

Mathematics in Chemical and Biochemical Kinetics and Engineering (MACKiE-2)

Program

Wednesday, February 7

1:30 pm Guy Marin, Welcome and opening remarks

1:40 pm *Invited Lecture:* Ioannis Kevrekidis (Princeton University)
Equation-free modeling for complex/multi-scale reacting systems

Presentations

2:30 pm Hao Song*, and Jong H. Byrne** (*Department of Biomedical Engineering, Duke University, and **The Department of Neurobiology and Anatomy, W.M.Keck Center for the Neurobiology of Learning and Memory, The University of Texas Medical School at Houston)
Nonlinear dynamics of minimal models of interlocked positive and negative feedback loops of transcriptional regulation by CREB proteins: deterministic and stochastic analysis

2:50 pm Kapil Mayawala*, Anne-Marie S. Niehaus*, Dionisios G. Vlachos*, and Jeremy S. Edwards** (*Department of Chemical Engineering, University of Delaware, Newark, DE, USA **Molecular Genetics and Microbiology, University of New Mexico, Albuquerque, NM)
Multiscale stochastic simulations for systems biology modeling: implications of spatial organization of EGF receptors

3:10 pm Istvan Lengyel and Ben Christenson (The Dow Chemical Company)
Automation of key steps in mechanistic kinetic model development

3:30 pm – 3:45 pm Coffee break

3:45 pm Dionisios Vlachos (Department of Chemical Engineering and Center for Catalytic Science and Technology (CCST), University of Delaware, Newark)
Multiscale simulations of nucleation and growth in porous media

4:05 pm Jonas Sjoblom and Derek Creaser (Department of Chemical and Biological Engineering, Chemical Reaction Engineering, Chalmers University of Technology, Goeteborg, Sweden)
Latent variable projections of sensitivity data used for experimental screening and kinetic modeling

**4:25 pm Deming Mao and David H. West (The Dow Chemical Company)
Calculation of residence time distribution in an Eulerian reference frame**

4:45 pm Eliodoro Chiavazzo*, Alexander N. Gorban, Iliya V. Karlin*
(*Aerothermochemistry and Combustion Systems Laboratory LAV, Swiss Federal Institute of Technology Zurich ETH; **Department of Mathematics, University of Leicester, Leicester UK)
Method of invariant grids for model reduction**

**5:05 pm Joseph Swisher, Eugene Redekop, Palghat Ramachandran, John T. Gleaves (Department of Energy, Environmental and Chemical Engineering, Washington University in St. Louis)
Application of method of lines to problems of complex transient kinetics**

5:25 – 6:00 pm Discussions

Thursday, February 8

**8:30 am *Invited lecture:* Neil St. John Forbes (Department of Chemical Engineering, The University of Massachusetts, Amherst)
Mathematical model of tumor metabolism and therapeutic efficacy based on mass balance, transport phenomena and reaction kinetics**

Presentations:

9:20 am Andreas Heyden*, Alex Bell, Fred Keil* (*Department of Chemical Engineering, Hamburg University of Technology, Hamburg, Germany; **Department of Chemical Engineering, University of California, Berkeley, California)
Efficient methods for finding transition states in chemical reactions; Comparison of improved dimer methods and partitioned rational function optimization methods**

9:40 am Renato Feres*, Gregory Yablonsky (* Department of Mathematics, and **Department of Energy, Environmental and Chemical Engineering Washington University, St. Louis)
Revealing surface structure from diffusion studies in rough channels**

10:00 am – 10:20 am Coffee break

**10:20 am Ravi Shekar, Patrick. L. Mills (Department of Chemical and Natural Gas Engineering, Texas A&M University-Kingsville, 700 University Blvd, MSC 188 Kingsville, TX 78363-8202)
Modeling and Simulation of Light Propagation and Image Reconstruction for Diffuse Optical Tomography in Single and Multiple Gas-Liquid Bubble Systems**

10:40 am Abhijit Chatterjee and Dionisios G. Vlachos (Department of Chemical Engineering and Center for Catalytic Science and Technology (CCST), University of Delaware, Newark, DE)

Nanopattern formation in heteroepitaxy

11:00 am Mark Lazman*, Gregory Yablonsky** (Aspen Technology, Calgary, Canada, and** Washington University, Department of Energy, Environmental and Chemical Engineering, St. Louis, MO)

Steady-state reaction rate equation of single-route complex catalytic reaction in terms of hypergeometric series

11:20 am Suresh Bhatia (University of Queensland, Brisbane, Australia)

Molecular transport in nanopores

11:40 pm – 1:30 pm Lunch

1:30 pm *Invited lecture:* Alexander Gorban* and Gregory Yablonsky**

(*University of Leicester, UK; **Department of Energy, Environmental and Chemical Engineering, Washington University, St. Louis)

Geometry of thermodynamic restrictions on kinetics

Presentations

2 :20 pm Andro Mikelic (Institute Carnille Jordan, UFR Mathematique, Site de Gerland, Universite Lyon 1, Lyon, France)

Rigorous upscaling of the reactive transport under dominant Peclet and Damkoehler numbers

2:40 pm Suresh Bhatia (University of Queensland, Brisbane, Australia)

Molecular modeling of structure and connectivity of disordered carbon

3:00 pm Edward Baudrez*, Geraldine Heynderickx*, Juray De Wilde*, Guy, B. Marin*** (* Laboratrium voor Petrochemische Techniek, Department of Chemical Engineering , Ghent University, Ghent University, B-9000 Gent, Belgium; ** Material and Process Engineering Universite Catholique de Louvain, Batiment Reaumur, Louvain-la-Neuve, Belgium)

Accounting for large density variations in the steady-state simulation of fluid catalytic cracking

3:20 pm Juray De Wilde , Edward Baudrez* , Geraldine Heynderickx* , Guy, B. Marin* (* Laboratrium voor Petrochemische Techniek, Department of Chemical Engineering , Ghent University, Gent, Belgium, and ** Material and Process Engineering Universite Catholique de Louvain, Batiment Reaumur, Louvain-la-Neuwe, Belgium)**
Speeding up gas-solid flow calculations with variable gas density

3:40 – 4:00 pm Coffee break

4:00 pm Raf Roelant* , Denis Constales , Roger van Keer** , Guy B. Marin* (*Laboratrium voor Petrochemische Techniek, Department of Chemical Engineering, Ghent University, Ghent University, Gent, Belgium, and **Department of Mathematical Analysis, Ghent University, Gent, Belgium)**
Regression of transient kinetics data

4:20 Rachana Agrawal* , Vemuri Balakotaiah* , David H. West (*University of Houston, **The Dow Chemical Company)**
Hot-spot formation in adiabatic down-flow packed-bed reactors

4:40 pm Ahmed M. Sowedan and Almahdi A. Alhoig (Chemical Engineering Department, Almergeb University, Khoms, Libya)
Kinetic Model of the Claus Process: Analysis of Mathematical Properties

5:00 pm Mohammad A. Al-Meshragi and Mustafa Asma (Chemical Engineering Department, Al-Marghib University, Libya)
Kinetic Model of Phenolic Effluents Removal from Wastewater

5:20 pm Concluding remarks; MACKIE-2 adjourns