

### PCC Continues as a Centre of Excellence

Based on the application of our Process Chemistry Centre and evaluation by an international board, the Academy of Finland has appointed PCC as a Centre of Excellence, CoE, for the next six years.

The main project will be Chemistry in Forest Biorefinery. In this concept we will concentrate in speciality chemicals from wood related raw materials, metals in fibres and biofuels and –energy, where PCC's approach molecular process technology will be of importance and enable scientific solutions to practical problems. Application of process chemistry and molecular process technology will turn Green Chemistry to Green Engineering.

A big asset we have as an academic institution is our students who we would train in scientific research to serve industry and the society as whole. They are our "tools" in CoE to do high level research and they also will be the main legacy of PCC.

The new European Chemicals Agency that will be placed in Finland will definitely increase interest to chemistry in the society and also give a better image to chemistry and chemical engineering as whole and should be seen as a big opportunity for chemistry in Finland. In this context PCC will have a role of its own.

The status of Centre of Excellency in research requires continuous self-evaluation of our activities and continuous optimizing our research strategy as well.

**Prof. Ari Ivaska**  
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*Prof. Ari Ivaska is the head of the Process Analytical Chemistry Group. Photo: Andreas Bernas.*

### ARI IVASKA TO RESEARCH INSTITUTE

Professor Ari Ivaska has been appointed for 1.8.2006–31.7.2009 as the research director of the Research Institute of the Åbo Akademi University Foundation. His activities in PCC will still continue as the leader of the Process Analytical Group.

## MIKKO HUPA PRESIDENT OF IFRF



Process Chemistry Centre Professor Mikko Hupa has been appointed president of the organization International Flame Research Foundation, IFRF. IFRF, an International Centre of Excellence for combustion research, technology, and information, has approximately 1200 members in 23 countries including USA, Japan, and most of the western European nations (Germany, United Kingdom, France, Italy, the Netherlands, Finland, Sweden, etc.) IFRF is a co-operative research and technical service organization serving power generation and chemical industry, plus an industrial and academic network of organizations concerned with combustion and environment.

The head office and communication center of IFRF is located adjacent to the industrial zone of Corus, IJmuiden, the Netherlands. *"The task as president is challenging but exciting, especially now when the secretariat and the research laboratory will move from IJmuiden, where they have been acting for decades, to Pisa, Italy. IFRF has been one of the most important networks for our combustion engineering research here at the Åbo Akademi Process Chemistry Centre"*, Prof. Hupa says.

## ANDRZEJ LEWENSTAM TO THE CHAIR OF IFCC

Professor Andrzej Lewenstam was nominated and elected to the Chair of the International Federation of Clinical Chemistry (IFCC) Working Group on Selective Electrodes and Biosensors, starting 2006. The Group, a part of the Scientific Division of IFCC, is responsible for developing recommendations on the most frequent measurements in hospital laboratories and doctor offices, such as electrolytes, e.g. potassium and blood gases as well as light metabolites, e.g. glucose. The published recommendations are obligatory world-wide.

## BIORAFF GOT A FLYING START

PCC has initiated a new project, where the ultimate goal is a more efficient use of forest resources. The aim is to use renewable materials in a more intelligent way than before, utilising in-depth knowledge in chemistry. This

knowledge is generated through practical work in the research groups and is targeted to understand phenomena and chemical structures at the molecular level of the components found in trees. The chemistry in the Forest Biorefinery (BIORAFF) program is part of the activities of PCC, funded by Tekes. We will be able to characterise several useful products, propose new separation and modification technologies leading to increased production availability of existing production lines, and create added value in form of more valuable products. The program focuses on chemistry and the cumulating knowledge will be used in various biorefinery product and process development projects. The program will focus on three main areas:

**Specialty Chemicals and Materials.** A key to the development of the Forest Biorefinery concept is to find new means of producing specialty chemicals and materials from forest resources. Preferable sources are waste streams of pulp and paper production. There are numerous opportunities for such production of natural specialty chemicals.

**Metals in Trees and Fibres.** Management of the metal flows and balances is important in order to minimize the negative and maximize the positive effects that the different metal ions have on the processes and on the quality of the final products in today's pulp and paper mills, but also in the future in combined mills with additional chemical and energy production. Alkaline, earth alkaline, and transition metals are known to be important in the paper making process. Many transition metals are of significant environmental concern as well.

**Biofuels and -energy.** The new biorefinery concepts all include conversion of parts of the feedstock biomass into energy via some novel processes based on pyrolysis, gasification, or combustion. To be able to use the many new waste derived fuels or fuel mixtures with no increased flue gas emission or plant availability (corrosion, fouling) problems is a major challenge and requires deep understanding of the properties of the fuels. Conventional fuel analysis is not sufficient to evaluate the practical feasibility of these fuels.

We want the project to have as high an impact as possible on the competitiveness of our supporters. Therefore, it is vital that information of the scientific findings will find interested industrial partners for utilizing this in their own businesses. Therefore an industrial advisory board will be established starting from the beginning of 2007, the idea being that the members of the industrial advisory board get first hand information of the results of our projects. There will be a participation fee used for additional financing of our research activities. The membership is open for any interested partner and enquiries should be directed to Professor Markku Auer (mauer@abo.fi).

## 3rd AND 4th PCC WORKSHOPS WERE HELD

The 3rd PCC Workshop on the topic METALS FROM WOOD-BIOREFINERY ASPECTS was held on February 3, 2006. Speakers were Mr. Kim Granholm (Process Analytical Chemistry) "*Removal of Metal Ions from Pulps by Chelation*", Mr. Andrey Pranovich (Wood and Paper Chemistry) "*Metals in Wood*", and Dr. Maria Zevenhoven (Combustion and Materials Chemistry) "*Metals from wood to ash*". Dr. Stefan Willför (Wood and Paper Chemistry) also highlighted the topic "*Biorefinery - an Existing Proposal*". The 4th PCC Workshop was held on April 25, 2006. Topics and presenters were Dr. Johan Wärnå (Kinetics & Catalysis) "*Kinetics and Reactor Modeling*", Dr. Christian Mueller (Combustion and Materials Chemistry) "*Computational Fluid Dynamics*", Dr. Ville Nieminen (Kinetics & Catalysis) "*Molecular Modeling/Computational Chemistry*", Dr. Tomasz Sokalski (Process Analytical Chemistry) "*Does Analytical Chemistry Need Mathematical Modeling*", and Ms. Eija Bergelin (Wood and Paper Chemistry) "*Extractive Flows*".

## MISCHA ENJOYS TRAVELS BETWEEN TURKU AND TORONTO

Diplom-Ingenieur in Chemical Engineering Mischa Theis from Cologne, Germany, has studied the interaction of fly ashes with different fouling tendencies during biomass combustion at the Combustion and Materials Chemistry group within the Process Chemistry Centre. The date of his doctor dissertation is June 2, 2006 with the kustos Prof. Mikko Hupa, PCC, and the opponent Prof. Hartmut Spliethoff from Technical University of Munich, Germany. Mischa graduated at University of Dortmund in Germany and continued his hobby of travelling during his years as a researcher - cumulatively 18 months of experiments at the Pulp and Paper Centre, University of Toronto, Canada as well as course work in Denmark, Estonia, Germany, Sweden, and USA.



The objective of the research was to study the interaction of fly ashes with different fouling tendencies during biomass combustion and to provide consistent data for development and validation of deposition models based on computational fluid dynamics (CFD). Oat straw and eucalyptus bark were used to represent biomass fuels that containing large amounts of alkali metals, alkaline earth metals, chlorides, and sulfates in the ash and produce fly ashes with a high fouling tendency. Peat was used as an example fuel that contains large amounts of silica and alumina in the ash and produces fly ash with a low fouling tendency. The results showed that the deposition rate was highest for straw, intermediate for bark, and lowest for peat. This trend was correlated to decreasing alkali contents from straw ash to bark ash to peat ash. The composition of the deposits resembled the composition of the fuel ash when firing the fuels individually. However, when straw and bark were fired in mixtures with peat, they behaved differently. While the presence of approximately 30 wt% of ash from peat was sufficient to decrease the ash deposition rate of straw-peat mixtures to the same value as that of peat fired alone, it was necessary to mix approximately 70 wt% of peat ash with bark ash to obtain the same effect. Chemical analyses of the deposits suggested that erosion caused by silicate ash particles from the peat was the main mechanism for lowering the ash deposition rate of straw-peat mixtures. For bark-peat mixtures, sulfation reactions appeared to play an important role in minimizing deposit buildup.  $K_2SO_4$  was found in the deposits when the deposition rate was low, while KCl was found when the deposition rate was high. The low deposition rate obtained from firing bark depleted of alkali confirmed the important roles of potassium, sulfur, and chlorine in deposit buildup.

Finland has a pretty pristine nature, so for instance I liked running in the quiet forests into the sunrises before coming to work, biking in the evenings or swimming across to Hirvensalo from Uittamo beach in the summer. And of course I liked sauna and ice hole swimming on Ruissalo Island. On the other hand, Finland may occasionally get a bit small if one is used to crowds and people. So I had the most perfect arrangement with staying a couple of months here and then a couple of months across the miles in Toronto to enjoy the amenities of a five-million city, Mischa says.



## NEW BOOK BY MURZIN AND SALMI

A new engineering textbook with the title "*Catalytic Kinetics*" by authors Prof. Dmitry Yu. Murzin and Prof. Tapio Salmi at the Kinetics & Catalysis group has been published by Elsevier (ISBN: 0-444-51605-0, 492 pages, publication year: 2005). The target group is Chemical Engineers, Physical Chemists, and Organic Chemists. This book unifies the main sub disciplines forming the cornerstone of catalytic kinetics.

## EUROPACAT VIII 2007 - [www.europacat.org](http://www.europacat.org)

The Nordic Catalysis Society takes pleasure in inviting the catalysis community to Finland for the EUROPACAT VIII congress 2007, a co-operative effort between Denmark, Finland, Norway, and Sweden. The Nordic Catalysis Society has participated in the planning of the scientific programme of the conference. The second announcement and call for papers is now available. The abstract submission deadline is Jan 31, 2007. There will be 5 plenary lectures, 18 keynote lectures, 180 oral presentations, equipment and book exhibitions as well as poster sessions (3x250). The Berzelius Lecture is given by the 2005 Nobel Prize winner in Chemistry, Prof. R.H. Grubbs from California Institute of Technology. The plenary lectures are held by Prof. James A. Dumesic (University of Wisconsin-Madison), Prof. Irina I. Ivanova (Moscow State University), Dr. Herman Kuipers (Shell Global Solutions), Prof. Jens K. Nørskov (Technical University of Denmark), and Prof. Ferdi Schüth (Max-Planck-Institut für Kohlenforschung). The keynote speakers will be listed on the congress website.



## PCC Scientific and Industrial Advisory Boards

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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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