

Combustion engineering - more and more chemistry...

Two important recent agreements are dramatically influencing the development of combustion technologies. These are the Kyoto agreement of the control of greenhouse gases, and the new EU directive on waste incineration.

The Kyoto agreement and the European green house gas emission trade have turned the focus towards the efficiency of the power plant. The CO₂ emission quota will be used to produce maximum output of power or heat. Higher plant efficiency often means more demanding conditions for the materials in the plant - for example higher superheater tube metal temperatures. This calls for an improved understanding and control of high-temperature corrosion.

Many types of CO₂ neutral fuels such as biomasses and wastes or waste-derived fuels are rapidly entering the scene. Combustion of these fuels is not always straightforward, but requires understanding of the details of their burning behaviour. In particular, co-firing of several fuels together may cause problems due to unwanted interaction between the fuels or their ashes.

The new EU directive on waste incineration gives detailed limits for the flue gases when waste or waste-derived fuels are burned. Besides sulphur and nitrogen oxides and particulate matter, it gives strict limits to a number of other flue gas components including twelve trace metals. This directive is a very important agreement and paves the way for the extensive use of waste as an energy source also in Finland.

This directive for the first time lists the emission components of importance in the legislation. This way it also partly



Photo by F. Klingstedt and J. Wennström

Prof. Mikko Hupa is the head of the Combustion & Materials Chemistry Group

directs the future development of emission control in other combustion systems. Understanding the details of the complex behaviour of the trace metals in the various combustion process conditions requires significant research work.

Clearly, the challenges in combustion engineering are more and more related to chemistry. Our Process Chemistry Centre is well equipped to continue playing a part in supporting the development of the future clean and CO₂ neutral combustion technologies. We will also continue our broader study of the role of metals in wood processing throughout the whole life cycle of the product. This kind of holistic view of the fate of the metals is a prerequisite for a solid understanding and control of the effects of these metals to the processes and to the environment.

Prof. Mikko Hupa

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THE 2005 FINNISH SCIENCE AWARD TO HOLMBOM

Professor Bjarne Holmbom from PCC has received the 2005 Finnish Science Award (85 000 €) for his pioneering research work within the field of wood chemistry. The prize is granted every second year for international and high-quality scientific research. Holmbom and his group discovered high concentrations of the anticarcinogenic HMR lignan in knots. The group has investigated over 50 different wood species and there are indications that several health-promoting products can be found in the wood. HMR lignan will soon be available on the market.

FORTUM FOUNDATION AWARD TO HUPA

In February, Professor Mikko Hupa was granted the Fortum Foundation Award 2005. The award was given to Hupa for his successful and long-term fundamental and applied research and academic education in the energy area.

YOUNG SCIENTIST'S PRIZE TO TOUKONIITTY

Esa Toukoniitty from PCC received the young scientist's prize at the prestigious International Congress on Catalysis in Paris. He was awarded the prize for his research on asymmetric catalysis, which is an important technique in the production of pharmaceuticals.

NEW COMBUSTION PROJECT CHEMCOM

Altogether 14 people from the PCC participate in laboratory, modelling and field studies on biomass combustion within this new three year mega project funded by six international companies and Tekes. ChemCom is led by Prof. Mikko Hupa

CHEMISTRY FOUNDATION PRIZE TO BERNAS

Andreas Bernas from PCC received the Finnish Chemistry Foundation prize for the best Doctoral Thesis within the field of chemistry in Finland. Bernas has been studying the production technology of functional foods having health-enhancing effects.

WACHEUP FOR PCC

The Wood and Paper Chemistry group from PCC is involved in a new EU project on *New Concepts for Upgrading Pulp and Cork Mill Waste Streams to Value-added Chemicals (WacheUp)*. More information is given by Prof. Holmbom.

PCC INVOLVED IN EPNOE

European Polysaccharide Network of Excellence (EPNOE) started on May 1, 2005. The network is composed of 17 European research groups from 9 different countries, including the Wood and Paper Chemistry group from PCC.

NANOCAT STARTED

A new EU project focusing on tailored nanosized metal catalysts for improving activity and selectivity via engineering of their structure and local environment (NANOCAT) started. The project is coordinated by Professor Dmitry Murzin from the PCC.

PCC EXPLORING MICROREACTORS

A new project on microreactor technology has been accepted by the National Technology Agency of Finland (TEKES). The partners are ÅA/PCC, Lappeenranta University of Technology and several companies.

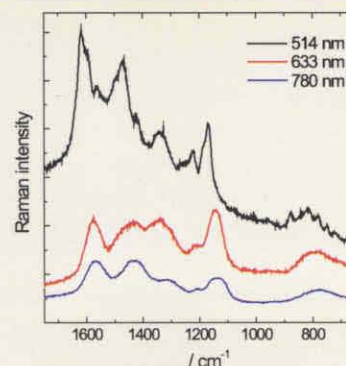
IN MEMORIAM KARI NURMI

Abo Akademi and Process Chemistry Centre have lost a faithful friend and colleague. Kari Nurmi passed away in the Tsunami catastrophe in Khao Lak, Thailand on the 26th of December 2004. Kari Nurmi did his Master's Thesis in physical chemistry and soon after graduation he started his career at Raisio Tehtaat OY, which later became Raisio Chemicals. During the years 1977-1978 Kari Nurmi completed his Licentiate thesis under the supervision of Professor Per Stenius at ÅA, being one of the pioneers of polymer research at ÅA. Shortly before passing away, Kari Nurmi had been appointed director for the R&D of surface treatment and coating of paper within Ciba Specialty Chemicals, Raisio. Kari Nurmi was a driving force in the Coating Technology Centre and Future Printing Center located in Raisio, as well as in the Turku Science Park. He was always in close contact with ÅA through several joint research projects. When PCC was appointed as a National Centre of Excellence in Research, he gave the centre his warmest support. During 1999-2005 Kari Nurmi was an extremely dedicated member of the PCC industrial advisory board. We will always remember Kari Nurmi for his boundless enthusiasm and optimism and for his personal kindness.

NEW RAMAN LASERS

The Raman spectrometer at PCC was recently updated with two lasers and the measurements can now be done with the 514, 633 and 780 nm lasers

Raman spectroscopy measures the wavelength shift of scattered light, which depends on the vibrational transitions of the sample. Certain vibrations are strongly enhanced for laser wavelengths approaching the electronic absorption band in the sample. This facilitates the measurements of i.e.: fullerenes, conducting polymers, dyes, and biologically important molecules. Sample pretreatment is usually not needed and spectra can be recorded directly from powders, films and liquids (e.g. water).



Raman spectra of electrically conducting polyaniline at pH 5 measured with different lasers

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NEW NMR INSTRUMENTATION IN TURKU

There are three spectrometers at our disposal operating at 400, 500 and 600 MHz for proton, respectively. All the instruments are equipped with two channels and field gradient units and are multi nuclear covering nearly whole the periodic system of



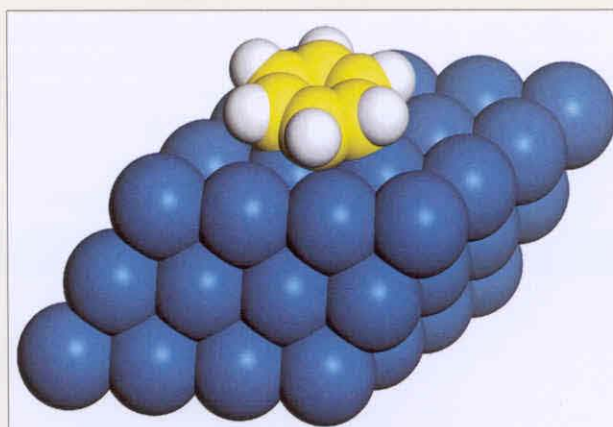
NMR active nuclei from ^{107}Ag to ^1H . Our instruments are also equipped with sample changers allowing automation of routine measurements. We have two types of probe head for the 600 and 500 MHz instruments. Both of the probe types are broadband and differ only in the geometry inside of the probe. The 400 MHz instrument is equipped with a classical broadband liquid probe-head. However, it is also equipped with a CP/MAS probe designed for solid state NMR. The solid system is also multinuclear with tunable probe covering nuclei from ^1H to ^{15}N . The spinner size is 4mm and the spinning speed goes up to 15kHz.

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Molecular modelling available at PCC

Molecular modelling including force field and quantum chemical calculations can be carried out at PCC. A cluster of six computers and resources at CSC together with a suitable set of software, such as Turbomole, Gaussian98 and Materials Studio provide an efficient computing environment. Possible applications are the evaluation of molecular interactions, conformational studies of organic molecules, and adsorption of molecules on different surfaces. Even reaction paths including activation barriers can be studied.

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Benzene adsorption on Pt(111) surface modeled by density functional theory

PREPARATION AND ANALYSIS OF NATURAL PRODUCTS

The Wood and Paper Chemistry group at PCC has procured a Shimadzu HPLC system suitable for both preparative and analytical scale operations. The system is equipped with two preparative pumps, a degasser, an autosampler, a column oven, a fraction collector, a recycle valve, UV- and RI detectors, and a data processing system. This system allows both isocratic and high-pressure gradient runs in flow rates between 0.1 and 150 ml/min. This enables large-scale isolation of, i.e., new natural bioactive compounds. The same data processing system is also used with the HPSEC system, which was recently upgraded with a new low-pressure gradient pump and a universal Sedex low-temperature evaporative light scattering detector (LT-ELSD).



Text by Stefan Willför and photo by Jarl Hemming

Doctoral defenses

- David Kubička: "Towards Clean Diesel Fuel Production" (04.03.2005). Opponent: Doctor Augustine Martínez Feliu from Instituto de Tecnología Química, Universidad Polytécnica de Valencia, Valencia, Spain.
- Johanna Lilja: "A Fibrous Polymer-Supported Sulphonic Acid Catalyst in Esterification Processes" (05.03.2005). Opponent: Professor Alirio Rodrigues from Department of Chemical Engineering, University of Porto, Portugal.
- Jeannette Aumo: "Structured Catalysts in Complex Three-Phase Hydrogenations" (02.04.2005). Opponent: Docent Ahmad Kalantar from Nynas Naphtenics AB, Sweden.
- Mercedes Vázquez: "Potentiometric Ion Sensors Based on Conducting Polymers" (04.05.2005). Opponent: Professor Ernö Pretsch from ETH Hönggerberg, Zürich, Switzerland.
- Lari Vähäsalo: "White Pitch Deposition, mechanisms and measuring techniques" (03.06.2005). Opponent: Doctor Lawrence H Allen from Pulp and Paper Research Institute of Canada, Pointe Claire, Canada.

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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 Chemical Engineering Faculty of Åbo Akademi University: *Combustion & Materials Chemistry* (Prof. Hupa), *Kinetics & Catalysis* (Prof. Salmi), *Process Analytical Chemistry* (Prof. Ivaska) and *Wood and Paper Chemistry* (Prof. Holmbom). In the year 2004, 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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