Mackie-2015 program

Thursday July 2, 2015

08:30 Opening by Prof. dr. ir. Guido Van Huylenbroeck, Dean of the Faculty of Bioscience Engineering, Ghent University.

08:40 Plenary lecture: *On the detailed modelling of high temperature nanoparticles synthesis*, by Markus Kraft (UK). Session chair: Kevin Van Geem.

09:40 Coffee break.

In **room 3 (Blanquaert)**, parallel session overlapping with ICCK in rooms 1 and 2, session chair Geraldine Heynderickx:

10:00 *A heterogeneous multi-scale dynamic model for simulation of catalytic reforming reactors*, by Grigorios Pantoleontos (Greece).

10:25 *Efficient method for the calculation of rate coefficients of elementary reactions in the gas phase*, by Andrey Koksharov (Germany).

10:50 *New observation of water gas shift equilibrium in flames*, by Wendong Wu (USA).

11:15 *On reactive settling of activated sludge*, by Raimund Bürger (Chile).

11:40 *Parameter fitting: Which algorithm to choose?* by Benoît Celse (France).

12:05 *Probing pore blocking effects on multiphase reactions at the particle level using a discrete model*, by Guanghua Ye (UK / China).

12:30 *A comparative study of optimization algorithms for a cellular automata model*, by Saurajyoti Kar (India).

12:55 Lunch and Poster session: *The Sectional Quadrature Method of Moments (SQMOM): An Application to Liquid-liquid Extraction Columns* by Semer Alzyod (Germany); *Slow Manifolds identification for dimensionality reduction of chemical kinetics: a computational route* by Alessandro Ceccato (Italy); *Traits of regularity in stochastic chemical kinetics: analogy with the "Slow Manifolds" feature in deterministic kinetics* by Paolo Nicolini (Italy / Czech Republic); *Mathematical description of the kinetics of photochemical reactions* by Katalin Ősz; *Exact analytical solution of a non-linear reaction-diffusion problem for full range of parameters values — multiplicity and dead zone coexistence* and *Modeling of gas flow — usefulness of the Laplace transform and CAS-type programs* by Mirosłav K. Szukiewicz (Poland).

Session chair for the afternoon: Denis Constales. Location: **room Vermeylen**.

14:00 Plenary lecture: *Quadrature-Based Moment Methods in Chemical Engineering*, by Rodney O. Fox (USA).

15:00 *Coping with heterogeneity and stochasticity in microbial processes*, by Denis Pischel (Germany).

15:25 *The switching point between kinetic and thermodynamic control of competitive reactions*, by Daniel Branco Pinto (Belgium)

15:50 *Fischer-Tropsch Synthesis SSITKA simulation: balancing between model complexity, computational effort and relevance of the included features*, by Jonas Van Belleghem (Belgium)

16:15 *Novel heuristics for mediating radical chain reactions: a stochastic simulation of the synthesis of copolymers with tailored monomer sequences*, by Paul H.M. Van Steenberge (Belgium)

16:40 *Calibration And Analysis Of A Direct Contact Membrane Distillation Model Using Monte Carlo Filtering and good modelling practice*, by I. Hitsov (Belgium)

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Friday July 3, 2015

08:40 Plenary seminar: *135 years in chemical kinetics: Bykov-Gorban-Yablonsky's problem*, by Valeriy I. Bykov, Alexander N. Gorban and Gregory S. Yablonsky. Session chair: Guy B. Marin. Location: **room Vermeylen**.

09:40 Coffee break.

	Room 1 (Vermeylen), chair: Geraldine Heynderickx	**Room 2 (Blancquaert)**, chair: Ingmar Nopens
10:00	*Optimal design of chemical processes with joint chance constraints*, by Gennadi M. Ostrovsky (Russia).	*Low-dimensional Modeling of Reactions and Transport in Stratified Microflows*, by Jason R. Picardo (India).
10:25	*Simulations of instationary operated heterogeneous catalytic reactions*, by Frerich J. Keil (Germany).	*Modeling the chaotic dynamics of heterogeneous catalytic reactions with fast, intermediate, and slow variables*, by N.A. Chumakova (Russia)
10:50	*Integration of DFT calculations into microkinetic analysis: Application to carbon dioxide hydrogenation on ceria*, by Cynthia S. Lo (USA).	*Modelling of Influence of Oxygen Bulk Diffusion in Nickel on Oscillatory Kinetics of Catalytic Oxidation of Methane*, by V. Ustyugov (Russia).
11:15	*Explicit formulas for reaction probability in reaction-diffusion experiments*, by Renato Feres (USA).	*Application of population balance concept in modeling of FCC riser reactions*, by Dariusz S. Orlicki (USA).
11:40	*Stochastic effects in autocatalysis*, by Gabor Lente (Hungary).	*Use of Hybrid Monte-Carlo Models in Online Control of Product Quality in Emulsion Copolymerization*, by Alexandr Zubov (Czech Republic).
12:05	*Oscillating regimes of first order phase transition* by Valeriy I. Bykov (Russia).	*Slow Manifolds identification for dimensionality reduction of chemical kinetics*, by Diego Frezzato (Italy).

12:30 Lunch and Mackie Award.

Session chair for the plenary lectures: Gregory S. Yablonsky. Location: **room Vermeylen**.

14:00 Plenary lecture: *Lyapunov functions and stability of kinetics: from Boltzmann to present days*, by Alexander N. Gorban (UK).

15:00 Plenary lecture: *Methods and tools for kinetic model identification*, by Rafiqul Gani (Denmark).

Chair Rafiqul Gani:

16:00 *Lack of fit and degrees of freedom in kinetic modelling*, by Bengt Andersson (Sweden).

16:25 *The nature of vortex breakdown*, by V. Shtern (U.S.A.).