

High Rated Chemistry Research at Åbo Akademi

The Academy of Finland has carried out an objective and extensive evaluation of the chemistry research in Finland. The concept “chemistry” was limited to classical fields of chemistry (biochemistry excluded) and to some extent chemical technology. Totally 41 units were evaluated based on their activity during 2005–2009.

The evaluation was done by an international panel consisting of seven foreign professors in chemistry and chemical technology. The opinion of the panel was based on self-evaluation forms comprising topics on the research and publication activity of the corresponding unit, as well as on the age and gender and the infrastructure and internationalization of the research. Even visits of the panel to different research centers in Finland were planned, but these visits were cancelled by the cloud from the volcano Eyjafjallajökull.

The following fields of chemistry were reviewed: analytical chemistry, physical chemistry, inorganic chemistry, material chemistry, polymer chemistry, and paper chemistry.

The assessment of the panel shows that chemistry research in Finland is on a high international level; some of the units are representing the international top within their fields. It was concluded that the infrastructure of the research is generally good and the financing is satisfying.

At Åbo Akademi University the following units were evaluated: analytical chemistry, physical chemistry, organic chemistry, inorganic chemistry, industrial chemistry and reaction engineering, as well as wood and paper chemistry. All these units achieved the grade “excellent” or “very good” in the evaluation. They were concluded to conduct innovative and productive research in an international environment with a good local infrastructure.

The number of international journal articles were particularly high at Åbo Akademi University in the period 2005–2009: 820 journal articles. The PCC had an excellent strategy and infrastructure for research and the evaluation panel recommends the PCC to continue its



Academy Professor Tapio Salmi

activities. The report “Chemistry Research in Finland” is found on the webpage of the Academy of Finland (www.aka.fi).

My inevitable conclusion is: The PCC shall and will continue!

Tapio Salmi

PCC Winter Colloquium

The PCC Winter Colloquium took place in Axelia on February 2, 2011. The speakers were **Tom Lindfors** (Water uptake in ion-selective membranes), **Daniel Lindberg** (Chemical thermodynamics of molten salts in biomass combustion and gasification), **Annika Smeds** (Liquid chromatography–mass spectrometry LC–MS – applications of forest industrial products), **Johan Bobacka** and **Tapio Salmi** (Conferences organized in 2011 by the groups at PCC), **Narendra Kumar** (Synthesis and characterization of micro-porous and meso-porous materials for production of fuels and chemicals), **Päivi Mäki-Arvela** (Engineering bio-chemo catalytic reactions), **Lari Vähäsalo** (Flow cytometry – for counting and sorting of particles), **Anders Brink** (Combustion modeling of industrial applications), and **Ari Ivaska** (Future activities of the PCC).



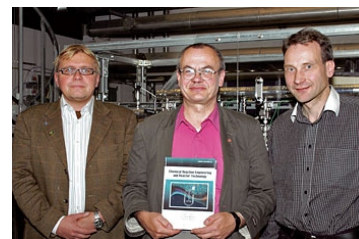
New Extensive Textbook on Chemical Reaction Engineering

The textbook "*Chemical Reaction Engineering and Reactor Technology*" by **Tapio Salmi**, **Jyri-Pekka Mikkola**, and **Johan Wärnå** was published in the autumn of 2010. The book was published by the prestigious publishing house CRC Press and is included in their series "*Chemical Industries Series*".

This is a textbook in modern chemical reaction engineering. It contains fundamental theory, historical aspects, and future perspectives as well as exercises. The idea of writing a book came up for a couple of years ago when Jyri-Pekka Mikkola translated my texts

to English and at the same time Johan Wärnå got involved in the project, Tapio Salmi says.

The content of this book is based partly on our own research, on results of our own experiments. The target group of the book is students, researchers, and industrial engineers. The three authors of the book states that this book differs from other textbooks in the field, because it contains a lot of solved exercises and many computer applications in the area. The trio will work together again. Finnish scientists seldom write



Jyri-Pekka Mikkola, Tapio Salmi, and Johan Wärnå.

textbooks that are published abroad. It feels good that we have published this book, Tapio Salmi concludes.

Interview with a Fresh Doctor: Elena Tokareva

Dr. Elena Tokareva, tell me about your research using time-of-flight secondary ion mass spectrometry (ToF-SIMS).

–ToF-SIMS is a chemical microscopy technique with great potential for simultaneous analysis of organic and inorganic constituents on the surfaces at an analysis depth of about 1–2 nm with a high lateral resolution, even better than 1 µm. The thesis work has aimed at simultaneous analysis of the spatial distribution of polymeric lignin and carbohydrates, and metals in wood.

What kind of results did you get - anything particularly interesting that you want to point out?

–Systematic studies using ToF-SIMS gave fundamentally new knowledge about the spatial distribution of various wood components. A new sample preparation procedure for wood analysis using ToF-SIMS was developed, evaluated and applied. It was found that in the case of freeze-dried or air-dried samples, extractives covered the wood section surfaces, masking the signals originating from individual wood components in ToF-SIMS images. However, after the extraction the distribution of lignin, carbohydrates and metal ions on wood surfaces could be assessed.

–ToF-SIMS analysis of pre-extracted spruce and aspen wood samples showed different distribution of metal ions (i.e. Na, Mg, K, Ca), pectin and lignin in ray cells, vessels and fibers. Carbohydrates (cellulose and hemicelluloses), however, were rather uniformly distributed across the wood sections.

–A new method for labeling of anionic groups (AGs) on wood surfaces was developed and applied. ToF-SIMS analysis of labeled samples showed that after alkaline-peroxide treatment the amount of AGs was higher than in alkali-treated and untreated samples. Since quantification of components on the surfaces by ToF-SIMS is difficult, the relative amount of AGs was monitored by laser ablation-inductively coupled plasma mass spectrometry (LA-ICP-MS). LA-ICP-MS revealed that after alkali-peroxide treatment, the concentrations of AGs in fibre walls and ray cells were correspondingly six times and five times higher than in untreated wood.

Did you come to Åbo Akademi right after becoming M.Sc.? Why did you choose it? How have you become interested in wood chemistry?

–I graduated from Moscow State University's Department of Analytical Chemistry in 1999. My diploma work was related to a development of a technique for dioxins analysis in natural tissues. After graduation, I spent several years in a laboratory of medicines control. This provided me with a lot of experience in the practical application of many modern analytical methods, such as GC, HPLC, ICP-MS etc. However, a job in laboratories intended for quality control is restricted by the need to implement standard procedures to give very high repeatability and reproducibility. The use of analytical skills and knowledge is limited by every day routine measurements. In contrast to this, an opportunity to make some real research was really desirable. Finland was not a random choice, since one year earlier, my husband chose ÅA as the place for his Ph.D. studies. A Ph.D. position related to the study of the wood nano-world was tempting for two reasons: the first reason was to do research and to try to obtain skills and knowledge in some real research. The second reason was to see what life was like outside Russia.

And what about Åbo Akademi and Finland now afterwards, what has been the positives and the negatives?

–After several years in Finland, I am pleased to say that I was not mistaken in my first impression. Finland is a small and friendly country best known for sauna, Nokia and tourism. It is also necessary to mention the high level of technology, which is based at research centers such as Åbo Akademi. Actually, many goods produced in Finland, starting with paper and ending with different construction paints and materials are very highly rated in the Russian market. This would not be possible without top level science, which goes hand in hand with technology. With respect to my laboratory, I would like to mention the very friendly and international team. Openness for discussions, willingness to help and professionalism make a creative environment for research.

Would you recommend Åbo Akademi and PCC to other young researchers.

–Certainly yes! I think that Åbo Akademi possess all of the factors needed for obtaining deep knowledge, while collaboration within the PCC broaden possibilities to do successful research.



Dr. Elena Tokareva

The Harry Elving Price to Docent Anna Sundberg

On August 31 Academy Lecturer and Docent **Anna Sundberg** was awarded a teacher price from Harry Elvings Legat proposed by the Department of Chemical Engineering. The motivation reads: She masters the entire scale of teaching, from basics to research level and her concern for students has been shown in her extensive supervising activity. She has been very active in the planning of education in the field of chemical engineering as well as on an academic level. Anna Sundberg is an experienced teacher who became academy lecturer in 2008. In her own research in fiber and paper chemistry, she has focused on the analysis of substances from mechanical pulp in the process water during paper manufacturing, and how these substances affect the paper quality. Anna Sundberg concludes that research on wood and biomass for other purposes than paper is becoming more and more important.



Docent Anna Sundberg

Improvement of Fine Chemical Synthesis in EU Project

The project POLYCAT, where the PCC is taking part, started on October 1st 2010 and is partially financed by the European Commission with a grant of 7 million € in the context of the EU Seventh Framework Programme for Research and Technological Development.

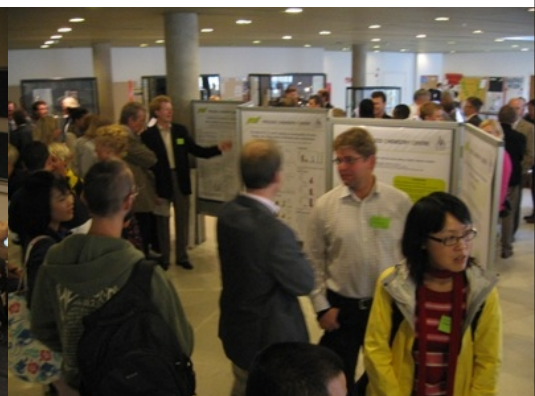
POLYCAT provides an integrated, coherent and holistic approach utilizing novel polymer-based nanoparticulate catalysts in pharmaceutical, crop protection and vitamin syntheses in conjunction with the enabling functions of micro process technology and “green” solvents. This provides a discipline-bridging approach between fine chemistry, catalysis and engineering. The project will lead to the replacement of a number of chemical or microbiological reaction steps in fine chemical syntheses by catalytic ones using more active, selective and stable nanoparticulate catalysts. In addition, POLYCAT will lead to the development of novel chiral modifiers immobilized on the polymeric supports.

The Institut für Mikrotechnik Mainz GmbH (IMM) coordinates the project with a duration of 3.5 years. **Dmitry Murzin** is coordinating the project for the PCC's part. In addition to IMM and PCC, 17 other European companies and universities are involved in the project.

The PCC will contribute to the project with synthesis of chiral modifiers, immobilization of the chiral modifiers on polymeric supports and testing of the catalysts in, for example, asymmetric hydrogenation of alkenes.

Åbo Akademi Process Chemistry Centre Annual Meeting

The Åbo Akademi Process Chemistry Centre Annual Meeting 2010 took place on August 26 in the Gadolinia Building. The event was opened with an introduction by **Academy Professor Tapio Salmi** and the PCC Activity Review by **Professor Mikko Hupa**. Introductions of posters were given by researchers **Maija Blomquist, Valerie Eta, Henrik Gustafsson, Oskar Karlström, Petri Kilpeläinen, Alexey Kirilin, Jens Krogell, Johan Lindholm, Tao Song, Pasi Tolvanen, Michał Wagner** and **Emil Vainio**. A FiDiPro Presentation was held by **Professor Kalle Levon** and recent doctoral theses were presented by **Dr. Markus Engblom, Dr. Fredrik Sundfors, and Dr. Pasi Virtanen**. Lectures on new tools and discoveries were presented by **Henrik Grénman** and **Dr. Mikael Bergelin**. After the comments from the Scientific Advisory Board and the IAB-SAB Conclusion Meeting, the PCC members enjoyed the evening dinner at the restaurant Pikku Pukki.



GUEST LECTURERS

Prof. Tadashi Kokubo, Department of Biomedical Sciences, College of Life and Health Sciences, Chubu University, Japan: "*Preparation of Novel Bioactive Ti-based Metals by Simple Chemical and Heat Treatments*" on September 10, 2010.

Prof. Adam Pron, Laboratoire d'Electronique Moléculaire Organique et Hybride, CEA Grenoble, France: "*Organic and Hybrid (Organic/Inorganic) Electronics - A Chemist Approach*" on October 6, 2010.

Prof. Rufat Abiev, St. Petersburg State University of Technology, Russia: "*Hydrodynamics of Taylor Flow in Capillaries*" on October 18, 2010.

Prof. John Villadsen, Department of Chemical and Biochemical Engineering, Technical University of Denmark: "*Bio-reaction Engineering - a Multidisciplinary Research Field*" on November 26, 2010.

Prof. Dage Sundholm, Department of Chemistry, University of Helsinki, Finland: "*Magnetically Induced Current Densities in Molecules*" on December 2, 2010.

Docent Mika Jokinen, Turku University of Applied Sciences, Turku, Finland: "*About Catalysts & Reactors in Bioprocesses*" on December 8, 2010.

Assoc. Prof. Harry Brumer, Division of Glycoscience, School of Biotechnology, Royal Institute of Technology (KTH), Stockholm, Sweden: "*Polysaccharide Functionalization: XG and Beyond*" on December 8, 2010.

Prof. James A. Anderson, University of Aberdeen, Scotland: "*Controlling Selectivity in Alkyne Hydrogenation Reaction*" on February 3, 2011.

DOCTORAL DEFENSES

Fredrik Sundfors: "*Solid-Contact Ion Sensors: Materials and Properties*" on September 3, 2010. Opponent: **Prof. Philippe Bühlmann**, University of Minnesota, USA.

Antti Taskinen: "*Molecular Modeling of Asymmetric Induction in Heterogeneously Catalyzed Hydrogenation of the C=O Bond*" on October 29, 2010. Opponent: **Dr. Philippe Sautet**, University of Lyon, France (presented at the Laboratory of Physical Chemistry, University of Turku).

Henrik Grénman: "*Solid-liquid Reaction Kinetics - Experimental Aspects and Model Development*" on November 26, 2010. Opponent: **Prof. John Villadsen**, Department of Chemical and Biochemical Engineering, Technical University of Denmark.

Serap Sahin: "*Engineering Chemo-Bio Catalytic Reactions*" on December 3, 2010. Opponent: **Docent Esa Toukonniitty**, Helsinki Metropolitan University of Applied Sciences, Finland.

Mats Käldestrom: "*Cellulose Valorization by Heterogeneous Catalysis*" on February 4, 2011. Opponent: **Prof. James A. Anderson**, University of Aberdeen, Great Britain.

Elena Tokareva: "*Spatial Distribution of Components in Wood by ToF-SIMS*" on February 18, 2011. Opponent: **Prof. Em. Ulla Westermark**, Luleå Tekniska Universitet, Sweden.

Olatunde Jogunola: "*Reaction Intensification Approach to Formic Acid Production*" on March 4, 2011. Opponent: **Prof. Andrzej Kraslawski**, Lappeenranta University of Technology, Finland.

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PCC FACTS AND MISSION

A Centre of Excellence in research appointed by the Academy of Finland for the periods 2000–2005 and 2006–2011. The Åbo Akademi Process Chemistry Centre (ÅA-PCC) studies physico-chemical processes at the molecular level in environments of industrial importance, in order to meet the needs of tomorrow's processes and product development. Our particular focus on the understanding of complex process chemistry we call *Molecular Process Technology*.

The Centre consists of four research groups at the Department of Chemical Engineering, Åbo Akademi University:

- Combustion & Materials Chemistry (Prof. Mikko Hupa),
- Catalysis and Reaction Engineering (Academy Prof. Tapio Salmi),
- Process Analytical Chemistry (Prof. Ari Ivaska) and
- Wood and Paper Chemistry (Prof. Bjarne Holmbom).

In the year 2009, about 130 people (including 20 senior researchers) took part in the PCC activities with a total funding of approximately 6 million euros.

PCC EXECUTIVE BOARD

Prof. Bjarne Holmbom | email: bjarne.holmbom@abo.fi
Prof. Mikko Hupa | email: mikko.hupa@abo.fi
Prof. Ari Ivaska | email: ari.ivaska@abo.fi
Prof. Tapio Salmi | email: tapio.salmi@abo.fi

COORDINATING ASSISTANT

Maria Ljung | email: pcc@abo.fi
Biskopsgatan 8, 20500 Turku / Åbo, Finland

EDITOR IN CHIEF

Prof. Mikko Hupa | email: mikko.hupa@abo.fi

EDITOR

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PROCESS CHEMISTRY CENTRE