Venue

The annual seminar on Mathematics in (bio)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).

Methusalem Funding by the Flemish Government

Faculty of Engineering and Architecture
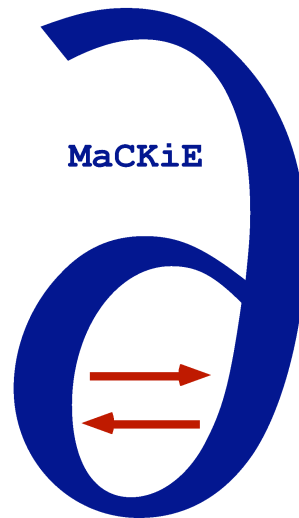
Faculty of Bioscience Engineering

UNIVERSITEIT GENT

Invitation

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Mathematics

in (bio)Chemical

Kinetics and Engineering

MACKIE

Annual Seminar

Ghent University, Belgium

Wednesday, May 28, 2014

Deadlines

* May 14, 2014: Registration deadline

Organizing Committee

– Denis Constales (NaM²)

– Geraldine J. Heynderickx (LCT)

– Guy B. Marin (LCT)

– Ingmar Nopens (BIOMATH)

– Kevin M. Van Geem (LCT)

Program

– 10:45 Coffee and registration

– 11:15 Introduction

– 11:30 Renato Feres, *From Knudsen diffusion to stochastic thermodynamics*

– 12:30 Question time and discussion

– 12:45 Lunch

– 13:45 Marc-Olivier Coppens on *Random Walks in Porous Media – Diffusion under Confinement*

– 14:45 Question time and discussion

– 15:00 Concluding remarks and closing address

Welcome to the 2014 annual seminar on Mathematics in (bio)Chemical Kinetics and Engineering

The *Research Group for model-based analysis and optimisation of (bio)processes* (BIOMATH), the *Laboratory for Chemical Technology* (LCT) and the *Research Group for Numerical analysis and Mathematical Modelling* (NaM^2) of Ghent University are pleased to invite you to attend the annual seminar on "Mathematics in (bio)Chemical Kinetics and Engineering" which will be held on May 28, 2014 in Ghent, Belgium.

After the successful international Mackie-20(02,07,09,11,13) conferences and Mackie-20(03,04,05,06,08,10,12) annual seminars, the local organizers at Ghent University have again invited two world-class experts from the fields of mathematics and (bio)chemical engineering, Prof. M.-O. Coppens (University College London) and Prof. R. Feres (Washington University in St. Louis) to give seminar talks during a one-day mini-symposium.

Participation to the seminar is free, but registration is strongly recommended before May 14, 2014. Please e-mail to Denis.Constales@UGent.be to register. A complimentary lunch is offered to the participants at the venue.

From Knudsen diffusion to stochastic thermodynamics

Prof. Renato Feres
Department of Mathematics
Washington University in St. Louis.

The theory of stochastic dynamical systems provides a conceptually satisfying set of links connecting models of surface-gas interaction to (1) the classical distributions of Knudsen and Maxwell-Boltzmann, (2) to the mathematical determination of Knudsen diffusivity in channels and, finally, (3) to the foundations of stochastic thermodynamics of simple ("nano-mechanical") heat engines.
The central character of the story is a classical surface scattering operator, P, derived from the interaction model. The random dynamical system we study is then a multiple scattering Markov chain (a "random billiard" system) with transition probabilities operator P.
Among other things we will see how the cosine law arises as stationary distribution of the multiple scattering process, how Knudsen diffusivity relates to the geometrical-mechanical gas-surface interaction model via the spectrum of P, and how a variation on the theme can also describe the workings of a minimalistic heat engine, which we explore via numerical simulation.

Random Walks in Porous Media Diffusion under Confinement

Prof. Marc-Olivier Coppens
University College London.

Molecular transport in nanoporous materials is important to a variety of chemical engineering applications. We will discuss methods to calculate the influence of pore geometry and chemical structure of the pore walls on diffusion in nanopores. In short pores, an incorrect analysis based on the mean-square displacement of molecules may bias diffusion results, even qualitatively. A first-passage time analysis gives correct and more complete information on diffusion in nanopores than a mean-square displacement analysis. In chemical engineering applications, we are most interested in macroscopic results, on the scale of a membrane, adsorbent or catalyst particle. To include heterogeneity requires multiscale methodologies that enable us to bridge wide ranges of length and time scales.
Finally, could materials be designed to tune molecular transport to enhance transport-dependent properties, such as membrane permeation and selectivity, or catalyst yield and stability? We propose a nature-inspired chemical engineering (NICE) approach to optimize hierarchical transport networks and nanopore designs.