

Newsletter

ÅBO AKADEMI
PROCESS CHEMISTRY GROUP
Centre of Excellence

Åbo Akademi Process Chemistry Group

No. 1

1 / 2001

Molecular Process Technology

"We have to dive into the world of molecules and then make our way back to the surface"

This statement was recently written by one of our students in the introduction of her thesis. It eloquently describes what Molecular Process Technology, our common approach, is all about. With this term we stress the importance of detailed understanding of the chemistry in industrial processes and products down to the molecular level.

We want to advance chemical process engineering from traditional material and energy balance calculations which involved modelling and simulation using coarse process parameters, towards a more complete understanding and controlling of various chemical phenomena in the processes.

The year 2000 was the first full year for the Åbo Akademi Process Chemistry Group (ÅA-PCG) as a National Centre of Excellence in Research. This nomination was an important recognition of our previous research efforts and also supplied major thrust to future work.

In this newsletter, Johan Bobacka writes about robust all-solid-state ion sensors based on electrically conducting polymers. Johan's work is an excellent example of molecular process technology. In his work, the key molecules are electrically conducting conjugated polymers. Johan was recently recognised by our University with the 2000 Per Brahe Prize.

In the year 2000, our Group produced five Doctoral theses, the titles of which are listed at the end of this newsletter. The key molecules under study in each of the theses are different, but all five are excellent examples of our focus on detailed chemistry in



Prof. Mikko Hupa is the chairman of the Åbo Akademi Process Chemistry Group Board.

complex applications.

For example, take the research conducted by Keijo Salmenoja. Keijo's key molecules were the chlorides of alkali metals and iron in hot furnace gases. These compounds were shown to significantly influence corrosion processes at the heat exchangers in biomass combustion systems. His thesis was recently awarded the IVO Foundation Prize for outstanding Doctoral thesis research.

On the centrespread, Heimo Ylänen describes his bioactive glass systems. The porous bioactive glass microspheres discussed in Heimo's article have shown remarkable properties in facilitating growth of new bone in medical applications. His key molecules are silicates and phosphates of calcium in the complex environment of human body fluids.

I hope that these delightful examples of success will inspire all of us in our future projects.

Congratulations to all our new Doctors!

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Durable Chemical Sensors

by Johan Bobacka



Dr. Johan Bobacka was awarded the 2000 Per Brahe Prize. His research focuses on various aspects of chemical sensors based on electrically conducting polymers.

A chemical sensor can be defined as a device that converts a chemical state (concentration, activity, partial pressure) into a quantifiable signal. The chemical sensing process involves molecular recognition of a chemical species (analyte) and transduction of the chemical information into a measurable signal. Chemical sensors give information about the chemical composition of a sample, which may originate e.g. from an industrial process, the environment or the human body.

Selective recognition of many ions can be achieved by using supramolecular structures in combination with conjugated polymers as ion-to-electron transducers. An example is the all-solid-state ion-selective electrode (ISE) utilizing valinomycin as the recognition site for K^+ in conjunction with poly(3,4-ethylene-dioxythiophene) as the solid-state transducer (see Figure).

The development of such all-solid-state potentiometric ion sensors would hardly be possible without the discovery of electrically conducting polymers by Alan J. Heeger, Alan G. MacDiarmid and Hideki Shirakawa in 1977. Their study on conjugated polymers gave them the *Nobel Prize in Chemistry* in 2000. Conjugated polymers (called synthetic metals) are electroactive organic materials with mixed electronic and ionic conductivity. The unique combination of electrical and optical properties make conjugated polymers interesting materials for applications such as chemical sensors, electrochromic devices and light-emitting diodes.

The research on conjugated polymers resulting in today's robust ion sensors was initiated by Prof. Ari Ivaska in 1988. The group's focus on this subject further intensified with the addition of Prof. Andrzej

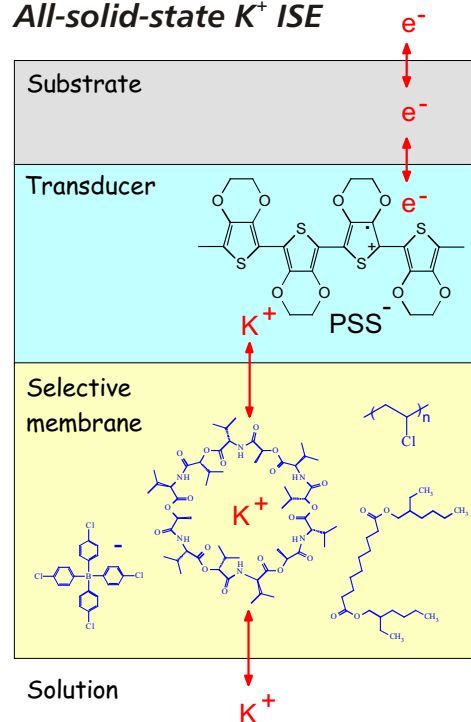
Lewenstam. Today our activities range from basic materials research to specific chemical sensors for on-line process analysis.

Durable chemical sensors that can be used for continuous analysis of a variety of samples without any pretreatment are very attractive analytical tools from the users' point of view, and the development of such sensors is a great challenge. The trends in ion sensor research point towards more robust, miniaturized sensors with a wide dynamic range and low detection limit, even down to 10^{-12} M. Durable chemical sensors will be important in on-line process analysis, while miniaturized sensors will find applications in clinical and biochemical analysis. Thus far, we have focused mainly on the determination of inorganic ions. There are a number of biochemically active organic compounds, however, which may also be determined by chemical sensors in the future.

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All-solid-state K^+ ISE



Bioactive Glass

by Heimo Ylänen



Bioactive glass, first introduced by Professor Larry Hench in 1969, exhibits the unique property of bonding firmly to host bone. In this article, Heimo Ylänen presents a concise synopsis of his doctoral thesis.

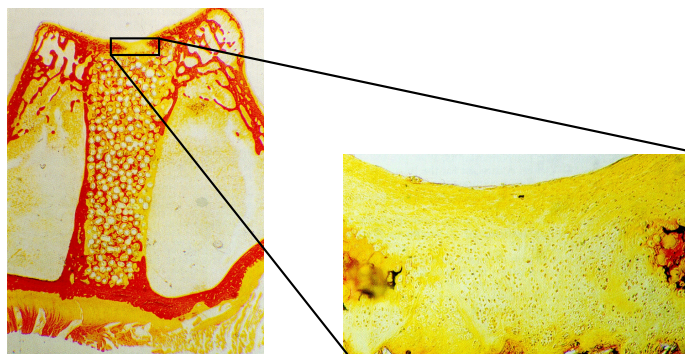
New bioactive glass types (of the $\text{Na}_2\text{O} - \text{K}_2\text{O} - \text{MgO} - \text{CaO} - \text{B}_2\text{O}_3 - \text{P}_2\text{O}_5 - \text{SiO}_2$ system) developed at ÅAU during the early nineties can be repeatedly reheated without the risk of devitrification, in stark contrast to first generation bioactive glass. This improvement has increased the number of possible clinical applications for which this advanced biomaterial may be used. As a first step towards the development of new clinical applications, an interdisciplinary study focusing on the behaviour of porous sintered bioactive glass microsphere implants in living tissues was initiated between Åbo Akademi University and the University of Turku's Department of Surgery. The porosity of a bioactive glass implant not only noticeably increases the total reactive surface area of the glass, but also allows healing bone tissue to grow three-dimensionally.

The collaborative studies have confirmed that the three dimensional microenvironment inside

the sintered bioactive glass microspheres does in fact promote bone growth. The porosity of the glass allows continuous transport of organic matter within the implant. For example, when sintered bioactive glass microspheres are inserted into a defective rabbit knee joint, bone forms within the bioactive glass implant while cartilage forms on the joint surface (see Figure). This suggests that stromal cells from the bone marrow occupy the pores in the bioactive glass microspheres during the implantation. Whether bone or cartilage forms depends on the location of the cells within the implant.

In conclusion, porous bioactive glass implants may provide a means to guide and promote the growth of new bone into selected anchoring areas. For instance, bioactive glass microspheres affixed to prostheses would facilitate bonding of the device to existing bone. Such implants may also facilitate healing of cartilage damage on joint surfaces.

Bioactive glass research within the Åbo Akademi Process Chemistry Group continues, making use of both national and international collaborations in order to focus on the further development of clinical applications for this unique biomaterial.



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New bone formation under the joint surface and surface formation of cartilage on a porous bioactive glass implant (white spheres) 8 weeks after implantation into the rabbit knee. Bone appears in red. Higher magnification shows more clearly how the joint surface defect has been covered by cartilage cells.

New Professor to PCG

Dmitry Yu. Murzin, Dr.Sci., (BASF, Moscow) was appointed as Professor of Chemical Technology 1.8.2000. His special interest is research in chemical kinetics and heterogeneous catalysis.

For more information: www.abo.fi/institut/pcg; *Kinetics & Catalysis*



Visitors

Dr. Pedro Fardim, *Universidade Estual de Campinas*, Brazil, from 1.3.2000

Dr. Konstantin Mikhelson, *St. Petersburg State University*, Russia, 1.2-30.4 and 1.10-31.12.2000

Dr. Li Niu, *Changchun Institute of Applied Chemistry, Chinese Academy of Sciences*, China, from 1.2.1999

Dr. Awni al Otoom, *University of Newcastle*, Australia, 11.6-8.7.2000

Dr. Tomasz Sokalski, *Warsaw University*, Poland, from 1.2.2000

Doctoral Theses 2000

Keijo Salmenoja: "Field and Laboratory Studies on Chlorine-Induced Superheater Corrosion in Boilers Fired with Biofuels"

Valentina Serra-Holm: "Aldolization of butyraldehyde and propionaldehyde with formaldehyde over resin catalysts"

Bengt Skrifvars: "Chemical Equilibrium Analysis in the Study of Corrosion"

Esko Tirronen: "A Methodological Approach to Process Development in the Fine Chemical Industry"

Heimo Ylänen: "Bone Ingrowth into Porous Bodies Made by Sintering Bioactive Glass Microspheres"

Please check our website for M.Sc. and Licentiate Theses: www.abo.fi/instut/pcg

PCG Mission

The Åbo Akademi Process Chemistry Group (ÅA-PCG) is studying 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

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