PROGRAMME

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International Conference on Mathematics in (bio)Chemical Kinetics and Engineering 2017

May 25–27, 2017 – Budapest, Hungary

Hotel Mercure Budapest Buda****
Krisztina krt. 41–43, H-1013 Budapest, Hungary

AKCongress
Akadémiai Kiadó / AKCongress
P.O. Box 245, H-1519 Budapest, Hungary
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ISBN 978-963-454-095-3

WELCOME FROM THE CHAIR

Welcome to the Mathematics in (bio)Chemical Kinetics and Engineering (MaCKiE) 2017 conference.

Since its first event in 2002, MaCKiE conferences have been organized in every second year, whereas smaller scale seminars have been held in intermittent years. The previous conferences were hosted in Ghent (Belgium), Chennai (India), Heidelberg (Germany), and Houston (USA). The meeting aims to bring together scientists interested in the application of advanced mathematical methods to describe kinetic phenomena, especially chemists, mathematicians, physicist, biologists, and engineers. The acronym MaCKiE naturally comes from the title of the conference, but is also part of the German name of Mack the Knife in Brecht and Weill's Threepenny Opera, Mackie Messer, and is phonetically indistinguishable from "makkie" in Dutch, optimistically meaning "a cinch".

As a participant you will be able to meet about 70 fellow scientists from 30 countries representing 4 continents on our globe. In a rich program for two and a half days, there are 53 lectures and 15 poster presentations. The diversity of scientific topics and participants is quite notable and hopefully will contribute to the success of future meetings as well.

Welcome to Hungary! Welcome to Budapest! Welcome to MaCKiE 2017!

Gábor Lente
Conference Chair

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Mathematics in (bio)Chemical Kinetics
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	THURSDAY, May 25, 2017
12:00–14:30	**Registration**
14:30–14:40	**Opening remarks**
	SESSION 1 – Chair: *Guy Marin*
14:40–15:20	***Vladana Vukojevic*** (Karolinska Institute, Stockholm, Sweden) Quenching Analysis of Small-Amplitude Chemical and Biochemical Oscillations near a Supercritical Hopf Bifurcation
15:20–15:40	***Gregory S. Yablonsky*** (Saint Louis University, USA) A Skeletal Kinetic Mechanism for the SO_x–NO_x–O_2–H_2O–CO_2 System at Elevated Pressures
15:40–16:00	***Massimiliano Esposito*** (University of Luxembourg) Dynamics and Thermodynamics of Open Chemical Networks
16:00–16:30	**Coffee break**
	SESSION 2 – Chair: *István Szalai*
16:30–17:10	***Vemuri Balakotaiah*** (University of Houston, USA) Multi-scale Averaging Methods for Chemical Reactors and Reacting Flows
17:10–17:30	***Josef Hofbauer*** (Universität Wien, Austria) Oscillations in the Lotka–Farkas Reaction
17:30–17:50	***Marek Orlik*** (University of Warsaw, Poland) The Model of “Minimal Oscillator” of the H2O2–NaSCN–NaOH–CuSO4 Dynamical System
17:50–18:10	***Gábor Szederkényi*** (Institute for Computer Science and Control, Budapest, Hungary) Approximation of delayed chemical reaction networks
18:10–18:30	***Igor Schreiber*** (University of Chemistry and Technology, Prague, Czech Republic) Parameter fitting in models of complex reactions to experimentally observed oscillatory dynamics using reaction network theory
18:30–20:00	**Welcome reception**

	FRIDAY, May 26, 2017			
	SESSION 3 – Chair: *Valery Romanovski*			
09:00–09:40	***Laurence Calzone*** (Institut Curie, Paris, France) From Regulatory Networks to Mathematical Models: Applications to Cancer Biology			
09:40–10:00	***Hiroyuki Fujii*** (Hokkaido University, Sapporo, Japan) Numerical Calculation of Time-Resolved Light Reflectance from Biological Tissue Using the Radiative Transfer Equation			
10:00–10:20	***Stefan Müller*** (Austrian Academy of Sciences RICAM, Linz, Austria) Optimal Enzyme Allocation in Kinetic Metabolic Networks			
10:20–11:00	**Coffee break**			
	SESSION 4 – Chair: *Massimiliano Esposito*		**SESSION 5 – Chair: *Igor Schreiber***	
11.00–11.20	***Arun Pankajakshan*** (University College London, UK)	A model-based experimental design approach for the identification of kinetic models of Au catalysed HMF oxidation in a micropacked bed reactor	***Gurmeet Kaur*** (Ghent University, Belgium)	Compartmental Modeling of Top Sprayed Fluidized Bed Granulator Using Population Balances
11:20–11:40	***Dániel Sebők*** (University of Szeged, Hungary)	Comparative Study of Adsorption And Scattering Techniques to Determine the Surface Fractal Dimension of Nanostructured Materials	***Nenad D. Ristic*** (Ghent University, Belgium)	Application of Partial Least Squares Regression for Understanding and Prediction of Fouling in the Transfer Line Heat Exchanger of a Steam Cracker
11:40–12:00	***Éloïse Comte*** (Laboratoire MIA, La Rochelle, France)	Optimal control problems for groundwater stressed by agricultural fertilizers	***Virág Kiss*** (University of Debrecen, Hungary)	Full Mathematical Description of the pH-stat Kinetic Traces in the Photochemical Reactions of Quinone Derivatives
12:00–12:20	***Almaz Mustafin*** (Kazakh National Research Technical University, Almaty, Kazakhstan)	Quasi-harmonic and spiky oscillations in a harvest model with equable resource supply	***Mehakpreet Singh*** (Ghent University, Belgium)	Finite Volume Approximation of Two-Dimensional Aggregation Population Balances on Triangular Mesh
12:20–12:40	***Ling Xiao*** (East China University of Science and Technology, Shanghai, China)	Rational Catalyst Design for Propane Dehydrogenation from First Principles and Microkinetic Modeling	***Shahzad Muhammad*** (Hazara University, Mansehra, Pakistan)	Different Available Completion Routes in Complex Chemical Reactions
12:40–14:00	**Lunch break**			

	FRIDAY, May 26, 2017			
	SESSION 6 – Chair: *Paul G. Mezey*		**SESSION 7 – Chair: *Peter Salamon***	
14:00–14:20	***Artur Wachtel*** (University of Luxembourg)	Dissipation in Noisy Chemical Networks: the Role of Deficiency	***Tomislav Plesa*** (University of Oxford, UK)	Systematic Design of Reaction Systems with Prescribed Behaviors: Deterministic and Stochastic Methods
14:20–14:40	***Daniel Branco Pinto*** (Ghent University, Belgium)	Kinetic Intersections as a Source of Information on Rate Coefficients	***Meritxell Saez*** (University of Copenhagen, Denmark)	Positive Linear Elimination of Species
14:40–15:00	***Riccardo Rao*** (University of Luxembourg)	Glucans Monomer–Exchange Dynamics as an Open Chemical Network	***Casian Pantea*** (West VA University, Morgantown, USA)	Inheritance of Bistability in Mass Action Reaction Networks
15:00–15:20	***Anupam Abha*** (Indian Institute of Technology Madras, Chennai, India)	Experiments and modeling of NO reduction using gold and silver catalyst	***Brigita Hočevar*** (National Institute of Chemistry, Ljubljana, Slovenia)	Hydrotreatment of C6 Ketones and Secondary Alcohols Over Sulphided Nimo Catalyst: First–Principles Supported Microkinetic Study
15:20–15:40	***Nishithan Balaji Chidambarakani*** (Indian Institute of Technology Madras, Chennai, India)	Global Kinetic Modelling and Reactor Analysis of Lean NOx Traps (LNT) Catalysts	***Moritz Schulze*** (Technical University of Braunschweig, Germany)	Flatness–Based Model Selection of a Benzaldehyde Lyase Catalysed Biochemical Reaction Network
15:40–16:00	**Coffee break**			
	SESSION 8 – Chair: *Vemuri Balakotaiah*		**SESSION 9 – Chair: *Katalin Ősz***	
16:00–16:20	***Grzegorz Król*** (Rzeszow University of Technology, Poland)	New, Simple Method of Determining Necessary Conditions of Dead Zone Formation	***Jean-François Derivaux*** (Université libre de Bruxelles, Belgium)	Stochastic Thermodynamics of Reactive Systems: an Extended Local Equilibrium Approach
16:20–16:40	***Nils De Rybel*** (Ghent University, Belgium)	A Novel Solution Strategy for the Simulation of Bulk Raft Polymerization	***Victor Costa*** (IFP Energies Nouvelles, Lyon, France)	Hybrid Models: Using Kriging to Improve ODE–Based Kinetics
16:40–17:00	***Songjun Liu*** (Ghent University, Belgium)	Exploring the Fundamentals in Catalytic Partial Oxidation of Methane: the Interaction Between Diffusion and Reaction in a Packed Bed Reactor	***Matteo Polettini*** (University of Luxembourg)	The Interplay between Topology and Fluctuations in the Thermodynamics of Chemical Networks
17:00–17:20	***Guanghua Ye*** (East China University of Science and Technology, Shanghai, China)	An Analytical Method for Optimizing the Pore Network Architecture of Lithium–Ion Battery Electrodes	***Pedro L. Valencia*** (Universidad Técnica Federico Santa María, Valparaíso, Chile)	Modeling the Enzymatic Hydrolysis of Proteins Considering Variable Product Inhibition
17:20–19:30	**Poster session and wine**			

	SATURDAY, May 27, 2017
	SESSION 10 – Chair: *István Lagzi*
09:00–09:40	***Daishin Ueyama*** (Meiji University, Tokyo, Japan) Self–organized Regulation Resulting from Local Contacts
09:40–10:00	***Enrico Bibbona*** (Politecnico di Torino, Italy) Strong Approximations of Stochastic Models of Reaction Networks
10:00–10:20	***Gabriele Milani*** (Technical University of Milan, Italy) An Innovative Kinetic Model for NR–High Cis PB Blends
10:20–10:40	***Balázs Boros*** (Austrian Academy of Sciences RICAM, Linz, Austria) Existence, Uniqueness, and Stability of Steady States of Mass–Action Systems
10:40–11:00	**Coffee break**
	SESSION 11 – Chair: *János Tóth*
11:00–11:40	***Karl Heinz Hoffmann*** (Chemnitz University of Technology, Germany) Modeling the Structure Formation Process of Twin Polymerization
11.40–12.00	***Valery Romanovski*** (CAMTP and University of Maribor, Slovenia) Some Computer Algebra Tools for Investigation of Biochemical Models Described by Systems of ODEs
12.00–12.20	***Katalin Ősz*** (University of Debrecen, Hungary) Double Exponential Evaluation Under Non-Flooding Conditions: a Mixed Second Order Process Followed by a First Order Reaction
12:20–14:00	**Lunch break**

	SATURDAY, May 27, 2017
	SESSION 12 – Chair: *Gregory S. Yablonsky*
14:00–14:40	***István Z. Kiss*** (Saint Louis University, USA) Synchronization Engineering: Design of Pattern Formation with Oscillatory Chemical Reactions Using Experiment–Based Phase Models
14:40–15:00	***István Lengyel*** (SABIC Technology and Innovation, Sugar Land, USA) Bifurcation Analysis of Detailed Combustion Mechanisms
15:00–15:20	***Peter Salamon*** (San Diego State University, USA) Time Scales for Free Energy Landscapes
15:20–15:40	***Paul G. Mezey*** (Memorial University of Newfoundland, St. John's, Canada) Molecular Potential Energy Surfaces as Frameworks for Reaction Kinetics
	SESSION 13 – Chair: *Gábor Lente*
15:40–16:00	***Ágota Tóth*** (University of Szeged, Hungary) Modelling of the Hydrogenase Front Reaction
16:00–16:20	***Gregory S. Yablonsky*** (Saint Louis University, USA) Linear or Non–Linear: Procedures for Distinguishing the Models of Chemical Kinetics and Chemical Engineering
16:20–16:40	***János Tóth*** (Budapest University of Technology and Economics, Hungary) What did I learn?
16:40–17:00	**Closing remarks**