

NEWSLETTER

PROCESS CHEMISTRY CENTRE



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Long Live the PCC

The annual meeting of the Process Chemistry Centre (PCC) was held in August 2013. This research centre was founded in 1998 after thorough scientific and strategic discussions that had been initiated by Prof. Bjarne Holmbom. He represented the area of forest product chemistry research at our department, while the other members Mikko Hupa, Ari Ivaska, and Tapio Salmi had their competence within materials and combustion chemistry, process analytical chemistry, as well as industrial chemistry and reaction engineering. What were we then, what did we want to become? It shortly became clear that we vigorously should intensify our cooperation, our mutual correlation. We have certainly had common projects earlier, even co-publications; they had arisen spontaneously when researchers from the Axelia and Gadolinia buildings met and began to discuss research, but no strategic program of cooperation existed. However, four professors gathered at a common meeting and concluded that something should be done. Not only to consolidate the cooperation on the paper, but to create new research together, a new platform for interaction, not only so that the leaders sometimes meet to discuss, but on a new level where researchers are cooperating on the grass root level, planning experiments together, fulfilling their new visions. What is it that is connecting us, these four groups, four laboratories? Together we represent a bridge, from chemistry to chemical engineering, from fundamental science to industrial application.

It may sound surprising, but this bridge is missing at most universities in Europe and also in America. Chemistry and physics in Europe had a leading position globally for a long time, but the advance of fascism in Germany seventy years ago changed the situation totally: many eminent researchers fled to the USA to survive. It took many decades to repair this damage. Chemical engineering made a breakthrough in USA, where great names such as Amundson, Reid, Prausnitz, Aris, Thiele, Himmelblau and many other developed chemical engineering to an independent scientific discipline. Simultaneously a sharp borderline between chemistry and chemical engineering was generated. Many European countries, especially France and Great Britain, followed



Academy Professor Tapio Salmi

this development pattern. Chemical engineering should be based on stringent mathematic modeling of chemical processes. The breakthrough became possible through a powerful development of numerical methods of calculation and computers. This great trend coincided with a massive expansion of the chemical process engineering industry in Europe and America. Everything good; new chemical factories and oil refineries were built to cover the needs of an increased consumption everywhere in the industrialized world. New products were needed and accepted by the consumers: plastics, medicines, detergents, cosmetics, herbicides, pesticides.

Unexpected challenges arose. The increasingly growing mathematical field of chemical engineering bloomed, but at the same time tended to in some respects become off-side, because the industry was not capable to accept all new theories and models that were developed by the academic society. An experienced industrial researcher once accused me: Tapio, you are working at the university, solving simple

problems in an outmost sophisticated way, but you avoid difficult realistic issues. First my feelings were hurt because I was young and sensitive, but later I have understood that his criticism was not totally unfounded.

With time also the dark side of the chemical expansion appeared: compounds that did not degrade in the nature and that sometimes even poisoned it. It was obvious that a new paradigm had to be created. First one spoke about green chemistry, but then it became clear that green chemistry alone is not enough. Instead, the new pattern had to lead to green sustainable process technology, which utilizes renewable resources as raw materials and gives products that degrade to harmless compounds in nature. The rationalism that had been created by classical chemical engineering science should be used in this gigantic transformation from unsustainable technology to green technology.

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The mission statement of the Process Chemistry Centre was formulated based on this reasoning. We wanted to combine a deep chemical knowledge with the most modern methods in chemical engineering in order to prepare the way for the sustainable processes of the future and for environmentally friendly products. The discussions emerged in a new concept: molecular process technology. What is this, are further new slogans needed or is it just a matter of the Emperor's new clothes.

Molecular process technology implies that a deep understanding of processes on a molecular level is created and that new processes and products are developed based on detailed chemical knowledge. Many scientific research methods are involved in the concept, from laboratory experiments to kinetic modeling, thermodynamics, transport processes and fluid dynamics. A too broad spectra one could say. It should be kept in mind that all this is applied to industrial processes and that its bottom line a matter of the chemistry of industrial processes. Professor Jean-Claude Charpentier, who has been the president of the European Federation of Chemical Engineering EFCE, characterized this concept with a triangle; Processus Procédés Produits, where the first word means molecular processes, on which the industrial processes and products are based. Later Charpentier became a member of our scientific advisory board.

A research plan was prepared and sent to the Academy of Finland in 1998 in order to achieve the status as a national center of excellence in scientific research. The competition was tough already then; however we managed to get to the second round in the competition. Later on the finalists were more carefully inspected and

the Academy of Finland sent a delegation to Abo in order to inspect out research and our infrastructure. Researchers and postgraduate students were interviewed. It was exciting; I remember how I gave detailed directives: do not talk about problems, you should talk about challenges (later on this has become a fashion trend among politicians!), our guest researchers should have a prominent roll in the interviews in order to demonstrate the international atmosphere.

Months passed by and finally the decision came: our program had been accepted and we were about to become a national centre of excellence from the beginning of the year 2000. The exultation was big. We did it! We decided to start immediately already in 1999; the first annual meeting was held and the first year book was published. Some of the researchers were of course distrustful: will there only be an alliance between four of our laboratories to get resources, will there be a rigid and controlling roof organization? The executive board was convinced that so was not the case, but instead we would become a scientific forum where we implement research projects together. And so it turned out. We have a very thin and efficient organization: a executive board consisting of four professors and one coordinator. The activities are supported by one academic and one industrial expert group. We decided not to unite the participating laboratories. Their economic and scientific autonomy was preserved. Instead we instantly focused on common research projects, common supervision of postgraduate students, efficient exploitation of our experimental infrastructure, annual seminars, scientific workshops, winter colloquia, annual reports, and we invited top guest lecturers (the PCC Distinguished Lecture series). Over the years

the PCC has grown and developed quantitatively. In 2010 the Academy of Finland arranged a comprehensive evaluation of chemical sciences, including chemical engineering sciences in Finland. The research groups at the PCC consistently received the highest grade 'excellent' by the international panel. At the annual seminar on August 29 2013 it was concluded that PCC is stronger than ever. During the year 2012 125 scientific original articles were published and 10 doctoral theses were defended. Two professors of the centre have held the Academy Professor position, which is extremely hard to win: only about 5% of all applications are accepted. Countless national and international prizes have been awarded to the researchers of the centre. We actively organize international conferences; the highlight was the largest European Congress on Catalysis EuropacatVIII in August 2007 at the Turku Fair and Congress Center, with 1500 participants from all continents. The Nobel Price Laureate **Prof. Robert H. Grubbs** was one of the plenary speakers and Finland's Minister of Culture **Stefan Wallin** honored us with his presence. Is it allowed to brag like this? Not according to the old Finnish and Nordic tradition, but in today's world it has become a necessity. It is hard for me, but one gets hardened as the years pass by. I believe that the PCC has contributed to the development of the chemistry and the chemical engineering science in an imaginative and innovative way, with high class research results and through education of highly qualified researchers that have spread over our planet. The PCC continues. Long live the PCC!

Tapio Salmi
Academy Professor

Analytical Chemistry – Challenges and Opportunities for Ion-Selective Electrodes

The availability of chemical information becomes increasingly important in today's modern world to ensure a safe and clean environment, sustainable industrial production, personal health and welfare for the growing population on Earth. New analytical methods, instruments and strategies are continuously developed and applied in important areas like environmental monitoring, process analysis and healthcare diagnostics. It has been estimated that more than 10 000 chemical analyses are done in the world every minute!

Among a large variety of analytical methods and instrumentation, there is an increasing demand for portable, small-size and easy-to-use chemical sensors. Ion-selective electrodes (ISEs) are an important type of such chemical sensors which has grown to become a major research topic also in our group over the last two decades. A unique feature of ISEs is that they provide information about the free ion

concentration (ion activity), in contrast to most other analytical methods which give the total concentration. Here I will briefly mention some opportunities and challenges in the field of ISEs.

Back in the 1980s, conducting polymers became a hot research topic in the world and thanks to the visions of our former Professor Ari Ivaska we were fortunate to enter this field of research at an early stage. As a result of basic research with analytical applications in mind we were able to employ conducting polymers as solid contact in ISEs already in 1992 and this unique approach soon reached wide international acceptance. In 1997 it was further discovered that the lower detection limit of ISEs can be improved by almost six orders of magnitude to reach concentrations (activities) as low as 10^{-11} mol/l. This ground-breaking discovery resulted in renewed interest in ISEs and their application for trace metal analysis in environmental research became realistic goals.



Photo: Andreas Bernas

Professor Johan Bobacka

In addition to trace metal analysis, research on ISEs over the last two decades has been largely focused on improving the selectivity, making the sensors more durable and gaining deeper theoretical understanding of the response mechanism of ISEs.

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Recent progress in the area of solid-contact reference electrodes has opened up new opportunities for the development of disposable potentiometric sensor systems and wireless sensor networks. Our doctoral students and researchers have made a significant contribution to all these developments.

Despite such an impressive progress, ISEs still have shortcomings that need to be addressed in the future. Precise control of the analytical

performance of ISEs at extremely low ion concentrations and during long-time measurements is still a great challenge. Furthermore, ISEs still require frequent calibration due to potential drift, which is more pronounced for ISEs having a solid internal contact. In real-life applications, the ion-selective membrane surface is prone to contamination from chemical and biological species present in real samples. Such limitations still prevent wide-spread use of ISEs and call for

innovative and ground breaking approaches beyond the state-of-the-art in this field. It is therefore important to keep up the scientific curiosity and to constantly look for new advanced materials and new analytical approaches to be able to satisfy the increasing need for chemical information in the future.

Johan Bobacka
Professor in Analytical Chemistry

2013 Events and Highlights

The PCC Winter Colloquium including a distinguished lecture by **Prof. Lars J Petterson** was held on February 13 and the PCC Annual Seminar was held on August 29. Moreover, an internal workshop on microscopy was arranged on May 8 and a workshop on modeling methods and tools was arranged on December, 17. This year there has been 15 doctoral disputations at the PCC, which is a record number. **Marceline Neg Akieh-Pirkanniemi** was awarded "Alfthanska priset" for her excellent PhD thesis "*Electroactive Ion Exchange Membranes Based on Conducting Polymers*".

Professors Salmi and Murzin are Research Leaders of the Year at Åbo Akademi

On October 8, 2013, the recently established prize "*Kanslerpriset*" (The Chancellor's Prize) was awarded for the first time at Åbo Akademi. The prize went to the research leaders of the year and the prize sum was 50,000 euro. The prize was awarded by the Chancellor of Åbo Akademi **Jarl-Thure Eriksson**.

The first ever prize winners are **Academy Professor in Chemical Reaction Engineering Tapio Salmi** and **Professor in Chemical Technology Dmitry Murzin**.

- It is a fantastic idea to found such a prize and it is of course a great pleasure for me and my colleague to be the first prize winners at Åbo Akademi. Thanks to the prize money we now also have the opportunity to employ new researchers, the prize winner **Tapio Salmi** says.

Salmi and **Murzin** have with a great engagement managed to create an excellent environment for scientific research and education within their area at Åbo Akademi. Their work meets all parts of Åbo Akademi's expectations and gives rise to national as well as international interest.

Professor Mikko Hupa was also nominated and received a diploma for excellent research leadership.

In addition, the article "*Simultaneous Determination of Ascorbic Acid, Dopamine and Uric Acid with Chitosan-graphene Modified Electrode*" by **Dongxue Han, Tingting Han, Chansheng Shan, Ari Ivaska, and Li Niu** led to a price of 2,000 euro for considerable international recognition.



Photo: YLE/Peter Karlberg

GUEST LECTURERS

Prof. Lars J. Pettersson, Chemical Technology, KTH Royal Institute of Technology, Stockholm, Sweden: "*Thermal and Chemical Conversion of Biomass*" on February 13, 2013.

Dr. Lukasz John, Faculty of Chemistry, University of Wrocław, Poland: "*Functional Materials: from Metal Alkoxides to Hybrid Biocomposites*" on May 8, 2013.

Prof. Xiaojun Han, Department Biomolecular and Chemical Engineering, School of Chemical Engineering and Technology, Harbin Institute of Technology, China: "*Biofunctionalized Surfaces*" on 23 August, 2013.

Prof. Nomchit Kaewthai Andrei, Department of Biotechnology, Faculty of Agro-Industry, Rajamangala University Srivijaya, Thailand: "*Plant Cell Wall Remodelling: the Role of XTH Enzymes*" on September 11, 2013.

Prof. Richard G Compton, Oxford University, United Kingdom: "*Electrochemical Studies of Nanoparticles*" on October 1, 2013.

Prof. Nikos Papayannakos, National Technical University of Athens, Greece: "*Pillared Clay Systems as Hydrogenation Catalysts*" on October 4, 2013.

Prof. Roland De Marco, Faculty of Science, University of the Sunshine Coast, Queensland, Australia: "*New Horizons for Solid Contact Polymeric Ion-Selective Electrodes*" on October 11, 2013.

Dr. Juan Carlos Serrano Ruiz, Abengoa Research, Spain: "*From Biomass to Advanced Biofuels: Alternatives to Biodiesel and Bioethanol via Catalytic Conversion*" on November 29, 2013.

Prof. Alexander Kuhn, ENSCBP, University of Bordeaux, France: "*Breaking the Symmetry of Chemical Systems with Bipolar Electrochemistry: from Materials Science to Motion*" on December 17, 2013.

DOCTORAL DEFENSES

Pasi Tolvanen: "*Development of an Environmentally Friendly Method of Starch Oxidation by Hydrogen Peroxide and a Complex Water-Soluble Iron Catalyst*" on February 1, 2013. Opponent: **Docent Fredrik Sandelin**, TF-Engineers Oy, Finland.

Pierdomenico Biasi: "*Combination of Catalyst Development and Chemical Reaction Engineering: A Key Aspect to Improve the Hydrogen Peroxide Direct Synthesis*" on March 8, 2013. Opponent: **Prof. Gabriele Centi**, Università di Messina, Italy.

Elena Privalova: "*Towards Novel Biogas Upgrading Processes*" on March 26, 2013. Opponent: **Dr. Alistair King**, University of Helsinki, Finland.

Oskar Karlström: "*Oxidation Rates of Carbon and Nitrogen in*

Char Residues from Solid Fuels" on June 7, 2013. Opponent: **Prof. Kim Dam-Johansen**, Technical University of Denmark, Denmark.

Tao Song: "*Extraction of Polymeric Galactoglucomannans from Spruce Wood by Pressurised Hot Water*" on August 23, 2013. Opponent: **Prof. Arnis Treimanis**, Latvia State Institute of Wood Chemistry, Latvia.

Jerzy Jasielec: "*Modelling of Potentiometric Ion Sensors*" on September 23, 2013. Opponent: **Prof. Richard Compton**, Oxford University, Great Britain.

Teuvo Kilpiö: "*Mathematical Modeling of Laboratory Scale Three-Phase Fixed Bed Reactors*" on October 4, 2013. Opponent: **Prof. Nikos Papayannakos**, National Technical University of Athens, Greece.

Ann-Sofie Leppänen: "*Regioselective Modification of Galactose-Containing Polysaccharides in Aqueous Media*" on October 25, 2013. Opponent: **Prof. Ilkka Kilpeläinen**, University of Helsinki, Finland.

Hanna Lindqvist: "*Improvement of Wet and Dry Web Properties in Papermaking by Controlling Water and Fiber Quality*" on November 8, 2013. Opponent: **Prof. Raimo Alén**, University of Jyväskylä, Finland.

Anders Strand: "*The pH-Dependent Phase Distribution of Wood Pitch Components in Papermaking Processes*" on November 15, 2013. Opponent: **Prof. Emeritus Per Stenius**, Aalto University and Norwegian University of Science and Technology, Norway.

Alexey Kirilin: "*Aqueous-Phase Reforming of Renewables for Selective Hydrogen Production in the Presence of Supported Platinum Catalysts*" on November 29, 2013. Opponent: **D.Sc. Juan Carlos Serrano Ruiz**, Abengoa Research, Spain.

Bingzhi Li: "*Modeling of Fireside Deposit Formation in Two Industrial Furnaces*" on December 5, 2013. Opponent: **Prof. Roman Weber**, Clausthal University of Technology, Germany.

Frida Jones: "*Characterisation of Waste for Combustion - with Special Reference to the Role of Zinc*" on December 11, 2013. Opponent: **Prof. Johan Hustad**, Norwegian University of Science and Technology, Norway.

Juho Lehmusto: "*The Role of Potassium in Corrosion of Superheater Materials of Boilers Riving Biomass*" on December 13, 2013. Opponent: **Prof. Jan-Erik Svensson**, Chalmers University of Technology, Sweden.

Michal Wagner: "*Synthesis, Characterization and Chemical Sensor Application of Conducting Polymers*" on December 18, 2013. Opponent: **Prof. Alexander Kuhn**, Université de Bordeaux 1, Groupe Nanosystèmes Analytiques, France.

PCC FACTS AND MISSION

The Abo Akademi Process Chemistry Centre (AA-PCC) studies physio-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, Abo Akademi University:

- Combustion & Materials Chemistry (Prof. Mikko Hupa)
- Catalysis and Reaction Engineering (Academy Prof. Tapio Salmi)
- Process Analytical Chemistry (Prof. Johan Bobacka)
- Wood and Paper Chemistry (Prof. Stefan Willför)

In the year 2012, about 130 people (including 20 senior researchers) took part in the PCC activities with a total funding of approximately 7 million euro.

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