

MaCKiE

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

**Scientific Program of the
International Conference on Mathematics in (bio)Chemical Kinetics and Engineering
MaCKiE 2018**

**NOVEMBER 8, Thursday
Morning Session
RECTOR VERMEYLEN Hall**

Chairs: Professor Marina Slinko (Russia), Professor Kevin Van Geem (Belgium)

08.45 MaCKiE Opening (Greetings of the Dean)

09.00

Plenary Lecture

Professor William H. Green

CREATING AND USING BIG KINETIC MODELS: MECHANISM TRUNCATION ERROR AND OPERATOR SPLITTING

Massachusetts Institute of Technology (MIT), Cambridge, MA, USA

ORAL PRESENTATIONS

OM-1

10.00

Balakotaiah V.¹, Ratnakar R.R.²

MULTI-SCALE COARSE-GRAINED MODELS FOR SIMULATION OF COUPLED HOMOGENEOUS-CATALYTIC REACTIONS IN MONOLITHS

¹University of Houston, Houston, USA

²Shell International Exploration and Production Inc., Houston, USA

OM-2

10.20

Hardy B., De Wilde J., Winckelmans G.

A PENALIZATION METHOD FOR THE DIRECT NUMERICAL SIMULATION OF LOW-MACH REACTING GAS-SOLID FLOWS

Catholic University of Leuven, Louvain-la-Neuve, Belgium

OM-3

10.40

Zagoruiko A.^{1,2}, Smolikov M.³, Yablokova S.³, Belyi A.³

THERMODYNAMICALLY CONSISTENT KINETIC MODEL FOR THE NAPHTHA REFORMING PROCESS

¹Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

²Tomsk Polytechnic University, Tomsk, Russia

³Institute for Hydrocarbon Processing, Omsk, Russia

11.00 Coffee break

Chairs: Professor Vemuri Balakotaiah (USA), Professor Andrey Zagoruiko (Russia)

OM-4

11.30

Slinko M.M.¹, Makeev A.G.²

REACTION RATE OSCILLATIONS IN A CATALYTIC FLOW REACTOR OPERATING IN A MASS-TRANSFER LIMITED REGIME

¹Semenov Institute of Chemical Physics RAS, Moscow, Russia

²Lomonosow Moscow State University, Moscow, Russia

OM-5

11.50

Wang H., Sarathy S.M., Takanabe K.

MODELING THE TRANSITION FROM OXIDATIVE COUPLING TO PARTIAL OXIDATION OF METHANE BY Ir-DOPING ON La₂O₃/CeO₂ NANOFIBER CATALYST

King Abdullah University of Science and Technology, Jeddah, Saudi Arabia

OM-6

12.10

Greiner R.^{1,2}, Prill T.³, Iliev O.³, van Setten B.², Votsmeier M.^{1,2}

TOMOGRAPHY BASED SIMULATION OF REACTIVE FLOW AT THE MICRO-SCALE: PARTICULATE FILTERS WITH WALL INTEGRATED CATALYST

¹Technical University of Darmstadt, Darmstadt, Germany

²Umicore, Hanau, Germany

³Fraunhofer ITWM, Kaiserslautern, Germany

12.30 Lunch

NOVEMBER 8, Thursday

Afternoon Session

RECTOR VERMEYLEN Hall

Chairs: Professor Gregory Yablonsky (USA), Professor Geraldine Heynderickx (Belgium)

OM-7

13.30

Tóth J.¹, Ladics T.², Nagy T.³

PARAMETER ESTIMATION: A BRUTE AND A SMART METHOD

¹Budapest University of Technology and Economics, Budapest, Hungary

²John von Neumann University, Kecskemét, Hungary

³Institute of Material and Environmental Chemistry, Budapest, Hungary

OM-8

13.50

Pankajakshan A., Waldron C., Gavriilidis A., Galvanin F.

TOWARDS ONLINE REDESIGN OF STEADY STATE EXPERIMENTS FOR THE IDENTIFICATION OF KINETIC MODELS IN FLOW REACTION SYSTEMS

University College London, London, United Kingdom

OM-9

14.10

Pirro L.¹, Paret S.¹, Obradovic A.¹, Vandegehuchte B.², Marin G.B.¹, Thybaut J.¹

OCM CATALYSTS ASSESSMENT: CLUSTERING TECHNIQUES FOR THE DESIGN AND ANALYSIS OF NUMERICAL EXPERIMENTS

¹*Ghent University, Ghent, Belgium*

²*Total Research and Technology Feluy, Ghent, Belgium*

OM-10

14.30

Plehiars P.¹, Coley C.², Green W.H.², Marin G.B.¹, Stevens C.¹, Van Geem K.¹

MACHINE LEARNING FOR EFFICIENT AND CONTINUOUS RETROSYNTHETIC PRODUCT DESIGN: A NOVEL REACTION IDENTIFIER

¹*Ghent University, Ghent, Belgium*

²*Massachusetts Institute of Technology (MIT), Cambridge, USA*

OM-11

14.50

Quaglio M., Roberts L., Jaapar M.S., Dua V., Galvanin F.

AN ARTIFICIAL NEURAL NETWORK APPROACH TO CLASSIFY CHEMICAL REACTION TYPES FROM EXPERIMENTAL DATA

University College London, London, United Kingdom

OM-12

15.10

Qamar S.^{1,2}, Seidel-Morgenstern A.¹

ANALYSIS OF RADIAL EFFECTS IN NON-ISOTHERMAL FIXED-BED ADSORBERS AND REACTORS

¹*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*

²*COMSTAST Institute of Information Technology, Islamabad, Pakistan*

15.30 Coffee break

Chair: Professor Ingmar Nopens (Belgium)

OM-13

16.00

Bawareth B.^{1,2}, Di Marino D.², Nijhuis T.¹, Wessling M.²

UNRAVELLING ELECTROCHEMICAL LIGNIN DEPOLYMERIZATION: KINETICS MODELLING USING POPULATION BALANCE EQUATIONS

¹*RWTH Aachen University, Aachen, Germany*

²*SABIC, Riyadh, Saudi Arabia*

OM-14

16.20

Campet R., Riber E., Cuenot B.

GEOMETRICAL OPTIMIZATION OF STEAM CRACKING COILS

European Center for Research and Advanced Training in Scientific Computing (CERFACS), Toulouse, France

OM-15

16.40

Lissens M., Devocht B.R., Marin G.B., Thybaut J.

ADAPTIVE REACTION NETWORK SIZE CONTROL FOR THE CATALYTIC CONVERSION OF RENEWABLE RESOURCES

Ghent University, Ghent, Belgium

OM-16

17.00

Hočevar B.^{1,2}, Huš M.¹, Bjelić A.¹, Grilc M.¹, Likozar B.¹

BIOMASS HYDRODEOXYGENATION: A COMBINED EXPERIMENTAL, FIRST-PRINCIPLES AND MATHEMATICAL MODELLING STUDY

¹*National Institute of Chemistry, Ljubljana, Slovenia*

²*University of Ljubljana, Ljubljana, Slovenia*

OM-17

17.20

SriBala G., Carstensen H., Van Geem K., Marin G.B.

ON THE REACTIVITY OF MONO-LIGNOL DERIVATIVES

Ghent University, Ghent, Belgium

17.40 Poster Session

Welcome Reception

NOVEMBER 9, Friday
Morning Session
RECTOR VERMEYLEN Hall

Chairs: Professor János Tóth (Hungary), Professor Denis Constaes (Belgium)

OM-30

09.00

Knyazeva A.G.^{1,2}, Korosteleva E.N.^{1,2}, Kryukova O.N.², Demidov V.N.², Baranovsky A.², Bukrina N.²
TITANIUM BASED COMPOSITE SYNTHESIS AT THE CONDITIONS OF CONTROLLED HEATING

¹*National Research Tomsk Polytechnic University, Tomsk, Russia*

²*Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia*

OM-31

09.20

Lashina E.A.^{1,2}, Slavinskaya E.M.^{1,2}, Chumakova N.A.^{1,2}, Stadnichenko A.I.^{1,2}, Chumakov G.A.^{2,3}, Boronin A.I.^{1,2}
INVERSE HYSTERESIS IN THE CO OXIDATION OVER PALLADIUM: INFLUENCE OF THE CONVECTION ON THE DYNAMICS

¹*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

²*Novosibirsk State University, Novosibirsk, Russia*

³*Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia*

OM-32

09.40

Vandewalle L.A.¹, Lengyel I.², West D.², Van Geem K.¹, Marin G.B.¹

CATALYST IGNITION IN A GAS-SOLID VORTEX REACTOR FOR OXIDATIVE COUPLING OF METHANE: A NUMERICAL STUDY

¹*Ghent University, Ghent, Belgium*

²*SABIC Technology and Innovation, Sugarland, Houston, USA*

OM-18

10.00

Panfilov A.V.

NON-LINEAR WAVES AND CARDIAC ARRHYTHMIAS

Ghent University, Ghent, Belgium

OM-19

10.20

Aboulmouna L.¹, DeVilbiss F.¹, Gupta S.², Maurya M.², Subramaniam S.², Ramkrishna D.¹
A CYBERNETIC APPROACH TO MODELING LIPID METABOLISM IN MAMMALIAN CELLS

¹*Purdue University, Indianapolis, USA*

²*University of California, San Diego, San Diego, USA*

OM-20

10.40

Patsatzis D.¹, Tingas E.², Goussis D.^{1,3}, Sarathy M.²

CHEMICAL KINETICS OF BRAIN METABOLISM: EQUILIBRATIONS AND CONTROL OF THE PROCESS

¹*National Technical University of Athens, Athens, Greece*

²*King Abdullah University of Science and Technology, Clean Combustion Research Center, Thuwal, Saudi Arabia*

³*Khalifa University of Science, Technology and Research, Abu Dhabi, United Arab Emirates*

11.00 Coffee break

Chairs: Professor Anna Knyazeva (Russia), Professor Juray De Wilde (Belgium)

OM-21

11.30

Golman B.¹, Kusekbayev N.², Skrzypacz P.¹

TRANSIENT KINETIC ANALYSIS OF MULTIPATH REACTIONS USING STEP-RESPONSE AND TAP METHODS

¹*Nazarbayev University, Astana, Kazakhstan*

²*Drilling and Production Research Institute KazMunaiGas, Kazakhstan, Astana, Kazakhstan*

OM-22

11.50

Malkovich E.^{1,2}, Semeykina V.^{2,3}, Bazaikin Y.^{1,2}, Parkhomchuk E.^{2,3}, Lysikov A.^{2,3}, Kleymenov A.⁴, Fedotov K.⁴

MATHEMATICAL MODELLING FOR BIMODAL CATALYST DEACTIVATION

¹*Sobolev Institute of Mathematics of SB RAS, Novosibirsk, Russia*

²*Novosibirsk State University, Novosibirsk, Russia*

³*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

⁴*PJSC «Gazprom Neft», St. Petersburg, Russia*

OM-23

12.10

Omojola T.^{1,2}, Cherkasov N.², Lukyanov D.B.¹, Rebrov E.V.², van Veen A.C.²

ON THE INDUCTION PERIOD OF THE CONVERSION OF METHANOL OVER ZSM-5 CATALYSTS: TRANSIENT STUDIES USING A TAP REACTOR

¹*University of Bath, Bath, United Kingdom*

²*University of Warwick, Coventry, United Kingdom*

12.30 Lunch

NOVEMBER 9, Friday

Afternoon Session

RECTOR VERMEYLEN Hall

Chairs: Professor William Green (USA), Dr. Paul Van Steenberge (Belgium)

OM-24

13.30

Branco Pinto D.¹, Yablonsky G.², Marin G.¹, Constaes D.¹

NEW INSIGHTS IN CHEMICAL RELAXATION: INVARIANTS AND CONSERVATIVELY PERTURBED EQUILIBRIUM

¹*Ghent University (Ghent), Belgium*

²*Washington University in St. Louis, St. Louis, MO, USA*

OM-25

13.50

Gromotka Z.¹, Yablonsky G.², Constaes D.¹

ON TERMOLECULAR REVERSIBLE REACTION KINETICS: TYPICAL DEPENDENCIES EXPLAINED WITH AUTOCATALYTIC REACTIONS

¹*Ghent University, Ghent, Belgium*

²*Washington University in St. Louis, St. Louis, MO, USA*

OM-26

14.10

Marien Y.W.¹, Van Steenberge P.H.¹, Vir A.B.¹, Barner-Kowollik C.^{2,3}, Reyniers M.¹, Marin G.B.¹, D'hooge D.R.¹

KINETIC MONTE CARLO MODELING OF PULSED LASER (CO)POLYMERIZATION TO DETERMINE INTRINSIC RATE COEFFICIENTS

¹*Ghent University, Ghent, Belgium*

²*Karlsruhe Institute of Technology, Karlsruhe, Germany*

³*Queensland University of Technology, Brisbane, Australia*

OM-27

14.30

Skrzypacz P., Golman B.

FINITE ELEMENT SOLUTIONS TO REACTION-DIFFUSION PROBLEMS WITH DEAD-CORES

Nazarbayev University, Astana, Kazakhstan

OM-28

14.50

Minette F., De Wilde J.

MULTI-SCALE MODELING OF AN ANNULAR STRUCTURED CATALYTIC REACTOR: APPLICATION TO STEAM METHANE REFORMING

Catholic University of Leuven, Louvain-la-Neuve, Belgium

OM-29

15.10

Symoens S.H., Aravindakshan S.U., Vermeire F.H., Gorugantu S.B., Marin G.B., Reyniers M., Van Geem K.

DATA QUALITY ASSESSMENT BY CLUSTERING ANALYSIS AND PRINCIPLE COMPONENT ANALYSIS

Ghent University, Ghent, Belgium

OM-33

15.30

Minette F.¹, Lugo M.², Castaldi M.², De Wilde J.¹

EXPERIMENTAL STUDY OF THE INTRINSIC KINETICS OF STEAM METHANE REFORMING ON A THIN Ni COATING

¹*Catholic University of Leuven, Louvain-la-Neuve, Belgium*

²*City College of New York (CCNY), New York, USA*

15.50 Coffee break

Chairs: Dr. Evgeniy Redekop (Norway), Professor Gregory Yablonsky (USA)

16.20

TAP Round Table

Moderator: Dr. Evgeniy Redekop, University of Oslo, Norway

17.20 Closing address

POSTER PRESENTATIONS

PP-1. Bosia F.¹, Proppe J.², Reiher M.¹

EXPLORING CHEMICAL REACTION NETWORKS WITH KiNetX

¹ETH Zurich, Zurich, Switzerland

²Harvard University, Cambridge, MA, USA

PP-2. De Keer L.¹, Cavalli F.², Van Steenberge P.H.¹, Reyniers M.¹, Barner L.^{2,3}, D'hooge D.R.¹

MATHEMATICAL MODELING OF NETWORK POLYMERS

¹Ghent University, Ghent, Belgium

²Karlsruhe Institute of Technology, Karlsruhe, Germany

PP-3. Devlaminck D.J., Van Steenberge P.H., De Keer L., Reyniers M., D'hooge D.R.

STOCHASTIC SIMULATION OF MADIX/RAFT POLYMERIZATION AT THE MOLECULAR LEVEL

Ghent University, Ghent, Belgium

PP-4. Guellout Z.^{1,2}, Francois-Lopez E.¹, Benguerba Y.², Dumas C.¹, Ernst B.¹

KINETIC MODELING OF HYDROGEN PRODUCTION BY DARK FERMENTATION

¹Universite de Strasbourg, Strasbourg, France

²Universite de Sétif, Sétif, Algeria

PP-5. Uskov S.I.^{1,2}, Potemkin D.I.^{1,2}, Snytnikov P.V.^{1,2}, Shigarov A.B.¹, Kurochkin A.V.³, Kirillov V.A.¹, Sobyenin V.A.¹

LOW-TEMPERATURE STEAM REFORMING OF LIGHT HYDROCARBONS: KINETIC STUDY ON THE WAY TO SELECTIVE CONVERSION

¹Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

²Novosibirsk State University, Novosibirsk, Russia

³AET OG "INTECH", Ufa, Russia

PP-6. Tschentscher R., Stensrød R.

KINETICS OF CELLULOSE AND HEMICELLULOSE HYDROLYSIS

SINTEF Industry, Oslo, Norway