

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).

Tourist Attractions in Ghent

Belgium possesses a wealth of highly distinctive architectural, cultural and gastronomic traditions.

Ghent, founded in the 10th century AD, has today a population of over two hundred thousand. The official language is Dutch; knowledge of English is very widespread.

Major touristic attractions include the *Gothic Cathedral* and other medieval churches, the Van Eyck Altarpiece depicting the *Adoration of the Mystic Lamb*, the *City Museum of Contemporary Art (SMAK)*, and numerous shops selling Flemish specialities such as local beers, lace and many other renowned products of authentic handicraft.

Weather

The end of May is Spring in Ghent, with average temperature of 15 degrees Celsius. Some rain is to be expected.

Invitation

—

Mathematics in Chemical Kinetics and Engineering

MACKIE

Annual seminar



Ghent University, Belgium

Wednesday, May 30, 2012

Deadlines

* May 16, 2012: Registration deadline.

Organizing Committee

- Denis Constaes (LCT and NaM²)
- Geraldine J. Heynderickx (LCT)
- Guy B. Marin (LCT)
- Roger Van Keer (NaM²)

Program

- 10:00 Coffee and registration
- 10:45 Introduction
- 11:00 Bjarne Andresen on *Finite-time optimization of chemical and unrelated reactions*
- 12:00 Question time and discussion
- 12:30 Lunch
- 14:30 Vladimir N. Parmon on *Thermodynamic form of kinetic equations and an experience of its use for analyzing complex reaction schemes*
- 15:30 Question time and discussion
- 16:00 Concluding remarks and closing address

Welcome to the 2012 annual seminar on Mathematics in Chemical Kinetics and Engineering

The *Laboratory for Chemical Technology* (LCT) and the *Research Group for Numerical analysis and Mathematical Modelling* (NaM²) of Ghent University are pleased to invite you to attend the annual seminar on "Mathematics in Chemical Kinetics and Engineering" which will be held on May 30, 2012 in Ghent, Belgium.

After the successful international Mackie-20(02,07,09,11) conferences and Mackie-20(03,04,05,06,08,10) annual seminars, the local organizers at Ghent University have again invited two world-class experts from the fields of mathematics and chemical engineering, Prof. B. Andresen (Copenhagen) and Prof. V.N. Parmon (Novosibirsk) to give seminar talks during a one-day mini-symposium.

Participation to the seminar is free, but registration is strongly recommended before May 16, 2012. Please e-mail to Denis.Constaes@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.

Finite-time optimization of chemical and unrelated reactions

Prof. Bjarne Andresen
Niels Bohr Institute
Copenhagen, Denmark.

Finite-time thermodynamics is useful in providing bounds on the performance of processes at non-vanishing rates as well as determining the paths that achieve these bounds, in other words the price of haste. One of the methods used is thermodynamic geometry which is based on a natural metric in thermodynamic state space. I will present some of the tools of finite-time thermodynamics with special attention to chemical reactions like $A \leftrightarrow B \leftrightarrow C$ with the objective of capturing the most B at a given final time. Other reactions treated are the cytochrome chain in mitochondria and the light absorbing reactions in photosynthesis. It will be shown how these methods are equally applicable to other 'reactions' like distillation, economic trading, and data encoding.

Thermodynamic form of kinetic equations and an experience of its use for analyzing complex reaction schemes

Prof. Valentin N. Parmon
Boreskov Institute of Catalysis
Novosibirsk State University, Russia.

The presentation concerns an experience in the application of a 'thermodynamic form' of kinetic equations for providing joint kinetic-thermodynamic analysis of a large variety of detailed schemes of stepwise reactions. The basis of the thermodynamic form is the substitution of the parameter 'concentration' of a substance by a related value expressed via the chemical potential of the thermalized substance. The application of the above substitution allows dramatic simplification of expressions for the rate of stoichiometric stepwise reactions even far from their equilibria. Also, the application of the thermodynamic form of kinetic equations for analyzing complex reactions schemes, at least for those linear in respect to reaction intermediates, allows to receive a simple general Horiuti-Boreskov-like expression for the rate of the stepwise reaction at its steady state occurrence and to suggest both simple Lyapunov functions which are minimized in the stepwise reaction steady state as well as reciprocity equations which are analogous to the Onsager ones but valid for occurrence of the parallel stepwise reactions far from the reaction equilibria.