

Everybody is Needed

My friend and colleague, a high-level expert in chemical engineering, came to me with a depressing message: "Tapio, we are not needed anymore!". I was astonished, why? Because nowadays all research and development should be strictly oriented toward new products, but chemical skills in chemical engineering are abandoned, such as mathematical modeling of processes and computation of kinetics, transport phenomena and fluid dynamics. No, I opposed strongly. Life is cyclic, so is the life of chemical technology and chemical engineering.

Chemical innovation came first, and chemical technology was developed, mainly based on experience and intuition. Exact computations came much later on. The golden age of chemical technology transformed to the golden age of chemical engineering: many professionals believed that chemistry was ready, but we first need more and more refined models and super-efficient computers.

A new age of chemistry has appeared: we need better waste treatment, we need green and biodegradable chemicals, we need fuels based on renewables. Today, we watch a renaissance of chemical innovation. As soon as new innovations are implemented in industrial scale, kinetics and thermodynamic measurements, physical characterizations and modeling are needed for the new components and the new systems.

In general, the new systems are more complicated and challenging than the conventional ones: poly-functional molecules and mixtures of them but not simple hydrocarbons.

People with chemical skills are again needed, I



Prof. Tapio Salmi is the head of the Kinetics & Catalysis Group. Photo: Andreas Bernas.

tried to convince my friend. Engineers design, computers run, and quantum chemists explain as usual. My friend looked more happy when he left.

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EUROPACAT VIII - CONGRESS IN TURKU/ÅBO AUGUST 26-31, 2007

In 2007, EUROPACAT will take place at the Turku Fair and Congress Center. The abstract submission deadline is January 31, 2007. For more information see www.europacat.org.

JYRI-PEKKA MIKKOLA AT PCC TAKES RISKS

On November 24, 2006, the Academy of Finland awarded two young researchers. The recipient of the Incentive Award was Academy Research Fellow, Docent Jyri-Pekka Mikkola at PCC. The Incentive Award is granted to a researcher who has shown exceptional creativity, courage or independent thinking in his or her research. The prize can be awarded for a bold or unique research idea, the unbiased crossing of scientific boundaries or the ability to take risks in research. The prizes are awarded to Academy Research Fellows or Postdoctoral Researchers working on Academy funding. The prize trophy is a miniature sculpture "Path" by artist Mika Natri. The Awards were given out at the Academy of Finland's Science Gala in Helsinki. This is the fourth time the Awards have been presented. Jyri-Pekka Mikkola is blazing new trails for ionic fluids. The award statement emphasizes Mikkola's progressive and innovative style as well as his preparedness to take risks. Mikkola is especially interested in researching process development, a research field located between basic chemistry and industry. He has applied his expertise to ionic fluids, a new field of chemistry in Finland. Spearheading the field, Mikkola estimates that ionic fluids will in the future affect most processes in the chemical industry, and also in the energy industry. Mikkola describes ionic fluids as salt-like substances that have many unique features. As the name would suggest, ionic fluids are liquid over a wide temperature range. They do not vaporize and they have excellent solvency characteristics. Another typical aspect is that many chemical reactions occur faster in ionic fluids than in traditional solvents. They can be used in ore separation, medicine production, heat transfer, carbon dioxide recovery, production of more environmentally-friendly and affordable solar cells, as well as in fuel cells. The latest trend is to produce ionic fluids from biomaterial or natural compounds.

THE 5th and 6th PCC WORKSHOPS WERE HELD

The 5th PCC Workshop on the topic FUNCTIONAL MATERIALS - PART I was held on October 6, 2006. Speakers were Dr. Leena Hupa (Combustion and Materials Chemistry) "*Tailoring of Surfaces for Everyday Life Environment*", Dr. Narendra Kumar (Kinetics & Catalysis) "*Engineering Crystal Morphology and Metal Modification of Porous Materials*", Prof. Ronald Österbacka "*Organic Electronics*", and Prof. Johan Bobacka (Process Analytical Chemistry) "*Chemical Sensors Based on Functionalized Materials*". The 6th PCC Workshop on the topic FUNCTIONAL MATERIALS - PART II took place on November 10, 2006. Lectures were given by Ph.Lic. Tapio Mäkelä (FunMat, VTT) "*Patterning Methods for Inherently Conducting Polyaniline*", Prof. Markku Auer (Wood and Paper Chemistry) "*New Functions for Paper – A Challenge*", and Dr. Heimo Ylänen (Turku BMC) "*Bioactive Glasses*".

PCC ANNUAL SEMINAR

The Åbo Akademi Process Chemistry Centre Annual Meeting was held in Arken on August 24, 2006. The 2005 activities were presented by the group leaders and moreover selected technical presentations were held.

According to tradition, young PCC scientists had a chance to show their results in the form of a poster session. Later in the evening, the participants had the pleasure to visit Suomalainen Pohja, where the dinner was arranged. In 2005, 8 doctoral theses, 2 licentiate theses, and 15 master of science theses were produced. The number of articles in refereed international journals and series were 109, articles in refereed international edited volumes and conference proceedings 18, and books and book chapters 5.



RECENT DOCTORAL THESES - LA DOLCE VITA OF JYRKI KUUSISTO

Jyrki Kuusisto has studied the catalytic production of alternative sweeteners. The date of his academic dissertation was October 28, 2006. The aim of the work was to improve the catalytic hydrogenation of different sugar species, primarily D-lactose (an aldehyde and a disaccharide), D-fructose (a ketose and a monosaccharide) and D-xylose (an aldehyde and a monosaccharide), to sugar alcohols, lactitol, mannitol and xylitol. The challenge has been the development of catalysts with improved selectivity and activity for the production of these specialty sweeteners.



The endeavor has been to study and optimize various hydrogenation parameters, such as reaction temperature, hydrogen pressure, pH and catalyst loading, to obtain maximum yield. Studies on the catalyst deactivation, leaching and filtration properties have been of special interest. Research on these topics is important as the goal is in environmentally and economically benign industrial operations.

CTMP DEVELOPMENT BY JONAS KONN

Jonas Konn has studied the process chemistry of chemithermomechanical pulps (CTMP). The date of his academic dissertation was November 17, 2006. The wood raw materials used in production of CTMP are very different in morphology and chemical composition. Fundamental knowledge on the chemistry of the native wood components and of the dissolving components in pulping and peroxide bleaching is therefore required for process and product development.



This work aimed at understanding the chemistry of spruce and aspen CTMP and assessing the role of: (a) deacetylation of galactoglucomannans, (b) demethylation of pectins, and (c) sulphonation of lignin on the final pulp and paper properties. The central hypothesis in this work was that pectin demethylation is a key reaction in CTMP, besides the sulphonation of lignin. Both these reactions form new anionic groups specifically in the primary wall and middle lamella region between adjacent fibres in the wood structure. This research has resulted in a new and deeper understanding of the processes relevant for tailor-making specific end products and for optimisation and further development of CTMP processes.

BEATRIZ MEANA ESTEBAN FOCUSES ON CONDUCTING POLYMERS

Beatriz Meana Esteban has studied the synthesis and characterization of different fused ring systems. The date of her academic dissertation was December 8, 2006. The current research in the field of conducting materials (polymers and oligomers) moves towards the synthesis and characterization of novel structures with specific properties for a certain field of application, e.g. organic electronics.



The aim of this work is to study fused ring systems that belong to a subgroup of conducting polymers, due to the character of their backbone. Thus, the synthesis and characterization of films of 2-methoxynaphthalene, 1,1'-binaphthyl, azulene and 2-[(E)-2-azulen-1-ylvinyl] thiophene, considered as an azulene derivative, have been investigated in this thesis.

PRIZES TO CARITA KVARNSTRÖM AND KALLE ARVE

Carita Kvarnström was awarded the Per Brahe Prize on December 7, 2006 for her research on electrochemically active materials. Kalle Arve was awarded "Det Alfthanska Priset år 2006" for his doctoral thesis "Catalytic Diesel Exhaust Aftertreatment: From Reaction Mechanism to Reactor Design".

Guest Lectures

- **Prof. Toribio Fernández Otero**, Universidad Politécnica de Cartagena, Spain: "Intelligent devices from electrochemical properties of conducting polymers" on November 22, 2006.
- **Dr. Friedrike Jentoft**, Department of Inorganic Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany: "Modern Alkane Isomerization Catalysts: Complex Materials for a Simple Reaction?" on November 23, 2006.
- **Dr. Krisztián Kordás**, Microelectronics and Materials Physics Laboratories, EMPART Research Group of Infotech Oulu, University of Oulu, Finland: "Nanomaterials" on November 27, 2006.
- **Dr. Helmut Neugebauer**, Linz Institute for Organic Solar Cells, Institute of Physical Chemistry, University of Linz, Austria: "Optoelectronic Applications of Organic Semiconductors" on December 7, 2006.
- **Professor Magdalena Maj-Zurawska**, Faculty of Chemistry, University of Warsaw, Poland: "Electrochemical Screen-Printed DNA Biosensors" on December 13, 2006.

Doctoral Defenses

- **Mischa Theis:** "*Interaction of Biomass Fly Ashes with Different Fouling Tendencies*" on June 2, 2006. Opponent: Prof. Hartmut Spliethoff, Technical University of Munich, Germany.
- **Antero Moilanen:** "*Thermogravimetric Characterisations of Biomass and Waste for Gasification Processes*" on September 1, 2006. Opponent: Prof. Johan Hustad, Norges teknisk-naturvitenskapelige universitet (NTNU), Norway.
- **José Ignacio Villegas Perdomo:** "*Engineering Bifunctional Catalysts for Hydrocarbon Valorization*" on October 27, 2006. Opponent: Dr. Dmitry Lukyanov, University of Bath, England.
- **Jyrki Kuusisto:** "*Catalytic Production of Alternative Sweeteners - Lactitol, Mannitol and Xylitol*" on October 28, 2006. Opponent: Dr. Michèle Besson, Institut de Recherches sur la Catalyse-CNRS, Villeurbanne, France.
- **Jonas Konn:** "*Process Chemistry in Chemithermomechanical Pulping*" on November 17, 2006. Opponent: Prof. Göran Gellerstedt, Royal Institute of Technology, KTH, Stockholm, Sweden.
- **Beatriz Meana Esteban:** "*Aromatic Fused Ring Systems: Synthesis and Characterization by Electrochemical and Spectroelectrochemical Methods*" on December 8, 2006. Opponent: Dr. Helmut Neugebauer, Linz Institute for Organic Solar Cells (LIOS) Physical Chemistry, Johannes Kepler University Linz, Austria.
- **Anton Tokarev:** "*Applied Electrochemical Methods for Heterogeneous Catalysis*" on December 15, 2006. Opponent: Dr. Tamas Mallat, Swiss Federal Institute of Technology, Zurich, Switzerland.
- **Mathias Snåre:** "*Development of Next Generation Biodiesel Technology - Catalytic Deoxygenation of Renewables*" on December 16, 2006. Opponent: Dr. Irina Simakova, Boreskov Institute of Catalysis, Novosibirsk, Russia.

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PCC Facts and Mission

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 process 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, Faculty of Technology, Åbo Akademi University: *Combustion & Materials Chemistry* (Prof. Mikko Hupa), *Kinetics & Catalysis* (Prof. Tapio Salmi), *Process Analytical Chemistry* (Prof. Ari Ivaska) and *Wood and Paper Chemistry* (Prof. Bjarne Holmbom). In the year 2005, about 130 persons (including about 20 senior researchers) took part in the PCC activities with a total funding of approximately 6 Million €.

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