



**XXIII International conference on Chemical Reactors
CHEMREACTOR-23**

**Ghent, Belgium
November 5 – 9, 2018**

Scientific Program



**Scientific Program of the
XXIII International conference on Chemical Reactors
CHEMREACTOR-23**

Ghent, Belgium, November 5-9, 2018

EFCE Event 748

**Boreskov Institute of Catalysis of the Siberian Branch
of the Russian Academy of Sciences, Novosibirsk, Russia**

Ghent University, Ghent, Belgium

European Federation on Chemical Engineering

**Scientific Council on Theoretical Fundamentals of Chemical
Technology RAS Scientific Council on Catalysis RAS**

Conference Co-Chairs

**Professor Guy Marin
Ghent University
Belgium**

**Professor Alexandr Noskov
Boreskov Institute of Catalysis SB RAS
Russia**

Conference Organizing Team

**Professor Kevin Van Geem
Ghent University
Belgium**

**Tatiana Zamulina
Boreskov Institute of Catalysis SB RAS
Russia**

Conference Proceedings:
Special Issue
CHEMICAL ENGINEERING JOURNAL
ELSEVIER



MEDIA PARTNERSHIP
Reaction Chemistry & Engineering
Royal Society of Chemistry

Reaction Chemistry & Engineering

CONFERENCE WEBSITE:

http://conf.nsc.ru/CR_23

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INTERNATIONAL SCIENTIFIC COMMITTEE

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Jaap Schouten	Eindhoven University of Technology, The Netherlands
Valeryi Schvets	Mendeleev University of Chemical Technology of Russia, Moscow, Russia
Andreas Seidel-Morgenstern	Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany
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Krzysztof Warmuzinski	Institute of Chemical Engineering, Polish Academy of Sciences, Gliwice, Poland
Gregory Yablonsky	Washington University in St. Louis, St. Louis, MO, USA
Andrey Zagoruiko	Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Xing-Gui Zhou	East China University of Science and Technology, Shanghai, China

JOINT PROGRAM COMMITTEE

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Professor Kevin Van Geem, Vice-Chairman	Ghent University, Belgium
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Professor Denis Constaes	Ghent University, Belgium
Professor Dagmar D'hooge	Ghent University, Belgium
Dr. Marko Djokic	Ghent University, Belgium
Dr. Vladimir Galvita	Ghent University, Belgium
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Dr. Elena Lashina	Boreskov Institute of Catalysis SB RAS, Russia
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Professor Christian Stevens	Ghent University, Belgium
Professor Joris Thybaut	Ghent University, Belgium
Dr. Alexey Vedyagin	Boreskov Institute of Catalysis SB RAS, Russia
Dr. Nadezhda Vernikovskaya	Boreskov Institute of Catalysis SB RAS, Russia
Professor Grigorii Yablonsky	Washington University in St. Louis, St. Louis, MO, USA
Professor Vadim Yakovlev	Boreskov Institute of Catalysis SB RAS, Russia
Mr. Ilya Zolotarskii	Boreskov Institute of Catalysis SB RAS, Russia

LOCAL ORGANIZING COMMITTEE

Professor Denis Constaes	Ghent University, Belgium
Professor Gregory Yablonsky	Washington University in St. Louis, St. Louis, MO, USA
Professor Joris Thybaut	Ghent University, Belgium
Professor Mark Saeys	Ghent University, Belgium
Professor Geraldine Heynderickx	Ghent University, Belgium
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Dr. Frederik Ronsse	Ghent University, Belgium
Professor Maarten Sabbe	Ghent University, Belgium
Dr. Paul Van Steenberge	Ghent University, Belgium
Professor Dr. Ir. Wolter Prins	Ghent University, Belgium BTG Biomass Technology Group bv, Enschede, The Netherlands

SCIENTIFIC TRENDS

Advances in Chemical Reactor Fundamentals

Chemical Reaction Kinetics

Energy & Mass Transfer in Chemical Reactors and first principles calculations

Fundamentals of Hydrodynamics and Fluid Flow in Chemical Reactors

Chemical Reaction Engineering and Reactor Design – Novel Experimental Approaches, Modeling, Scale-Up and Optimization

Mathematical Simulation: Multiscale Analytic and Computational Studies of Chemical Reactors

Development of Chemical Reactors and Flow-Sheeting of Reactive Processes

New Chemical Reactor Designs (e.g., Structured Reactors, Membrane Reactors, Microreactors)

Process Intensification and Novel Approaches in Multifunctional Reaction Processes (e.g., Microwave/Induction Heated Reactors, Ultrasonic Reactors, Unsteady-State Forcing and Sorption Enhancement in Chemical Reactors, Multifunctional Reactors, Nature-Inspired Engineering of Reaction Processes, High-gravity, High-Shear Reactors)

Chemical Reactors and Technologies for Targeted Applications

Environmental Protection and Utilization of Waste

Reactors for Polymers and Other Novel Materials with Targeted Properties

Processing of Biomass and Renewable Feedstocks

Electrochemical and Photochemical Reaction Engineering

Biochemical Engineering

CO₂ Sequestration and Utilisation

Advanced Processing of Conventional and Unconventional Hydrocarbon Feedstocks

Modern Reactive Technologies for Natural Gas, Oil and Coal Processing

Chemical Processes for Intensification of Fuel Production

Chemical Reactors for In Situ Processing of Oil and Coal in Deposits

Chemical Reactors and Processes for Treatment of Heavy Hydrocarbon Feedstock and Shale Oil

November 5, Monday

Morning Session

REFTER Hall

08.45 Conference opening

PLENARY LECTURES

Chairpersons:

Professor Guy Marin, Belgium

Professor Mario Montes, Spain

09.00

PL-1

Professor Jens Kehlet Nørskov

Technical University of Denmark, Lyngby, Denmark

A Professor Mikhail Slin'ko Honorary Lecture

CATALYSIS FOR SUSTAINABLE PRODUCTION OF FUELS AND CHEMICALS

10.00

PL-2

Professor Vemuri Balakotaiah¹, Zhe Sun¹, David H. West²

¹*University of Houston, USA*

²*SABIC Technology Center, Sargarland, TX, USA*

AUTOTHERMAL REACTOR DESIGN FOR CATALYTIC PARTIAL OXIDATIONS

11.00 Coffee-break

KEYNOTE LECTURES

Chairperson: Professor Carlos Castillo-Araiza, Mexico

11.30

KL-1

Professor Manos Mavrikakis

University of Wisconsin, Madison, Wisconsin, USA

PREDICTION OF REACTION RATES FOR IMPROVED CATALYST DESIGN AT THE ATOMIC SCALE

12.00

KL-2

Professor José Carlos Brito Lopes

University of Porto, Portugal

The NETmix REACTOR: CONCEPTS, TECHNOLOGY AND PRODUCTS

12.30 Lunch

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Professor Evgeny Rebrov, United Kingdom

14.00

OP-I-1

Peng B.^{1,2}, Yablonsky G.³, **Constales D.**⁴, Marin G.⁴, Muhler M.^{1,2}

TESTING THE INVARIANT FOR THE NON-LINEAR CHEMICAL REACTION

¹*Ruhr-University Bochum, Bochum, Germany*

²*Max Planck Institute for Chemical Energy Conversion, Mulheim an der Ruhr, Germany*

³*Washington University in St. Louis, St. Louis, MO, USA*

⁴*Ghent University, Ghent, Belgium*

14.20

OP-I-2

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

A MODEL-BASED DATA MINING APPROACH FOR OUTLIER DETECTION IN KINETIC MODELLING STUDIES

Chemical Engineering Department, University College London, London, United Kingdom

14.40

OP-I-3

Till Z., Varga T., Chován T.

REDUCTION OF LUMPED REACTION NETWORKS BASED ON GLOBAL SENSITIVITY ANALYSIS

University of Pannonia, Veszprém, Hungary

15.00

OP-I-4

Slinko M.M.¹, Makeev A.G.², Luss D.³

MECHANISM OF CO OXIDATION OVER Pt-GROUP METALS UNDER HIGH PRESSURE CONDITIONS: Langmuir–Hinshelwood or Mars–van Krevelen?

¹*Semenov Institute of Chemical Physics RAS, Moscow, Russia*

²*Lomonosov Moscow State University, Moscow, Russia*

³*University of Houston, USA*

15.20

OP-I-5

Yablonsky G.¹, Stokie D.¹, Kumfer B.¹, Verma P.¹, Min Y.¹, Zhu Y.¹, Jun Y.¹, Suresh A.², Axelbaum R.²

THE KINETICS OF FLUE GAS PURIFICATION FOR PRESSURIZED OXY-COMBUSTION

¹*Washington University in St. Louis, St. Louis, MO, USA*

²*Indian Institute of Technology Bombay, Mumbai, India*

15.40 Coffee-break

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Professor Joris Thybaut, Belgium

16.00

OP-I-6

Kolb G.^{1,2}, Ortega C.², Hessel V.²

DIMETHYL ETHER CONVERSION TO GASOLINE GRADE HYDROCARBONS OVER ZSM-5: KINETIC STUDY IN A RECYCLE REACTOR

¹*Fraunhofer IMM (Fraunhofer Institute for Microtechnology and Microsystems), Mainz, Germany*

²*Eindhoven University of Technology, Eindhoven, The Netherlands*

16.20

OP-I-7

Standl S.¹, Kühlewind T.¹, Kirchberger F.M.¹, Tonigold M.², Lercher J.A.¹, Hinrichsen O.¹

METHANOL-TO-OLEFINS (MTO) on ZSM-5: SINGLE-EVENT KINETIC MODELING, MECHANISTIC ANALYSIS AND REACTOR DESIGN

¹*Technical University of Munich, Munich, Germany*

²*Clariant Produkte (Deutschland) GmbH, Bruckmühl, Germany*

16.40

OP-I-8

Petrov R.¹, Nazimov D.¹, Klimov O.¹, Noskov A.¹, Parakhin O.²

KINETIC MODEL FOR n-BUTANE TO BUTADIENE DEHYDROGENATION ON Cr-AI CATALYST

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

²*LLC «SPAC «Sintez», Barnaul, Russia*

17.00

OP-I-9

Alvarado Camacho C.¹, Thybaut J.², Ruiz Martinez R.¹, Morales A.¹, Castillo-Araiza C.O.¹

KINETIC ASSESSMENT OF THE OXATIVE DEHYDROGENATION OF ETHANE USING a NiSnO CATALYSTS

¹*Autonomous Metropolitan University-Iztapalapa, Iztapalapa, Mexico*

²*Ghent University, Ghent, Belgium*

17.20

OP-I-10

Chizhik S.A.^{1,2}, Popov M.P.¹, Nemudry A.P.¹

KINETICS OF OXYGEN EXCHANGE BETWEEN NONSTOICHIOMETRIC OXIDES AND GAS PHASE: ANALYSIS OF GIBBS ENERGY RELATIONS IN TERMS OF CONTINUOUS HOMOLOGOUS SERIES

¹*Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia*

²*Novosibirsk State University, Novosibirsk, Russia*

17.40

OP-I-11

Arutyunov V.S.^{1,2}, Troshin K.Y.^{1,3}, Nikitin A.V.^{1,3}, Kiryushin A.A.², Belyaev A.A.^{1,3},
Ozerskii A.V.^{1,3}, Komarov I.K.^{1,3}, Strekova L.N.¹

SELF-IGNITION DELAY OF METHANE-ALKANE FUEL COMPOSITIONS

¹*Semenov Institute of Chemical Physics RAS, Moscow, Russia*

²*ONCLEN LLC, Moscow, Russia*

³*Noncommercial Partnership Center of Pulse Detonation Combustion, Moscow, Russia*

19.00 Welcome Reception

Afternoon Session
RECTOR VERMEYLEN Hall

ORAL PRESENTATIONS

Section II.

CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION

Chairperson: Professor Yao Wang, China

14.00

OP-II-1

Bac S., Avci A.K.

CFD MODELING OF MICROCHANNEL ENABLED ETHYLENE OXIDE SYNTHESIS WITH INTEGRATED COOLING

Bogazici University, Istanbul, Turkey

14.20

OP-II-2

Ambrosetti M., Bracconi M., Balzarotti R., Maestri M., Groppi G., Tronconi E.

OPEN-CELL FOAMS AND PERIODIC OPEN-CELLULAR STRUCTURES AS ENHANCED SUBSTRATES FOR THE INTENSIFICATION OF ENVIRONMENTAL CATALYTIC PROCESSES

Politecnico di Milano, Milan, Italy

14.40

OP-II-3

Balzarotti R., Ambrosetti M., Beretta A., **Groppi G.**, Tronconi E.

INVESTIGATION OF PACKED FOAMS AS A NOVEL REACTOR CONFIGURATION FOR METHANE STEAM REFORMING

Politecnico di Milano, Milan, Italy

15.00

OP-II-4

Plachá M.¹, Šourek M.¹, Koci P.¹, Isoz M.¹, Vaclavik M.¹, Svoboda M.², Price E.³, Novak V.³, Thompson D.³

PORE-SCALE MODELING OF COATED CATALYTIC FILTERS

¹*University of Chemistry and Technology, Prague, Czech Republic*

²*University of West Bohemia, Pilsen, Czech Republic*

³*Johnson Matthey Technology Centre, Sonning Common, Reading, United Kingdom*

15.20

OP-II-5

Vernikovskaya N.V.^{1,2}, Ovchinnikova E.V.¹, Chumachenko V.A.¹, Gribovskii A.G.¹, Makarshin L.L.¹

MATHEMATICAL MODELING OF HIGHLY EXOTHERMAL PROCESSES IN MICRO-CHANNEL REACTORS

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

²*Novosibirsk State Technical University, Novosibirsk, Russia*

15.40 Coffee-break

**Afternoon Session
RECTOR VERMEYLEN Hall**

ORAL PRESENTATIONS

Section II.

CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION

Chairperson: Professor Paul Van Steenberge, Belgium

16.00

OP-II-6

Minette F., De Wilde J.

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

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

16.20

OP-II-7

Claes T., Leblebici M.E., Van Gerven T.

DESIGN AND EVALUATION OF PHOTOCATALYTIC MICROSTRUCTURED REACTOR MODULES

Catholic University of Leuven, Leuven, Belgium

16.40

OP-II-8

Boon J.^{1,2}

THE SORBENT AND THE PROCESS: CO₂ and H₂O SORPTION ENHANCEMENT IN CHEMICAL REACTORS

¹*Sustainable Process Technology, ECN, Energy Research Center of the Netherlands, Petten, The Netherlands*

²*Eindhoven University of Technology, Eindhoven, The Netherlands*

17.00

OP-II-9

Zazhigalov S., Zagoruiko A.

HYDROGEN PRODUCTION BY SORPTION-ENHANCED STEAM REFORMING OF HYDROCARBONS WITH AUTOTHERMAL SORBENT REGENERATION IN A SUPER-ADIABATIC HEAT FRONT OF CATALYTIC COMBUSTION REACTION

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

17.20

OP-II-10

Bremer J.¹, Sundmacher K.^{1,2}

FLEXIBLE PRODUCTION OF SYNTHETIC METHANE: DYNAMIC OPERATION AND CONTROL OF FIXED-BED METHANATION REACTORS

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

²*Otto-von-Guericke University Magdeburg, Magdeburg, Germany*

17.40

OP-II-11

Fukuhara C.¹, Watanabe R.¹, Ratchahat S.², Sudoh M.²

A POWERFUL CO₂ METHANATION REACTOR with Ni/CeO₂ STRUCTURED CATALYST: ESTIMATION OF MASS AND HEAT TRANSFER PROFILES

¹*Shizuoka University, Naka-ku Hamamatsu, Shizuoka, Japan*

²*Amano Institute of Technology, Hosoecho, Hamamatsu, Shizuoka, Japan*

19.00 Welcome Reception

November 6, Tuesday

Morning Session

REFTER Hall

PLENARY LECTURES

Chairpersons:

Professor Kevin Van Geem, Belgium

Professor Gregory Yablonsky, USA

09.00

PL-3

Professor Dionisios G. Vlachos

University of Delaware, Newark, Delaware, USA

MULTI-LEVEL BRIDGE BETWEEN REACTION ENGINEERING AND COMPUTATIONAL CATALYSIS

10.00

PL-4

Mr. Clayton C. Sadler, John Senetar, Geoffrey Fichtl

Honeywell UOP, Des Plaines, IL, USA

METHANOL TO OLEFINS: CONCEPT TO COMMERCIALIZATION

11.00 Coffee-break

KEYNOTE LECTURES

Chairperson: Professor José Carlos Brito Lopes, Portugal

11.30

KL-3

Professor Eugeniusz Molga

Warsaw University of Technology, Poland

APPLICATION OF NEURAL NETWORKS TO APPROXIMATE AND GENERALIZE EXPERIMENTAL DATA

12.00

KL-4

Professor Mario Montes, Oihane Sanz

University of the Basque Country, San Sebastián, Spain

INTENSIFICATION OF CATALYTIC PROCESSES WITH STRUCTURED CATALYSTS AND REACTORS

12.30 Lunch

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Dr. Frédérique Battin-Leclerc, France

14.00

OP-I-12

Skudin V., Gavrilova N.N.

KINETIC STUDY OF CARBON DIOXIDE CONVERSION OF METHANE ON MEMBRANE CATALYSTS UNDER KNUDSEN DIFFUSION CONDITIONS

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

14.20

OP-I-13

Sinev M., Lomonosov V., Gordienko Y., Ponomareva E.

OPTIMIZATION OF KINETIC DESCRIPTION OF GAS-PHASE AND CATALYTIC OXIDATION OF C1-C2 HYDROCARBONS

Semenov Institute of Chemical Physics RAS, Moscow, Russia

14.40

OP-I-14

Uskov S.I.^{1,2}, Potemkin D.I.^{1,2}, Snytnikov P.^{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

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

²*Novosibirsk State University, Novosibirsk, Russia*

³*AET OG "INTECH", Ufa, Russia*

15.00

OP-I-15

Li H., Gao M., Ye M., Liu Z.

MESO-SCALE MODEL OF REACTION-DIFFUSION PROCESS WITHIN A CATALYST PARTICLE FOR MTO PROCESS

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

15.20

OP-I-16

Ye G.¹, Zhou X.¹, Coppens M.²

PROBING CATALYST DEACTIVATION BY COKE AT THE PARTICLE LEVEL DURING PROPANE DEHYDROGENATION USING A DISCRETE MODEL

¹*East China University of Science and Technology, Shanghai, China*

²*Chemical Engineering Department, University College London, London, United Kingdom*

15.40 Coffee-break

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Professor Mikhail Sinev, Russia

16.00

OP-I-17

Bracconi M., Ambrosetti M., Maestri M., Groppi G., Tronconi E.

EFFECTIVE THERMAL CONDUCTIVITY IN OPEN CELLULAR STRUCTURES: ANALYSIS OF THE EFFECT OF THE GEOMETRICAL PROPERTIES AND PERFORMANCE COMPARISON

Politecnico di Milano, Milan, Italy

16.20

OP-I-18

Uglietti R., Bracconi M., Maestri M.

COUPLING MICROKINETIC MODELING WITH CFD-DEM FOR THE SIMULATION OF FLUIDIZED REACTIVE SYSTEMS

Politecnico di Milano, Milan, Italy

16.40

OP-I-19

Donaubauer P., Schmalhorst L., Hinrichsen O.

2D CONTINUUM MODELS FOR FIXED-BED REACTOR DESIGN: IMPACT OF 2D FLOW FIELD ON INLET REGION CHARACTERISTICS

Technical University of Munich, Munich, Germany

17.00

Flash presentations

Poster Session

Beer Reception

Afternoon Session
RECTOR VERMEYLEN Hall

ORAL PRESENTATIONS

Section II.

**CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL
APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION**

Chairperson: Professor Matteo Maestri, Italy

14.00

OP-II-12

Shoynkhorova T.B.¹, **Snytnikov P.**^{1,2,3}, Simonov P.^{1,3}, Potemkin D.^{1,2}, Rogozhnikov V.¹, Kulikov A.¹, Belyaev V.^{1,2,3}, Sobyandin V.¹

SYNGAS PRODUCTION FOR SOFC VIA CATALYTIC OXIDATION OF DIESEL FUEL

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

²*Novosibirsk State University, Novosibirsk, Russia*

³*UNICAT Ltd, Novosibirsk, Russia*

14.20

OP-II-13

He Z., Minette F., De Wilde J.

**NUMERICAL SIMULATION OF INDUSTRIAL SCALE AUTOTHERMAL CHEMICAL LOOPING
METHANE REFORMING FOR SYNGAS PRODUCTION IN A DUAL FLUIDIZED BED REACTOR**

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

14.40

OP-II-14

Cherkasov N.^{1,2}, Bai Y.¹, Exposito A.¹, Rebrov E.^{1,2}

**PERFORMANCE AND SELECTIVITY COMPARISON OF PACKED BED AND TUBE REACTORS IN
SELECTIVE HYDROGENATION**

¹*Stoli Catalysts Ltd, Coventry, United Kingdom*

²*University of Warwick, Coventry, United Kingdom*

15.00

OP-II-15

Guffanti S., Visconti C.G., Groppi G.

**THE EFFECTS OF INTRAPARTICLE DIFFUSION PHENOMENA ON DIMETHYL ETHER DIRECT
SYNTHESIS**

Politecnico di Milano, Milan, Italy

15.20

OP-II-16

Banzaraksaeva S., Ovchinnikova E.V., Chumachenko V.A.

**ETHANOL-TO-ETHYLENE DEHYDRATION ON RING-SHAPED ALUMINA CATALYST IN TUBULAR
REACTOR**

Boreshkov Institute of Catalysis SB RAS, Novosibirsk, Russia

15.40 Coffee-break

Afternoon Session
RECTOR VERMEYLEN Hall

ORAL PRESENTATIONS

Section II.

CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION

Chairperson: Dr. Pasi Tolvanen, Finland

16.00

OP-II-17

Driessen R.T., van der Linden J.J.Q., Bos M.J., Kersten S.R.A., Brilman D.W.F.

MODELING OF CO₂ ADSORPTION ON SUPPORTED AMINE SORBENTS IN A MULTISTAGE FLUIDIZED BED

Sustainable Process Technology, University of Twente, Enschede, The Netherlands

16.20

OP-II-18

Fernengel J.¹, Bolton L.², Hinrichsen O.¹

CHARACTERISATION AND DESIGN OF SINGLE PELLET STRING REACTORS USING NUMERICAL SIMULATION

¹*Technical University of Munich, Garching-Munich, Germany*

²*BP, Sunbury-on-Thames, United Kingdom*

16.40

OP-II-19

Frey M., Violet L., Seyidova L., Richard D., Fongarland P.

HYBRID CATALYSIS: A NEW REACTOR DESIGN FOR ONE-POT SYNERGISTIC COUPLING OF ENZYMATIC AND HETEROGENEOUS CATALYSIS

Laboratory of Catalytic Process Engineering, CNRS-CPE-Lyon, Villeurbanne, France

17.00

Flash presentations

Poster Session

Beer Reception

November 7, Wednesday

Morning Session

REFTER Hall

PLENARY LECTURE

Chairpersons:

Professor Manos Mavrikakis, USA

Professor Andrey Zagoruiko, Russia

09.00

PL-5

Professor Dr.-Ing. Kai Sundmacher^{1,2}, Steffen Linke², Kevin McBride¹

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

²*Otto-von-Guericke University, Magdeburg, Germany*

SOLVENT SELECTION AND TUNING FOR SUSTAINABLE CHEMICAL PROCESSES

KEYNOTE LECTURES

10.00

KL-5

Dr. Bénédicte Cuenot

*CERFACS - European Centre for Research and Advanced Training in Scientific Computation,
Toulouse, France*

NUMERICAL SIMULATION OF COMBUSTION: FROM FUNDAMENTALS TO APPLICATIONS

10.30

KL-6

Dr. Marco Van Goethem

Technip Benelux B.V., Zoetermeer, The Netherlands

TechnipFMC's SWIRL FLOW TUBE® RADIANT COIL: FROM PATENT TO APPLICATION

11.00 Coffee-break

**Morning Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Professor Dr. Gunther Kolb, Germany

11.30

OP-I-20

Castillo-Araiza C.O., Gómez-Ramos G.A., Couder-Garcia M., Buenrostro-Figueroa J., Huerta-Ochoa S., Prado-Barragan L.A.

CHARACTERIZATION OF HYDRODYNAMICS, HEAT AND MASS TRANSPORT UNDER ABIOTIC AND BIOTIC CONDITION IN A TRAY BIOREACTOR FOR THE PRODUCTION OF PROTEASES OUT OF AGROINDUSTRIAL WASTES

Autonomous Metropolitan University-Iztapalapa, Iztapalapa, Mexico

11.50

OP-I-21

Chezeau B., Fontaine J.-P., **Vial Ch.**

EXPERIMENTAL ANALYSIS OF HYDROGEN PRODUCTION, LIQUID-TO-GAS MASS TRANSFER AND MIXING IN DARK FERMENTATION PROCESS

Clermont Auvergne University, CNRS, Sigma Clermont. Institut Pascal, Clermont-Ferrand, France

12.10

OP-I-22

Danican A., Chezeau B., Fontaine J., Vial C.

CHARACTERIZATION OF THE LOCAL HYDROMECHANICAL STRESS THROUGH EXPERIMENTAL AND NUMERICAL ANALYSIS OF HYDRODYNAMICS UNDER DARK FERMENTATION OPERATING CONDITIONS

Clermont Auvergne University, CNRS, Sigma Clermont. Institut Pascal, Clermont-Ferrand, France

12.30 Lunch

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section I.

ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS

Chairperson: Professor Sascha Kersten, The Netherlands

14.00

OP-I-23

Dorokhov I., Hellgardt K., Hii K.K.(M)

SPATIALLY-RESOLVED REACTION CALORIMETRY WITH PACKED BED REACTOR

Imperial College London, London, United Kingdom

14.20

OP-I-24

Gomez N.^{1,2}, Vandewalle L.², Reyniers P.², Molina A.¹, Van Geem K.², Marin G.²

CAPTURING THE EFFECT OF PARTICLE CLUSTERS IN A DOWNFLOW REACTIVE SYSTEM VIA LARGE EDDY SIMULATIONS

¹National University of Colombia, Medellin, Colombia

²Ghent University, Laboratory for Chemical Technology, Ghent, Belgium

14.40

OP-I-25

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

¹Darmstadt University of Technology, Darmstadt, Germany

²Umicore AG & Co. KG, Hanau, Germany

³Fraunhofer ITWM, Kaiserslautern, Germany

Section III.

CHEMICAL REACTORS AND TECHNOLOGIES FOR TARGETED APPLICATIONS

15.00

OP-III-1

Rodriguez-Vega P., Ateka A., Aguayo A., Bilbao J.

DIRECT SYNTHESIS OF DIMETHYL ETHER (DME) from CO/CO₂ in a MEMBRANE REACTOR

University of the Basque Country UPV/EHU, Bilbao, Spain

15.20

OP-III-2

Ozturk N.F., Avci A.K.

INTENSIFIED DME PRODUCTION FROM SYNTHESIS GAS WITH CO₂

Bogazici University, Istanbul, Turkey

15.40 Coffee-break

Morning Session
RECTOR VERMEYLEN Hall

ORAL PRESENTATIONS

Section II.

**CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL
APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION**

Chairperson: Professor Choji Fukuhara, Japan

11.30

OP-II-20

Hernández-Ortiz J.C.¹, Van Steenberge P.¹, Duchateau J.², Toloza C.², Schreurs F.², Reyniers M.¹, Marin G.¹, D'hooge D.R.¹

MULTIPHASE REACTOR MODELING FOR REACTIVE PROCESSING OF POLYOLEFINES

¹*Ghent University, Ghent, Belgium*

²*SABIC Geleen, Geleen, The Netherlands*

11.50

OP-II-21

Nuñez Manzano M., Kulkarni S.R., Marin G.B., Nopens I., Heynderickx G.J., Van Geem K.

PROOF OF CONCEPT CFD STUDY OF POLYSTYRENE PYROLYSIS IN A GAS-SOLID VORTEX REACTOR

Ghent University, Ghent, Belgium

12.10

OP-II-22

Mohammad A.F.¹, El-Naas M.H.², Al-Marzouqi A.H.¹, Al-Marzouq M.H.¹, Suleiman M.I.³, Al-Musharfy M.³, Firmansyah T.³

CFD SIMULATION OF A NOVEL GAS-LIQUID REACTOR SYSTEM

¹*United Arab Emirates University, Al-Ain, United Arab Emirates*

²*Qatar University, Doha, Qatar*

³*ADNOC Refining Research Center, Abu Dhabi, United Arab Emirates*

12.30 Lunch

Afternoon Session
RECTOR VERMEYLEN Hall

ORAL PRESENTATIONS

Section II.

CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION

Chairperson: Professor Eugeniusz Molga, Poland

14.00

OP-II-23

Möller K., Khazali A.

X-GTL: A STUDY OF THE PROCESS OPTIONS USING A MULTI-PHASE PROCESS MODELLING FRAMEWORK

University of Cape Town, Cape Town, South Africa

14.20

OP-II-24

Ovchinnikova E.V., Chumachenko V.A., Andrushkevich T.V.

NICOTINIC ACID PRODUCTION AT ELEVATED β -PICOLINE LOADING: THEORETICAL STUDIES OF THE POSSIBILITY TO INTENSIFY THE PROCESS

Boreshkov Institute of Catalysis SB RAS, Novosibirsk, Russia

14.40

OP-II-25

Rebrov E.^{1,2}, Fernández-García J.², Matveeva V.¹, Cherkasov N.², Sulman E.¹

TRANSIENT OPERATION: A NOVEL WAY TO ENHANCE SELECTIVITY IN GLUCOSE ISOMERIZATION REACTION

¹*Tver Technical University, Tver, Russia*

²*University of Warwick, Coventry, United Kingdom*

15.00

OP-II-26

Chakraborty S., Paul S.K., Dutta S.K.

SPATIOTEMPORAL OSCILLATIONS IN BATCH REACTORS PROMOTE LIGNOCELLULOSIC BIOFUEL PRODUCTION

Indian Institute of Technology Kharagpur, Kharagpur, India

15.20

OP-II-27

Zagoruiko A.

LOW-TEMPERATURE CHEMISORPTION-ENHANCED CATALYTIC DECOMPOSITION OF HYDROGEN SULFIDE: THERMODYNAMIC ANALYSIS AND PROCESS CONCEPT

Boreshkov Institute of Catalysis SB RAS, Novosibirsk, Russia

15.40 Coffee-break

November 8, Thursday

Morning Session

REFTER Hall

ORAL PRESENTATIONS

Section III.

CHEMICAL REACTORS AND TECHNOLOGIES FOR TARGETED APPLICATIONS

Chairperson: Professor Klaus Möller, South Africa

10.00

OP-III-3

Currie R.¹, Nikolic D.², Petkovska M.², Simakov D.¹

CO₂ CONVERSION ENHANCEMENT IN A PERIODICALLY OPERATED SABATIER REACTOR: NONLINEAR FREQUENCY RESPONSE ANALYSIS AND SIMULATION-BASED STUDY

¹University of Waterloo, Waterloo, Ontario, Canada

²University of Belgrade, Belgrade, Serbia

10.20

OP-III-4

Lan L., Wang A., Wang Y.

APPLICATION OF DIELECTRIC-BARRIER DISCHARGES REACTOR in CO₂ HYDROGENATION

Dalian University of Technology, Dalian, China

10.40

OP-III-5

Moioli E., Gallandat N., Züttel A.

OPTIMAL REACTOR DESIGN for CO₂ METHANATION on Ru/Al₂O₃

Swiss Federal Institute of Technology in Lausanne, Lausanne, Switzerland

Empa Materials Science & Technology, Dübendorf, Switzerland

11.00 Coffee-break

Chairperson: Professor David Simakov, Canada

11.30

OP-III-6

Dubin Y.V.^{1,2}, Yazykov N.¹, Simonov A.¹, Yakovlev V.^{1,2}

COMBUSTION IN THE FLUIDIZED BED OF CATALYST AS AN EFFECTIVE METHOD OF OIL WASTE UTILIZATION

¹Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

²Novosibirsk State University, Novosibirsk, Russia

11.50

OP-III-7

Frassoldati A.¹, Cuoci A.¹, Saufi A.E.¹, Faravelli T.¹, Calabria R.², Chiariello F.², Massoli P.²
AN EXPERIMENTAL AND MODELLING STUDY OF FAST BIOMASS PYROLYSIS OIL DROPLET COMBUSTION

¹*Politecnico di Milano, Milan, Italy*

²*Istituto Motori, Department of Engineering, ICT and Technologies for Energy and Transportation, National Research Council of Italy, Napoli, Italy*

12.10

OP-III-8

Krasnikov D.V.¹, Iakovlev V.Ya.¹, Gilshteyn E.P.¹, Kopylova D.S.¹, Grebenko A.K.¹, Tsapenko A.P.¹, Nasibulin A.G.^{1,2}

THERMOPHORETIC DEPOSITION COMBINED WITH AEROSOL CVD SYNTHESIS OF SINGLE-WALLED CARBON NANOTUBES FOR THIN, CONDUCTIVE, AND TRANSPARENT FILMS OF EXCEPTIONAL CHARACTERISTICS

¹*Skolkovo Institute of Science and Technology, Moscow, Russia*

²*Aalto University, Espoo, Finland*

12.30 Lunch

**Afternoon Session
REFTER Hall**

ORAL PRESENTATIONS

Section III.

CHEMICAL REACTORS AND TECHNOLOGIES FOR TARGETED APPLICATIONS

Chairperson: Professor Ahmet Kerim Avci, Turkey

14.00

OP-III-9

Marathe P., Westerhof R., **Kersten S.**
PYROLYSIS OF LIGNIN: EFFECTS OF MOLECULAR WEIGHT AND BOND TYPE
University of Twente, Enschede, The Netherlands

14.20

OP-III-10

Hočevar B.^{1,2}, Huš M.¹, Grilc M.¹, Likožar B.¹
MUCIC ACID HYDRODEOXYGENATION OVER METAL CATALYSTS
¹*National Institute of Chemistry, Ljubljana, Slovenia*
²*University of Ljubljana, Slovenia*

14.40

OP-III-11

Möller K., Mhlongo M., Dalton R., Embling N., Collins R.

MULTI-PHASE, MULTI-SPECIES MODEL FOR THE CONVERSION OF RECYCLED PLASTIC TO DIESEL

University of Cape Town, Cape Town, South Africa

15.00

OP-III-12

Violet L., Mifleur A., Vanoye L., Favre-Réguillon A., Philippe R., Fongarland P.

CATALYTIC DEHYDROGENATION COUPLING OF ALCOHOLS TO ESTERS: MECHANISM AND KINETIC STUDIES FOR MODELLING PURPOSES

Laboratory of Catalytic Process Engineering, UMR CNRS-CPE-Lyon, University Lyon 1, Villeurbanne-Lyon, France

15.20

OP-III-13

Sulman A.¹, Matveeva V.^{1,2}, Lakina N.¹, Golikova E.¹, Sulman M.¹, Tikhonov B.¹, Sidorov A.¹, Sulman E.¹

MAGNETICALLY SEPARABLE BIOCATALYSTS BASED ON IMMOBILIZED ENZYMES

¹*Tver State Technical University, Tver, Russia*

²*Tver State University, Tver, Russia*

15.40

OP-III-14

Venezia B.¹, Ellis P.², Gavriilidis A.¹

CONTINUOUS CATALYTIC AEROBIC OXIDATION OF BENZYL ALCOHOL IN A SLURRY TUBE-IN-TUBE REACTOR USING Au-Pd/TiO₂ CATALYST

¹*Chemical Engineering Department, University College London, London, United Kingdom*

²*Johnson Matthey Technology Centre, Sonning Common, Reading, United Kingdom*

16.00

OP-III-15

Shivaprasad P., Patterson D., Jones M., Emanuelsson E.

PROCESS INTENSIFICATION OF ENZYME CATALYSED KINETIC RESOLUTION OF 1-PHENYLETHANOL IN A SPINNING MESH DISC REACTOR

University of Bath, Bath, United Kingdom

16.20 Closing

November 8, Thursday

**Morning Session
BLANCQUAERT Hall**

ORAL PRESENTATIONS

Section II.

CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN – NOVEL EXPERIMENTAL APPROACHES, MODELING, SCALE-UP AND OPTIMIZATION

Chairperson: Professor Saikat Chakraborty, India

10.00

OP-II-28

Cordero-Lanzac T., Aguayo A.T., Castaño P., Bilbao J.

MODELING THE CONVERSION OF DIMETHYL ETHER INTO OLEFINS CONSIDERING THE HZSM-5 BASED CATALYST DEACTIVATION

University of the Basque Country, Bilbao, Spain

10.20

OP-II-29

Santos E., Rijo B., Lemos M.A., Lemos F.

PLASTIC WASTE PYROLYSIS IN A SEMI-BATCH REACTOR

Instituto Superior Técnico, Lisboa, Portugal

10.40

OP-II-30

Freites Aguilera A.¹, Tolvanen P.¹, Leveneur S.^{1,2}, Mikkola J.^{1,3}, Marchant T.⁴, Salmi T.¹

MODELING OF MICROWAVE IRRADIATED AND HETEROGENEOUSLY CATALYSED EPOXIDATION OF VEGETABLE OILS

¹*Åbo Akademi University, Turku, Finland*

²*Rouen Normandie University, Saint-Étienne-du-Rouvray, France*

³*Umea University, Umeå, Sweden*

⁴*University of Wollongong, Wollongong, Australia*

11.00 Coffee-break

Chairperson: Dr. Dominique Richard, France

11.30

OP-II-31

Jokiel M.¹, Sundmacher K.^{1,2}

NOVEL REACTOR DESIGNS FOR THE HYDROFORMYLATION OF LONG-CHAIN OLEFINS: FLEXIBILITY AND AUTOMATION ASPECTS

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

²*Otto-von-Guericke University Magdeburg, Magdeburg, Germany*

Section IV.

ADVANCED PROCESSING OF CONVENTIONAL AND UNCONVENTIONAL HYDROCARBON FEEDSTOCKS

11.50

OP-IV-1

Song Y.¹, Marrodán L.², Vin N.¹, Herbinet O.¹, Assaf E.³, Fittschen C.³, Stagni A.⁴, Faravelli T.⁴, Alzueta M.U.², Battin-Leclerc F.¹

THE SENSITIZING EFFECTS OF NO₂ and NO ON METHANE LOW TEMPERATURE OXIDATION IN A JET STIRRED REACTOR

¹Reactions and Process Engineering Laboratory, CNRS, Lorraine University, Nancy, France

²University of Zaragoza, Zaragoza, Spain

³Université Lille, Lille, France

⁴Politecnico di Milano, Milan, Italy

12.10

OP-IV-2

Fedotov A.¹, Uvarov V.², Tsodikov M.¹

INNOVATIVE HYBRID MEMBRANE-CATALYTIC TECHNOLOGY FOR SYNGAS, HYDROGEN AND VALUABLE MONOMERS PRODUCTION

¹A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

²The Institute of Structural Macrokinetics, RAS, Moscow, Russia

12.30 Lunch

Afternoon Session BLANCQUAERT Hall

ORAL PRESENTATIONS

Section IV.

ADVANCED PROCESSING OF CONVENTIONAL AND UNCONVENTIONAL HYDROCARBON FEEDSTOCKS

Chairperson: Professor Vladimir Arutyunov, Russia

14.00

OP-IV-3

Cheula R.¹, Soon A.², Maestri M.¹

STRUCTURE-DEPENDENT MULTISCALE MODELLING OF CATALYTIC PROCESSES: AN APPLICATION TO THE CATALYTIC PARTIAL OXIDATION OF METHANE ON RHODIUM

¹Politecnico di Milano, Milan, Italy

²Yonsei University, Seoul, South Korea

14.20

OP-IV-4

Belinskaya N.S.¹, Ivanchina E.D.¹, Frantsina E.V.¹, Lutsenko A.S.¹, Nazarova G.Y.¹, Glik P.A.¹, Dementyev A.Y.²

PROGNOSTIC MODELLING OF DESTRUCTIVE PROCESSES OF HYDROCARBON FEEDSTOCK CONVERSION

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

²*PJSC "KINEF", Tomsk, Russia*

14.40

OP-IV-5

Maksimov A.L., Magomedova M.V., Peresyphkina E.G., Afokin M.I.

INTEGRATED TECHNOLOGY OF OLEFINS SYNTHESIS FROM DYMETHYL ETHER

A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

15.00

OP-IV-6

Mekki-Berrada A., Zani M., Souchon V., Pereira De Oliveira L.C., Chainet F.

COMPARATIVE STUDY OF THE SULFUR SPECIATION by GC and GC×GC for GAS OIL CHARACTERIZATION in HDT PROCESS SIMULATION

IFP Energies Nouvelles, Solaize, France

15.20

OP-IV-7

Madlokazi M.¹, Möller K.²

A THERMODYNAMICALLY CONSISTENT REACTOR MODEL FOR THE FURNACE BLACK PROCESS

¹*Orion Engineered Carbons, Port Elizabeth, South Africa*

²*University of Cape Town, Cape Town, South Africa*

15.40

OP-IV-8

Palos R., **Gutiérrez A.**, Castaño P., Azkoiti M.J., Arandes J.M., Bilbao J.

MODELING THE REMOVAL OF SULFUR, AROMATICS AND HEAVIER COMPOUNDS OF LIGHT CYCLE OIL

University of the Basque Country, Bilbao, Spain

REFTER Hall

16.20 Closing

CHEMREACTOR-23 Special Sessions
OUDE INFIRMERIE Hall

Oral presentations

BIOLEUM session

November 6, Tuesday, afternoon

Chairperson: Professor Wolter Prins, Belgium

14.00

Introduction to BIOLEUM: Kevin Van Geem 10 min

14.10

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

ON THE REACTIVITY OF MONO-LIGNOL DERIVATIVES

Ghent University, Ghent, Belgium

14.30

Kulkarni S.R., **Gonzalez Quiroga A.**, Heynderickx G.J., Van Geem K., Marin G.B.

EXPERIMENTAL DEMONSTRATION OF BIOMASS FAST PYROLYSIS IN THE GAS-SOLID VORTEX REACTOR

Ghent University, Ghent, Belgium

14.50

Kulkarni S.R., Schuerewegen C., Manzano M.N., Heynderickx G.J., Van Geem K., Marin G.B.

EXPERIMENTAL HEAT TRANSFER MODELLING IN A GAS-SOLID VORTEX UNIT

Ghent University, Ghent, Belgium

15.10

Pala M., Guo K., PrévotEAU A., Rabaey K., Ronsse F., Prins W.

ELECTROCHEMICAL UPGRADING OF FAST PYROLYSIS BIO-OIL

Ghent University, Ghent, Belgium

15.30

Jia C.¹, Bueken B.¹, Van Geem K.², De Vos D.¹

ISOLATION OF PHENOLICS FROM BIO-OIL USING FLEXIBLE MIL-53 AS HIGHLY SELECTIVE ADSORBENT

¹*Centre for Surface Chemistry and Catalysis K.U. Leuven, Leuven, Belgium*

²*Ghent University, Ghent, Belgium*

15.50

Boerjan W.

GENETIC ENGINEERING OF LIGNIN AMOUNT AND STRUCTURE TO IMPROVE BIOMASS PROCESSING

Ghent University, Ghent, Belgium

IMPROOF session
November 8, Thursday, afternoon

Chairperson: Dr. Marko Djokic, Belgium

14.00

Introduction to IMPROOF: Kevin Van Geem 10 min

14.10

Namysl S.¹, Pelucchi M.², Herbinet O.¹, Ranzi E.², Frassoldati A.², Faravelli T.², Battin-Leclerc F.¹
THE OXIDATION OF LINEAR C₄-C₆ ALDEHYDES: AN EXPERIMENTAL AND KINETIC MODELLING STUDY

¹*Reactions and Process Engineering Laboratory, CNRS, Lorraine University, Nancy, France*

²*Politecnico di Milano, Milan, Italy*

14.30

Pelucchi M.¹, Namysl S.², Herbinet O.², Frassoldati A.¹, Faravelli T.¹, Battin-Leclerc F.²
AN EXPERIMENTAL AND KINETIC MODELLING STUDY OF C₄-C₅ CARBOXYLIC ACIDS PYROLYSIS AND OXIDATION IN A JET STIRRED REACTOR

¹*Politecnico di Milano, Milan, Italy*

²*Reactions and Process Engineering Laboratory, CNRS, Lorraine University, Nancy, France*

14.50

Virgilio M.¹, Van Geem K.², Arts T.¹, Marin G.B.²
EXPERIMENTAL AERO-THERMAL INVESTIGATIONS OF SWIRLING FLOWS IN THREE-DIMENSIONAL RIBBED TUBES

¹*von Karman Institute for Fluid Dynamics, St. Gilles/Brussel, Belgium*

²*Ghent University, Ghent, Belgium*

15.10

Dedeyne J.N.¹, Virgilio M.², Arts T.², Van Geem K.¹, Marin G.B.¹
PROCESS INTENSIFICATION IN STEAM CRACKING: FLOW CHARACTERISTICS OF SPHERICAL DIMPLES

¹*Ghent University, Ghent, Belgium*

²*von Karman Institute for Fluid Dynamics, St. Gilles/Brussel, Belgium*

15.30

Vangaever S., Reyniers P., Heynderickx G.J., Van Geem K.
COMPUTATIONAL FLUID DYNAMIC-BASED STUDY OF THE STEAM CRACKING PROCESS USING A HYBRID 3D-1D APPROACH

Ghent University, Ghent, Belgium

15.50

Symoens S.¹, Djokic M.¹, Zhang J.¹, Bellos G.², Jakobi D.³, Weigandt J.³, Klein S.³, Battin-Leclerc F.⁴, Heynderickx G.¹, Thielen J.V.⁵, Cuenot B.⁶, Faravelli T.⁷, Theis G.⁸, Lenain P.⁹, Munoz A.E.¹⁰, Olver J.¹¹, Van Geem K.¹

"PAS DE DEUX" OF HIGH-TEMPERATURE ALLOY AND 3D REACTOR TECHNOLOGY FOR STEAM CRACKING COILS: IMPACT ON PRODUCT YIELDS AND COKE FORMATION

¹*Ghent University, Ghent, Belgium*

²*DOW Benelux B.V., Terneuzen, The Netherlands*

³*Schmidt + Clemens GmbH + CO. KG, Lindlar, Germany*

⁴*National Center for Scientific Research, Nancy, France*

⁵*CRESS B.V., Breskens, The Netherlands*

⁶*European Centre for Research and Advanced Training in Scientific Computation, Toulouse, France*

⁷*Politecnico di Milano, Milan, Italy*

⁸*John Zink International, Luxembourg SARL, Luxembourg*

⁹*Ayming France, Lyon, France*

¹⁰*AVGI, Ghent, Belgium*

¹¹*Emmisshield Inc, Blacksburg, Virginia, USA*

November 6, Tuesday
Afternoon Session

17.00

POSTER SESSION

FLASH PRESENTATIONS
REFTER Hall

Sanz O., Egaña A., Montes M.

FISCHER-TROPSCH SYNTHESIS INTENSIFICATION IN METALLIC FOAM STRUCTURES

University of the Basque Country, San Sebastián-Donostia, Spain

Méndez D., Cambra J.F., Barrio V.L.

POWER-TO-GAS: BIMETALLIC CATALYSTS SUPPORTED ON Al_2O_3 FROM A SULPHUR CONTAINING BIOGAS

University of the Basque Country, Bilbao, Spain

Lissens M., Mendes P.S., Sabbe M.K., Thybaut J.

METHANOL-TO-OLEFINS: A DETAILED DESCRIPTION FOR THE AROMATIC HYDROCARBON POOL

Ghent University, Ghent, Belgium

Bac S.¹, Say Z.², Bulutoglu P.¹, Ozensoy E.², **Avci A.K.**¹

CO₂ REFORMING OF GLYCEROL OVER Rh-BASED CATALYSTS

¹*Bogazici University, Istanbul, Turkey*

²*Bilkent University, Ankara, Turkey*

Rijo B.¹, Lemos F.¹, Fonseca I.², Vilelas A.³

STUDY OF DIFFERENT KINETIC EXPRESSIONS ON THE ACETYLENE HYDROGENATION

¹*Instituto Superior Técnico, Lisboa, Portugal*

²*Universidade Nova de Lisboa, Caparica, Portugal*

³*REPSOL Polímeros, Sines, Portugal*

Yamada H.¹, Kashifuku H.¹, Tagawa T.²

REACTION RATE ENHANCEMENT IN GAS-LIQUID-LIQUID-SOLID FOUR-PHASE CONTINUOUS FLOW REACTOR

Nagoya University, Nagoya, Japan

National Institute of Technology, Toyota College, Japan

Hao Z., Lapkin A.

AN EFFICIENT APPROACH TO KINETIC PARAMETER ESTIMATION THROUGH DYNAMIC-MODEL-BASED DESIGN OF EXPERIMENT

University of Cambridge, Cambridge, United Kingdom

Gavrilova N.N., **Myachina M.A.**, Ardashev D.V., Nazarov V.V., Skudin V.V.

SYNTHESIS OF MEMBRANE CATALYSTS BASED ON MESOPOROUS SUPPORT FOR DRY REFORMING OF METHANE

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

POSTER PRESENTATIONS

KAPITTELZAAL Hall

- PP-1** Aksenov D.G., Kodenev E.G., **Ovchinnikova E.V.**, Echevskii G.V., Chumachenko V.
PROCESSING of C4-FRACTION CONTAINED IN THE WASTE GASES OF REFINERIES BY CATALYTIC ISOMERISATION TO ISOBUTANE on Pd/SULFATED ZIRCONIA
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
- PP-2** Al-Dalama K.
INCREASING THE EFFICIENCY OF THE HDS PROCESS BY THE MODIFICATION OF Ni/Mo/W HYDROTREATING CATALYST SUPPORTED ON MODIFIED SUPPORTS
Kuwait Institute For Scientific Research, Kuwait City, Kuwait
- PP-3** **Alghamdi N.**, Bavykina A., Gascon J., Sarathy S.
MODELING CO₂ to METHANOL CONVERSION IN A STAGNATION FLOW REACTOR
King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia
- PP-4** **Authayanun S.**¹, Saebea D.², Patcharavorachot Y.³, Arpornwichanop A.⁴
MODEL BASED EVALUATION OF ALKALINE ANION EXCHANGE MEMBRANE FUEL CELLS WITH UNBALANCED PRESSURE OPERATION
¹*Srinakharinwirot University, Nakhon Nayok, Thailand*
²*Burapha University, Chonburi, Thailand*
³*King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*
⁴*Chulalongkorn University, Bangkok, Thailand*
- PP-5** Bac S.¹, Say Z.², Bulutoglu P.¹, Ozensoy E.², **Avci A.K.**¹
CO₂ REFORMING OF GLYCEROL OVER Rh-BASED CATALYSTS
¹*Bogazici University, Istanbul, Turkey*
²*Bilkent University, Ankara, Turkey*
- PP-6** Bazaikin Y.^{1,3}, Malkovich E.^{1,3}, Okunev A.^{1,2}, **Derevschikov V.**^{2,3,4}
NEW MODELS FOR THE DESCRIPTION OF SORPTIVE AND TEXTURAL PROPERTIES OF CaO-BASED SORBENTS CHANGING DURING REPETITIVE SORPTION/REGENERATION CYCLES
¹*Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia*
²*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
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- PP-87 Yemelyanova V.S., Dossumova B.T., Shakiyev E.M., Baizhomartov B.B., Shakiyeva T.V.**
ELECTROPHYSICAL METHODS OF PRE-TREATMENT OF SEEDS
"Scientific and Production Technical Center "Zhalyn" LLP, Almaty, Kazakhstan
- PP-88 Yemelyanova V.S., Dossumova B.T., Shakiyev E.M., Baizhomartov B.B., Shakiyeva T.V., Kalinichenko O.G.**
MAGNETIC ENRICHMENT OF SLUDGE WASTE FROM TPP TO OBTAIN A CONCENTRATE OF RARE AND SCATTERED ELEMENTS
"Scientific and Production Technical Center "Zhalyn" LLP, Almaty, Kazakhstan
- PP-89 Zaichenko A., Podlesniy D.N., Zhirnov A.A., Salganskaya M.V., Tsvetkov M.V., Polianczyk E.V.**
CONVERSION OF HYDROCARBON LIQUIDS TO SYNTHESIS GAS BY PARTIAL OXIDATION IN A MOVING BED REACTOR
Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow region, Russia
- PP-90 Rodikova Y., Zhizhina E., Gogin L. Pai Z.**
EFFICIENT TWO-PHASE PROCESSES OF OXIDIZING SUBSTITUTED ALKYLPHENOLS INTO THE CORRESPONDING PARA-QUINONES IN THE PRESENCE OF HETEROPOLY ACID SOLUTIONS
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
- PP-91 Zagoruiko A.^{1,2}, Mikenin P.¹, Lopatin S.¹, Golyashova K.^{1,2}**
SO₂ OXIDATION IN STRUCTURED CATALYTIC CARTRIDGES WITH GLASS-FIBER CATALYST FOR CONDITIONING OF FLUE GASES FROM COAL-FIRED POWERPLANTS
¹*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*
²*Novosibirsk State University, Novosibirsk, Russia*
- PP-92 Krivtsova K.B., Mityanina O.E.**
FUTURE DEVELOPMENT OF UPGRADING PROCESSES FOR HEAVY OIL FEEDSTOCKS
National Research Tomsk Polytechnic University, Tomsk, Russia

VIRTUAL PRESENTATIONS

VP-1. Aliyev G.S., Nagiyeva R.N.

MODELING OF ISOTHERMAL ADSORPTION OF SULPHANOL ON THE QUARTZ SAND

Institute of Catalysis and Inorganic Chemistry named after Academician M.F. Nagiyev, Baku, Azerbaijan

VP-2. Bykov V.I., Tsybenova S.B., Lomakin S.M., Varfolomeev S.D.

MATHEMATICAL MODELING OF PYROLYSIS IN TUBULAR REACTORS OF VARIOUS TYPES

Emanuel Institute of Biochemical Physics RAS, Moscow, Russia

VP-3. Chernyshev D.O., Dubrovsky V., Nechepurenko N., Varlamova E., Suchkov Y., Staroverov D.V.

INVESTIGATION OF THE CATALYTIC EFFICIENCY OF COBALT AND NICKEL PYROPHOSPHATES IN THE PROCESS OF DEHYDRATION OF METHYL LACTATE

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-4. Dossumov K.¹, Yergaziyeva G.², Tairabekova S.Zh.², Churina D.H.¹, Telbayeva M.²

CATALYSIS OF TRANSFORMATION OF BIOETHANOL TO ACETALDEHYDE AND HYDROGEN

¹*Center of Physical and Chemical Methods of Research and Analysis, Almaty, Kazakhstan*

²*Institute of Combustion Problems, Almaty, Kazakhstan*

VP-5. Enikeeva L.¹, Khursan S.², Gubaydullin I.^{1,3}

MATHEMATICAL MODELING OF INTRAMOLECULAR TRANSFORMATIONS OF ORTHO-SUBSTITUTED AROMATIC NITROSO OXIDES

¹*Ufa State Petroleum Technological University, Ufa, Russia*

²*Ufa Institute of Chemistry RAS, Ufa, Russia*

³*Institute of Petrochemistry and Catalysis RAS, Ufa, Russia*

VP-6. Knyazev D., Chernyshev D., Dubrovsky V., **Varlamova E.**, Makarov M., Kozlovsky R.

THE STUDIED OF ALTERNATIVE METHOD FOR PRODUCTION OF ACRYLIC ACID BY DEHYDRATION OF BUTYL LACTATE

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-7. Kozlovskiy R., Luganskiy A., Zolotareva M., Suchanova M., Dyagileva A.

RESEARCH OF DIESEL FUEL CLEANING ON THE ALUMINOSILICATE ADSORBENT

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-8. Kukueva V.V.

PREDICTIONS OF CHEMICAL REACTIVITY BY THEORETICAL CALCULATIONS

State Institution "Institute of Environmental Geochemistry", Kiev, Ukraine

VP-9. Menshchikova A., **Varlamova E.**, Filatova E., Suchkov Y.

PRODUCTION OF PLASTICIZERS BASED ON SUCCINIC ACID AND 2-ETHYLHEXANOL AND CYCLOHEXANOL

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-10. Shulyaka S.E., Sinitin S.A., Bukharkina T.V.

XYLENES OXIDATION IN THE PRESENCE OF TRANSITION METALS SALTS MIXTURE

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-11. Polovinkin M.A.¹, Kostiuchenko V.V.¹, Gavrilov Y.V.¹, **Sinitsin S.A.¹**, Danilov E.A.², Cheblakova E.G.², Vodoleyev V.V.³

SYNTHESIS AND EXTRUSION MOLDING OF Fe-Mo CATALYST FOR OXIDATIVE DEHYDROGENATION OF METHANOL TO FORMALDEHYDE

¹*D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia*

²*State Research Institute for Graphite-Based Structural Materials, Moscow, Russia*

³*JSC Tehmetall-2002, Kirovograd, Russia*

VP-12. Staroverov D., Zudilin D.M., Efimov I.V., Makarov M.G.

INFLUENCE OF PALLADIUM CONTENT ON THE ACTIVITY AND STABILITY OF THE CATALYST OF THE BENZYL ALCOHOL AQUEOUS ALKALINE OXIDATION

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-13. Zhila M., Sapunov V., Voronov M., Shpakova P., Gladysheva A.

MODIFIED FATTY ACID METHYL ESTERS DISTILLATION BOTTOMS AS A NOVEL STABILIZER FOR POLYMER COMPOSITIONS

D. Mendeleev University of Chemical Technology of Russia, Moscow, Russia

VP-14. Bachurikhin A.¹, Efendiev M.²

ELECTROMAGNETIC INSTALLATION FOR NEUTRALIZATION OF WASTEWATER PRODUCTION OF OLIVE OILS

¹*Gubkin I.M. Russian State University of Oil and Gas, Moscow, Russia,*

²*OJSC DagNefteProduct, Makhachkala City, Russia*

XXIII International Conference on Chemical Reactors CHEMREACTOR-23, Ghent, Belgium, November 5-9, 2018

Nov 4, Sunday	November 5, Monday		November 6, Tuesday		November 7 Wednesday		November 8, Thursday		Nov 9, Friday	Nov 10, Saturday	
	08.45	Opening						08.45	MaCKiE Opening		
Registration, from 12.00 17.00 Boat trip "Ghent completely"	09.00	PL-1 Nørskov		PL-3 Vlachos		PL-5 Sundmacher		09.00	MaCKiE PL Green		
	10.00	PL-2 Balakotaiah		PL-4 Sadler		KL-5 Cuenot		10.00	OP-III-3 Simakov	OP-II-28 Cordero-Lanzac	
						KL-6 Van Goethem		10.20	OP-III-4 Wang	OP-II-29 Rijo	
	11.00	Coffee break						10.40	OP-III-5 Moiola	OP-II-30 Tolvanen	
	11.30	KL-1 Mavrikakis		KL-3 Molga		11.30	OP-I-20 Castillo-Araiza	OP-II-20 Van Steenberge	Coffee break		
						11.50	OP-I-21 Vial	OP-II-21 Nunez Manzano	11.30	OP-III-6 Dubinin	OP-II-31 Jokiel
	12.00	KL-2 Lopes		KL-4 Montes		12.10	OP-I-22 Danican	OP-II-22 Mohammad	11.50	OP-III-7 Frassoldati	OP-IV-1 Song
	12.30	Lunch						12.10	OP-III-8 Krasnikov	OP-IV-2 Fedotov	
	14.00	OP-I-1 Constales	OP-II-1 Bac	OP-I-12 Gavrilova	OP-II-12 Snytnikov	14.00	OP-I-23 Dorokhov	OP-II-23 Möller	Lunch		
	14.20	OP-I-2 Quaglio	OP-II-2 Ambrosetti	OP-I-13 Sinev	OP-II-13 He	14.20	OP-I-24 Gomez	OP-II-24 Ovchinnikova	14.00	OP-III-9 Kersten	OP-IV-3 Maestri
	14.40	OP-I-3 Till	OP-II-3 Groppi	OP-I-14 Potemkin	OP-II-14 Cherkasov	14.40	OP-I-25 Greiner	OP-II-25 Rebrov	14.20	OP-III-10 Hočevnar	OP-IV-4 Belinskaya
	15.00	OP-I-4 Slinko	OP-II-4 Šourek	OP-I-15 Li	OP-II-15 Guffanti	15.00	OP-III-1 Rodriguez-Vega	OP-II-26 Chakraborty	14.40	OP-III-11 Mhlongo	OP-IV-5 Maksimov
	15.20	OP-I-5 Yablonsky	OP-II-5 Vernikovskaya	OP-I-16 Ye	OP-II-16 Banzaraktsaeva	15.20	OP-III-2 Ozturk	OP-II-27 Zagoruiko	15.00	OP-III-12 Violet	OP-IV-6 Mekki-Berrada
	15.40	Coffee break						15.20	OP-III-13 Sulman A.	OP-IV-7 Madlokazi	
	16.00	OP-I-6 Kolb	OP-II-6 Minette	OP-I-17 Bracconi	OP-II-17 Driessen	16.30 Excursion around Ghent		15.40	OP-III-14 Venezia	OP-IV-8 Gutiérrez	
	16.20	OP-I-7 Standl	OP-II-7 Claes	OP-I-18 Uglietti	OP-II-18 Fernengel			16.00	OP-III-15 Shivaprasad		
	16.40	OP-I-8 Petrov	OP-II-7 Boon	OP-I-19 Donaubaauer	OP-II-19 Richard			16.20	Closing		
17.00	OP-I-9 Alvarado Camacho	OP-II-9 Zazhigalov	17.00 Flash presentations Poster Session Beer Reception		17.30 Evening overview of Brussels Time for beer bars						
17.20	OP-I-10 Chizhik	OP-II-10 Bremer									
17.40	OP-I-11 Arutyunov	OP-II-11 Fukuhara									
19.00	Welcome Reception				20.00 Banquet						

November 6-BIOLEUM & November 8-IMPPOOF Special Sessions

**MaCKiE,
09.00 Excursion to Brugge**

09.00 Excursion to Antwerpen

Section I. ADVANCES IN CHEMICAL REACTOR FUNDAMENTALS
Section II. CHEMICAL REACTION ENGINEERING AND REACTOR DESIGN

Section III. CHEMICAL REACTORS AND TECHNOLOGIES FOR TARGETED APPLICATIONS
Section IV. ADVANCED PROCESSING OF HYDROCARBON FEEDSTOCKS



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ABSTRACTS



<http://catalysis.ru/resources/institute/Publishing/Report/2018/Abstracts-Chemreactor-23.pdf>