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

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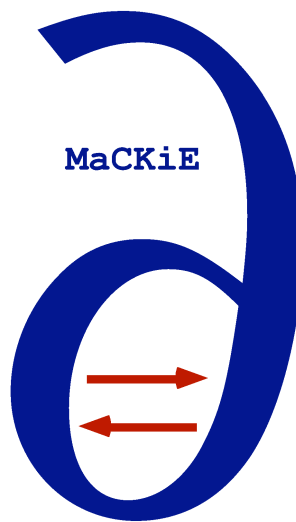

Invitation

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Mathematics in Chemical Kinetics and Engineering

MACKIE

Annual seminar

MaCKiE

Ghent University, Belgium

Friday, May 23, 2008

Deadlines

* May 9, 2008: Registration deadline.

Organizing Committee

– Denis Constales (NFaM^2)

– Geraldine Heynderickx (LPT)

– Guy Marin (LPT)

– Roger Van Keer (NFaM^2)

Program

– 10:00 Coffee and registration

– 10:45 Introduction

– 11:00 Andro Mikelic on *Effective Dispersion Equations For Reactive Flows With Dominant Peclet and Damkohler Numbers*

– 12:00 Question time and discussion

– 12:30 Lunch

– 14:30 Harry van den Akker on *Computational Reactor Engineering: pretty extreme, extremely pretty.*

– 15:30 Question time and discussion

– 16:00 Concluding remarks and closing address

Welcome to the 2008 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 23, 2008 in Ghent, Belgium.

After the successful international Mackie-200(2,7) conferences and Mackie-200(3,4,5,6) Annual Seminars, the local organizers at Ghent University have again invited two world-class experts from the fields of mathematics and chemical engineering, Prof. Andro Mikelic (Lyon) and Prof. Harry van den Akker (Delft) to give seminar talks during a one-day mini-symposium.

Participation to the seminar is free, but registration is strongly recommended before May 9, 2008. 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.

Effective Dispersion Equations For Reactive Flows With Dominant Peclet and Damkohler Numbers.

Prof. dr. Andro Mikelic
Institut Camille Jordan, UFR Mathématiques
Université Claude Bernard Lyon 1, Lyon, France.

We study reactive flows through a capillary tube. The transport and reaction parameters are such that we have large, dominant Peclet and Damkohler numbers with respect to the ratio of characteristic transversal and longitudinal lengths (the small parameter epsilon). Using the anisotropic singular perturbation technique we derive the effective equations. The result is compared with the turbulence closure modeling and with the center manifold approach. Furthermore, we present a numerical justification of the model by a direct simulation of the full problem and of the effective equations. Next, we use the Laplace transform in time to get precise dependence on the parameter epsilon and rigorously show that our effective equations, with Taylor dispersion terms and chemical reactions contributions, give an approximation in the energy norm, which is uniform in time and always better than constant times the ratio between the characteristic transversal diffusion time and the characteristic longitudinal transport time. This result confirms the numerical experiments and justifies the dimensional reduction.

Computational Reactor Engineering: pretty extreme, extremely pretty.

Prof. dr ir. Harry E.A. van den Akker
Department of Multi-Scale Physics
Technical University Delft, The Netherlands.

Computational simulations of chemical reactions combined with flow, mixing and transport phenomena in realistic 3-D geometries are very promising with a view of improving the performance of chemical reactors. Turbulent-flow conditions present enormous challenges compared to laminar-flow conditions, multi-phase flow being even more challenging. The seminar covers Reynolds-Averaged Navier-Stokes, Large-Eddy and Direct Numerical Simulations. Various mathematical techniques (Finite Volume, Lattice-Boltzmann, Monte Carlo) are available for solving the set of transport equations. The challenge is to control computational time. The potential success of the approach is illustrated by means of detailed simulation results as to a commercial-scale high-pressure low-density polyethylene polymerization reactor.

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