

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 200 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

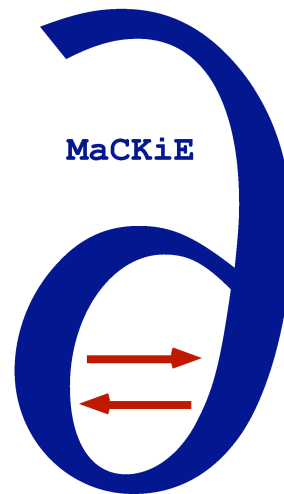
Early May is Spring in Ghent, with average temperature of 15 degrees Celsius. Some rain is to be expected.

Invitation

Mathematics in Chemical Kinetics and Engineering

MACKIE

Annual seminar



Ghent University, Belgium

Wednesday, May 3rd, 2006

Deadlines

* April 19th, 2006: Registration deadline.

Organizing Committee

- Denis Constaes (NFaM²)
- Geraldine Heynderickx (LPT)
- Guy Marin (LPT)
- Roger Van Keer (NFaM²)

Program

- 10:00 Coffee and registration
- 10:45 Introduction
- 11:00 Wolfgang Marquardt on *Model-based experimental analysis: a systems approach to mechanistic modeling of reactive systems*
- 12:00 Question time and discussion
- 12:30 Lunch
- 14:30 Alexander Gorban on *The thermodynamic projector and model reduction in chemical kinetics*
- 15:30 Question time and discussion
- 16:00 Concluding remarks and closing address

Welcome to the 2006 annual seminar on Mathematics in Chemical Kinetics and Engineering

The *Laboratory for Petrochemical Technology* (LPT) and the *Research Group for Numerical functional analysis and Mathematical Modelling* (NfaM²) 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 3rd, 2006 in Ghent, Belgium.

After the successful international Mackie-2002 conference and Mackie-2003, 2004 and 2005 Annual Seminars, the local organizers at Ghent University have again invited two world-class experts from the fields of mathematics and chemical engineering, Prof. Wolfgang Marquardt (RWTH Aachen) and Prof. Alexander Gorban (University of Leicester) to give seminar talks during a one-day mini-symposium.

Participation to the seminar is free, but registration is strongly recommended before April 19th, 2006. A complimentary lunch is offered to the participants at the venue.

Model-based experimental analysis: a systems approach to mechanistic modeling of reactive systems.

Prof. Wolfgang Marquardt
Lehrstuhl für Prozesstechnik
RWTH Aachen, Germany.

This contribution will introduce a novel concept for mechanistic modelling of complex kinetic phenomena and will explore its potential for single- and multi-phase reaction systems modelling.

The approach aims at the integration of high resolution measurements, modelling on multiple scales and the formulation and solution of inverse problems in a unifying framework.

An incremental and iterative approach based on gradual refinement of experimental techniques, mathematical models and identification problems forms the core of the suggested methodology.

The foundations of the approach developed in a collaborative interdisciplinary research center at RWTH Aachen will be reviewed.

Illustrative examples focussing on chemical reaction kinetics will be presented.

The thermodynamic projector and model reduction in chemical kinetics.

Alexander Gorban
Department of Mathematics
University of Leicester, UK.

Model reduction should respect thermodynamics: we should not violate the Second Law (entropy growth), and all operations of model reduction should preserve positivity of entropy production. Kinetic equations with thermodynamic Lyapunov functions are studied. Uniqueness of the thermodynamic projector is proven: there exists only one projector which transforms any vector field equipped with the given Lyapunov function into a vector field with the same Lyapunov function for a given ansatz manifold which is not tangent to the Lyapunov function levels. Explicit construction of the thermodynamic projector for chemical kinetics is presented. Various approximations are discussed: from classical Quasi-Steady-State (QSS) and Quasi-Equilibrium (QE) approximations to their recent modifications and improvements.

For the latest information, consult the annual seminar's Web site at www.mackie-workshops.com