Sun, Yunhao,* Luleå University of Technology, reviewer, *Päivi Mäki-Arvela*

*Xu, Kequan*, KTH, Sweden, opponent, *Tom Lindfors*

## 8.5 Editorial boards

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*

Catalysis Today, editorial board member, *Dmitry Murzin*

Catalysts, editor of special issue Metal Modified and Acidic Mesoporous Catalytic Materials for Valorization of Lignocellulosic Biomass, Synthesis of Speciality, Fine Chemicals and Pharmaceuticals, *Narendra Kumar*

Catalysts, editor of special Issue Microporous Zeolites and Related Nanoporous Materials: Synthesis, Characterization and Application in Catalysis, *Narendra Kumar*

Catalysts, editor of special issue Microporous and Mesoporous Materials for Application in Catalysis, *Narendra Kumar*

Catalysts, guest editor of special issue Process Intensification in Chemical Reaction Engineering, *Pasi Tolvanen*

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

ChemEngineering, scientific advisor board, *Dmitry Murzin*

Clean Technologies, editorial board member, *Dmitry Murzin*

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

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

Electroanalysis, editorial board member, *Andrzej Lewenstam*

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

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

Frontiers in Bioengineering and Biotechnology, Guest editor*, Chunlin Xu*

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

Frontiers in Chemical Engineering, topic editor of Innovators in Chemical Reaction Engineering, *Narendra Kumar*

Frontiers in Chemical Engineering, topic editor of Supported Metal Naoparticles for synthesis of value-added products, *Narendra Kumar*

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

Industrial crops and products, Associate editor, *Chunlin Xu*

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 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 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*

Processes, guest editor of special issue Catalytic Epoxidation Reaction, *Pasi Tolvanen*

Reactions*,* editor-in-chief*, Dmitry Murzin*

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, editor, *Johan Bobacka*

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

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

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

*Wood Science & Technology,* Member of editorial board, Bjarne Holmbom

## Member of committees and boards

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

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

Biocity Turku Research Programme: Biomaterials and Biomedical Devices Research Programme of Biocity, Director, *Chunlin Xu*

Clic Innovation Ltd (innovation cluster in bioeconomy, energy, and cleantech), ÅAU representative, *Chunlin Xu*

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

European Federation of Catalysis Societies, *Dmitry Murzin*

Finnish Chemical Society, the Division of Analytical Chemistry (DAC) of the European Chemical Society (EuChemS), representative, *Johan Bobacka*

GlucoModicum Oy, member of the board, *Johan Bobacka*

19th Nordic Symposium on Catalysis, Member of Organizing Committee, *Henrik Grénman*

9th International Conference on Engineering for Waste and Biomass Valorisation, June 27-30, 2022, Copenhagen, Denmark, Member of Scientific Committee, *Narendra Kumar*

Industrial Biotechnology Cluster Finland (IBC Finland), Member of the board, *Stefan Willför*

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

Subject cluster: Chemistry and Chemical Technology at the Faculty of Science and Engineering, head of the subject cluster, *Johan Bobacka*

Walter Ahlström foundation, Member of the board, *Anna Sundberg*

Åbo Akademi strategic research profile: Technologies for a Sustainable Future, chairman of the steering group, *Johan Bobacka*

Åbo Akademi strategic research profile: Molecular Process and Material Technology, member of the steering group, *Henrik Grénman*

# 9. Doctoral Theses in Progress at PCC

*Aalto-Setälä, Laura* (MSc 2014, Aalto University), Dissolution mechanisms of bioactive glass – based scaffolds, FINLAND

*Ahamed, Ashiq* (MSc 2012, Nanyang Technological University), Life cycle assessment of plastic waste, its treatment, and application of the upcycled product: a comprehensive circular approach, SINGAPORE, Defended 2021

*Alopaeus, Marie* (MSc 2022, Åbo Akademi University), Lignin-carbohydrate complexes, FINLAND

*Alvear, Matias* (MSc 2019, Politecnico di Milano), Kinetics, mechanism and reactor/catalyst technology for epoxidation reactions, CHILE.

*Araujo Barahona, German* (M.Sc. 2021, Universidad de Valladolid) New technology for hydrogenation processes in alimentary industry (double degree with Universidad de Valladolid), EL SALVADOR

*Badazhkova, Veronika* (MSc 2020, Saint-Petersburg State Chemical Pharmaceutical University), From forest industry waste streams to new chemicals and Materials: value from lignin degradation, RUSSIAN FEDERATION

*Balint, Roland* (MSc 2018, Åbo Akademi University), Ash deposit aging in combustion of biomass, GERMANY

*Bruun, Nina* (MSc 1984, Åbo Akademi University), Challenge of bio-oil in marine engines, FINLAND

*Cogliano, Tommaso* (MSc 2019, Università di Napoli 'Federico II'), Vegetable oils epoxidation: from batch to continuous process, double-degree with Università di Napoli 'Federico II', ITALY

*Delgado, Jose Emilio* (MSc 2019, INSA-Rouen), Production of γ-valerolactone – a green platform molecule, double-degree with INSA-Rouen, DOMINIC REPUBLIC

*Fagerlund, Rasmus* (MSc 2021, Åbo Akademi University), Machine-learning based prediction of NOx-emission formation kinetics in biomass combustion CFD modeling, FINLAND

*Hachhach, Mouad* (MSc 2016 ENSA Agadir) Techno-economic and environmental analysis of hemicellulose valorization, ROYAUME DU MAROC

*Han, Tingting* (MSc 2008, Åbo Akademi University), Novel signal readout principle for solid-contact ion-selective electrodes, CHINA, Defended 2021

*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), Microfibrillated cellulose composites for paper and packaging, CHINA

*Hupa, Elisa* (MSc 2014, Åbo Akademi University), New approach to determine initial melting of corrosive deposits, FINLAND

*Joon, Narender* (MSc 2016, Åbo Akademi University), Continuous dynamic extraction and on-line determination of metals from solid environmental samples, INDIA

*Kaka Khel, Taimoor A.* (MSc 2019, Åbo Akademi University), A comprehensive catalytic study for the production of diesel range cycloalkanes from biomass molecules, PAKISTAN

*Kholkina, Ekaterina* (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, RUSSIAN FEDERATION

*Kråkström, Matilda* (MSc 2015, Åbo Akademi University), Evaluation of advanced oxidation processes for removal of antibiotics in wastewater treatment plants, FINLAND, Defended 2021

*Korotkova, Ekaterina* (MSc 2011, Åbo Akademi University), Mild-alkaline extraction of spruce lignin and its applications, RUSSIAN FEDERATION

*Kvikant, Minette* (MSc 2022 Åbo Akademi University), Hemicellulose modification and coating, 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

*Li, Zhiqiang* (MSc 2013, Åbo Akademi University), Dissolving pulp, 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

*Lund, Sara* (MSc 2013, Åbo Akademi University), From exfoliation of graphite to graphene-nanocellulose composites for bioelectrochemical applications, FINLAND

*Lu, Zonghong* (MSc 2020, Tianjin University of Science &Technology), Bioactive packaging, CHINA

*Mastroianni, Luca* (MSc 2021, Università di Napoli 'Federico II') Transient and stationary studies of avant-garde catalysts and reactors (double degree with Università di Napoli 'Federico II'), ITALY

*Matamala, Veronica* (MSc 2014, Åbo Akademi University), The effect of raw materials on production of dissolving pulp, CHILE

*Martínez Klimov, Mark* (M.Sc. 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

*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

*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

*Salucci, Emiliano* (M.Sc. 2018, Università di Napoli 'Federico II'), Reduction of iron oxides with hydrogen, ITALY

*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 scale bubbling fluidized bed in conditions typical for biomass and agrofuel firing, FINLAND

*Siekkinen, Minna* (MSc 2019, Åbo Akademi University), Interaction between bio-active glass and bio-degradable polymers, FINLAND

*Sinitsyna, Polina* (MSc 2018, Åbo Akademi University), Novel understanding of dissolution kinetics of bioactive glasses, RUSSIAN FEDERATION

*Stiller, Adrian* (MSc 2019, Universität Ulm), The impact of fluid-flow rate of dissolution of bioactive glasses, GERMANY

*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

*Wang, Luyao* (MSc 2018, Qingdao Institute of Bioprocess and Bioenergy Technology, Chinese 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

*Wei, Liangyuan* (MSc 2014, Huazhong University of Science and Technology), Sorption enhanced $CO_2$ methanation for large scale energy storage - catalyst & process development, CHINA

*Xu, Jiayun* (MSc 2019, Qilu University of Technology), Lignin and LCC from novel fractionation processes, CHINA

*Yrjänä, Ville* (MSc 2018, Åbo Akademi University), Developing potentiometric ion-selective electrodes for anions, FINLAND

*Zhang, Yidong* (MSc 2021, Qingdao University of Science and Technology), Preparation of dialdehyde cellulose with molten salt hydrates pretreatment and its potential applications, CHINA

*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), Multifaceted applications of nanocellulose-based materials for water remediation, CHINA

*Zhu, Lulu* (BSc 2018, Nanjing Forestry University), Lignin reactive extrusion, CHINA

*Örn, Anton* (MSc 2019, Åbo Akademi University), Synthesis of rare sugars through site selective epimerization, FINLAND