Newsletter

Åbo Akademi Process Chemistry Centre

No. 7 1 / 2004

Process analytical chemistry - a metrological science

Without analysis chemical engineering is blind!

The Division of Analytical Chemistry of the Federation of European Chemical Societies gives the following definition: "Analytical chemistry is a scientific discipline that develops and applies methods, instruments and strategies to obtain information on the composition and nature of matter in space and time". Process analytical chemistry can be defined as "analytical determinations in industrial and environmental processes". Lord Kelvin understood the importance of measurements by stating: "When you can measure what you are speaking about and express it in numbers, you know something about it; and when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meager and unsatisfactory kind".

Analytical chemistry in general and process analytical chemistry in particular is a metrological (i.e. based on measurements) science that develops measurement procedures in order to solve scientific, technical and even social problems.

A certain cybernetic feature is always connected to analytical determinations. The information received through analytical measurements is primarily used to characterize an object and secondarily to take an action to bring the object to the desired state. The object can be an industrial process, environment or even a human being whose state is defined by clinical analyses. A control will be activated if the measurement shows the state to be outside predetermined acceptable parameters. In a chemical process, some variable affecting the stream composition might be changed. If the state of the environment, e.g. quality of wastewater discharged to a river, is not within set limits, legal action might even be taken against the responsible party. In the case of human beings, the action to be taken may be a change in lifestyle or starting a certain medication.

Photo: Tom Lindfors

Prof. Ari Ivaska is the head of the Process Analytical Chemistry group.

The importance of analysis and measurements was reflected in the key slogan of a recent international fair in process engineering and instrumentation: "Without analysis chemical engineering is blind!"

Prof. Ari Ivaska
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The Distinguished Lecturer Series continues

Wilhelm Jost Prize to PCC for CFD based combustion research

Photo: IFRF (Roberts)

Docent Christian Mueller receiving the "Wilhelm Jost Medal" from Prof. Dr. Dr. h.c. Heinz Georg Wagner.

During the 21st German Flame Days in Cottbus, Germany, the German Flame Research Committee, in co-operation with the Association of Engineers (VDI) and the German Section of the Combustion Institute, honoured Docent Christian Mueller with the Wilhem Jost Prize for extraordinary achievements regarding prediction of particle deposition in furnaces and boilers using Computational Fluid Dynamics (CFD).

The prize, named after the well-known German combustion scientist and former director of the Göttingen physicochemical institute, Wilhem Jost is awarded every second year to a young researcher in the combustion community.

The long term goal of ash research at Åbo Akademi Process Chemistry Centre has been to increase the knowledge of ash behaviour in different types of thermal conversion systems and to develop practical tools for predicting it. After many years of basic theoretical and experimental research, combination of the collected knowledge and experiences with novel CFD methods opened new possibilities for the research in the group. Fundamental results and findings regarding fuel specific ash deposition in furnaces and boilers can now be used to address design aspects of these units. In particular, the inclusion of models for describing the chemistry of ash deposition into CFD allows for the prediction of which parts of the boiler might face problems of significant ash deposition.

Next to the particle deposition model a variety of other CFD submodels for combustion modelling have been developed over the last few years. All are now compiled in the *Åbo Akademi Furnace Model*, a customized version of a commercial CFD software package.

Text by Frauke Mueller

The Doctoral thesis of M.Sc. Andreas Bernas "Heterogeneous Catalytic Isomerization of Linoleic Acid for Production of Anticarcinogenic Food Constituents" was presented for public criticism on December 12th. The opponent appointed by the Faculty of Chemical Engineering was Prof. Angelo Vaccari from Alma Mater Studiorum Università di Bologna (Italy).

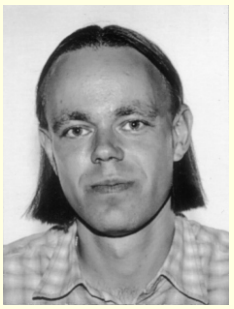

Photo: Åbo Akademi University

A new and clean technology using heterogeneous catalysts is reported for the first time for preparing conjugated linoleic acids (CLA). The environmentally friendly method is based on batchwise isomerization of linoleic acids with mild conditions in the solvent phase over a solid catalyst. New catalytic materials were synthesized, characterized and tested.

Fore more information: Andreas.Bernas@abo.fi

The distinguished lecturer series within the PCC group features lectures held by prominent scientists with connections to the Process Chemistry Centre. The following lecturers have been scheduled:

14.5, Prof. Lynn Gladden, University of Cambridge, England

Prof. Alan MacDiarmid, University of Pennsylvania, USA
Prof. Douglas Reeve, University of Toronto, Canada
Prof. Roger Sheldon, TU Delft, The Netherlands
Prof. Gordon Wallace, University of Wollongong, Australia

The distinguished lectures will take place at the Axelia building of the Faculty of Chemical Engineering, Åbo Akademi University, Biskopsgatan 8. Exact dates and times will be announced later on our web page: www.abo.fi/instut/pcc

Photo: Ari Ivaska

Prof. Jiri Janata (Georgia Tech, USA) lecturing January 15th at the PCC about "Organic microelectronics".

A natural path for process chemistry

Long ago our materials and chemicals were natural. In Finland, wood tar produced from resin-rich pine trees was by far the most important "industrial" product until the middle of the 19th century.

At the end of the century, fossil raw materials became the basis for the growing production of organic chemical products, first coal and later oil. Synthetic polymers emerged in the 1930´s. The petrochemical industry started to grow tremendously after the second world war. A whole new oil-based synthetic polymer industry grew up.

In the 1970´s, it was a common belief that natural materials and chemical products would gradually disappear. We would be reading books made of plastic paper, wearing cloth of only synthetic fibres, living in houses built of synthetic polymer materials and even eating synthetic oil-based products. Certainly, synthetic drugs would come to replace natural medicines.

by Bjarne Holmbom

Head of the Wood and Paper Chemistry group.

Now we are living in a world full of artificial materials and chemicals, well functioning, but not necessarily good for our health and for nature. The image of the chemical industry has suffered badly from disasters in large chemical mills, and from the unexpected negative effects of synthetic chemicals on health and the environment. Chemistry and the chemical industry have gradually become ever less attractive to the younger generation.

Can we change the path of process chemistry? It has already changed! The predictions that natural materials and chemicals would be totally replaced by synthetic, artificial ones have not been realised. We are still reading books made of natural paper, wearing clothes of cotton, wool, linen and silk, building houses and furniture of wood, and eating mostly natural food grown in nature. Natural medicine has made a comeback. Big chemical companies are now actively looking for natural, renewable raw materials in order to produce biocompatible, natural products.

Finland has been a forerunner along this path. Well known products such as tall oil, xylitol and Benecol were originally developed in Finland. We do not have any oil or coal, but have more biomass per capita in the form of wood than any other country in the world. We must use our "green gold" wisely. Polysaccharides, fatty and resin acids and polyphenols can be extracted from wood, bark or industrial process streams and can be utilised for new materials and chemicals that cannot be synthesized by chemists, at least not as elegantly as by nature. New biomass-derived products will not be replacing bulk products, but will be small-scale niche products where the profit margins may be very healthy, thanks to help from nature.

We in Åbo Akademi Process Chemistry Centre are working intensively to develop functional natural materials and chemicals. We have several projects going on related to the chemistry and utilisation of polysaccharides, fatty acids and polyphenols, in addition to the traditional uses of wood and other biomass for pulp and paper and as biofuels.

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Photo: Thomas Holmbom

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Recent Doctoral Theses

- **Andreas Bernas**: "Heterogeneous Catalytic Isomerization of Linoleic Acid for Production of Anticarcinogenic Food Constituents"
- **Tea Hannuksela**: "Mannans in Mechanical Pulping and Papermaking - Naturally Existing Aids and Promising Wet-End Additives"
- **Jatta Partanen**: "Chemistry of HCl and Limestone in Fluidised Bed Combustion"

Visitors

- M.Sc. **Iwona Bedlechowicz**, *Warsaw University*, Poland, 1.3-31.8.04
- Dr. **Klaus Bauer**, *Albert-Ludwigs Universität*, *Freiburg*, Germany, 16-29.2.04
- M.Sc. **Pamela Espindola**, *Albert-Ludwigs Universität*, *Freiburg*, Germany, 16-29.2.04
- M.Sc. **Petya Konova**, *Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences*, 5.2-5.10.04
- Dr. **Livia Nagy**, *University of Pecs*, Hungary, 14.11-3.12.03
- M.Sc. **Daniela Nastac**, *Polytechnic University of Bucharest*, Romania, 19.1-19.8.04

PCC Scientific and Industrial Advisory Boards

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 2002, about 170 people (including 40 senior researchers) took part in the PCC activities with a total funding of approximately 5.8 Million €.

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Layout ••• Tom Lindfors