Venue

The annual seminar on Mathematics in Chemical Kinetics and Engineering will be held in the Pand, a renovated ancient building owned by Ghent University, and situated in the heart of Ghent's historical centre (address: Onderbergen 1).

G.S. Yablonsky dr.h.c.

On *Dies Natalis* (March 19, 2010) of Ghent University, Prof. Yablonsky has received a honorary doctorate by proposal of the Engineering Faculty. Prof. Yablonsky (1940) obtained his Ph.D. and Habilitation in physical chemistry at the Boreskov Institute for Catalysis in Novosibirsk. During his long career in the former USSR he developed mathematical methods in chemical technology to decode complex chemical reactions. In particular, his results have found industrial and ecological applications for CO- and H-oxidation reactions.
In 1995 he moved to the famous Washington University in St. Louis (Missouri, USA). Since then he developed a theory for pulse response investigations which is at the basis of accurate characterization of catalysts.
A significant part of these results were obtained together with an interdisciplinary team of chemical engineers and applied mathematicians at *LCT* and *NaM*[2] of Ghent University.

Invitation

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Mathematics in Chemical Kinetics and Engineering

MaCKiE

Sixth Annual Seminar
on the occasion of 175 Years of Engineering Study at Ghent University and of the honorary doctorate of Gregory S. Yablonsky

Ghent University, Belgium

Wednesday, May 19, 2010

Organizing Committee

– Denis Constales *(NAM*[2]*)*

– Geraldine Heynderickx *(LCT)*

– Guy Marin *(LCT)*

– Roger Van Keer *(NAM*[2]*)*

Program

– 9:30 Coffee and registration

– 10:00 Gregory S. Yablonsky on *What happens at the crossroads between Chemical Engineering and Applied Mathematics?*

– 11:00 Question time and discussion

– 11:30 **Speech by the Dean of the Faculty of Engineering**

– 11:45 **Reception in honor of G.S. Yablonsky dr.h.c.**

– 13:00 Lunch

– 14:30 Oliver Trapp on *Precise Determination of Reaction Rate Constants by Combining Reactions and Separations: New Routes in the High-Throughput Screening of Catalysts*

– 15:30 Question time and discussion

– 16:00 Concluding remarks and closing address

Welcome to the 2010 annual seminar on Mathematics in Chemical Kinetics and Engineering

The *Laboratory for Chemical Technology (LCT)* and the *Numerical Analysis and Mathematical Modelling Research Group (NAM²)* of Ghent University are pleased to invite you to attend the annual seminar on "Mathematics in Chemical Kinetics and Engineering" and/or to the reception in honor of Prof. Yablonsky, which will both be held on May 19, 2010 in Ghent, Belgium.

After the successful international MaCKiE-200(2,7,9) Conferences and MaCKiE-200(3,4,5,6,8) Annual Seminars, the local organizers at Ghent University have again invited two world-class experts from the fields of applied mathematics and chemical engineering, Prof. Gregory S. Yablonsky (Saint Louis) and Prof. Oliver Trapp (Heidelberg) to give seminar talks during a one-day mini-symposium.

Participation to the **seminar** and/or **reception** is free, but registration is strongly recommended by May 3, 2010. Please e-mail to **Denis.Constales@UGent.be** to register. A complimentary lunch is offered to the participants at the venue. Vegetarian and other special requirements can be met if mentioned in the registration e-mail.

What happens at the crossroads between Chemical Engineering and Applied Mathematics?

Prof. dr. Gregory S. Yablonsky
Department of Energy, Environmental and Chemical Engineering,
Washington University in St. Louis, USA.

A panoramic view on the interaction between Chemical Engineering and Applied Mathematics will be presented. A variety of different mathematical dialects of contemporary Chemistry and Chemical Engineering, in particular formal approaches based on linear and non-linear algebra and theory of differential equations, will be characterized. Special attention will be paid to the problem of decoding the complexity of temporal chemical transformations using mathematical tools. The Temporal Analysis of Products (TAP) approach will be presented as an application of mathematical calculus to experimental chemistry. The importance of this approach for precise catalyst characterization, catalyst design and development of sustainable processes will be stressed. The effectiveness of the collaboration between chemical engineers and mathematicians will be discussed, using as examples the MaCKiE-workshops and the activity of the interdisciplinary *LCT–NAM²* group at Ghent University in this area during the last decade.

Precise Determination of Reaction Rate Constants by Combining Reactions and Separations: New Routes in the High-Throughput Screening of Catalysts

Prof. dr. Oliver Trapp
Organisch-Chemisches Institut
Ruprecht-Karls-Universität Heidelberg,
Germany.

Searching for highly efficient and selective catalysts is of great importance to develop benign chemical processes for industrial applications. To understand a catalyzed reaction on a molecular level rate-controlling elementary steps need to be identified and comprehensive experimental kinetic data of a broad variety of substrates need to be acquired. An overview over existing and promising techniques in the screening of catalysts will be given.
The combination of separation selectivity and catalytic activity in the same chromatographic stationary phase allows performing high-throughput kinetic analysis of catalyzed reactions. Results for the screening of (enantioselective) hydrogenation catalysts, C-C-cross coupling catalysts, enantioselective rearrangements and the investigation of Grubbs type metathesis catalysts will be shown. Furthermore results for higher order reactions will be discussed and strategies to determine reaction rate constants will be shown.