

CONFERENCE PROGRAMME

15 – 17 May 2023

DECHEMA-Haus · Frankfurt/Main · Germany

Annual Meeting on Reaction Engineering 2023

www.dechema.de/react_2023



GENERAL INFORMATION

VENUE

DECHEMA-Haus
Theodor-Heuss-Allee 25
60486 Frankfurt / Main

INTERNET ACCESS

WiFi access is available for free throughout the conference venue. As WiFi can be used by all participants, a loss of efficiency is possible.

Network: **DECHEMA Foyer** or **Max Buchner Foyer**
Password: **DECHEMA14**

BOOK OF ABSTRACTS

A book of abstracts from all lectures and posters is available online for all participants of the meeting at www.dechema.de/react2023_BOA

OFFICE HOURS CONFERENCE DESK

Monday, 15 May 2023	10:00 – 18:00
Tuesday, 16 May 2023	08:30 – 17:30
Wednesday, 17 May 2023	08:30 – 14:00

ORGANISER

DECHEMA-Haus
Theodor-Heuss-Allee 25
60486 Frankfurt / Main

CONTACT

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CONTENTS

PLENARY LECTURES

4

SCIENTIFIC COMMITTEES

4

CONFERENCE DINNER

5

SPONSORS / EXHIBITORS

6

PROGRAMME AT A GLANCE

10

LECTURE PROGRAMME

12

Monday, 15 May 2023

12

Tuesday, 16 May 2023

13

Wednesday, 17 May 2023

14

POSTER PROGRAMME

16

PLENARY LECTURES / COMMITTEES

PLENARY LECTURES

Digitalization in Catalysis and Reaction Engineering: More than just a Buzzword

Prof. Dr. Olaf Deutschmann, Karlsruhe Institute of Technology
Dr. Stephan Andreas Schunk, hte GmbH & BASF SE

Adventures in computer generated microkinetic mechanisms

Prof. C. Franklin Goldsmith, Brown University, Providence Rode Island, USA

Cellulosic Ethanol a Key Intermediate for Sustainable Mobility and Chemical Production

Dr. Henning Marckmann, Clariant AG

SCIENTIFIC COMMITTEE

Dr. Jonathan Bloh	DECHEMA Forschungsinstitut, Frankfurt
Dr. Marion Börnhorst	TU Dortmund (Representative of NaWuRet)
Prof. Markus Busch	TU Darmstadt
Dr. Kai Ehrhardt	BASF SE, Ludwigshafen
Prof. Hannsjörg Freund	TU Dortmund
Dr. Jens Friedland	University of Ulm (Representative of NaWuRet)
Prof. Olaf Hinrichsen	TU München
Prof. Elias Klemm	University of Stuttgart
Prof. Ulrike Krewer	Karlsruhe Institute of Technology
Dr. Ricarda Leiberich	Lanxess
Dr. Stefan Palkovits	RWTH Aachen University
Prof. Jörg Sauer (Chairman)	Karlsruhe Institute of Technology
Dr. Kristina Schiffer	CLARIANT, Frankfurt
Prof. Thomas Turek	TU Clausthal
Dr. Olaf Wachsen	formerly CLARIANT
Prof. Gregor Wehinger	TU Clausthal
Prof. Horst-Werner Zanhoff	Evonik Operations GmbH, Marl

CONFERENCE DINNER

TUESDAY, 16 MAY 2023

18:30 – 22:30

CONFERENCE DINNER

The conference dinner will take place at **ALEX Frankfurt Skyline Plaza**.

The evening will start with a reception on the restaurant's terrace with an impressive view on the surrounding skyscrapers. You will meet all colleagues in a relaxed atmosphere to continue your discussions and increase networking.

The restaurant provides us a delicious buffet dinner to meet the taste of every participant (also vegetarian and vegan options will be available).

Food & beverages are included in dinner ticket. Please book a ticket in advance.

Address:

Skyline Plaza
Europa-Allee 6
60327 Frankfurt am Main

Access via the shopping center. Please take the elevator and go to the top floor.



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REACNOSTICS is modeling, constructing and building chemical research reactors for the spatially resolved investigation of catalytic processes. Our methodology comprises simulations and operando measurements of concentration & temperature profiles in combination with spectroscopic catalyst characterization. By applying patented methods we provide insight in catalytic reactors during time on stream required for knowledge based optimization.

www.reacnistics.com

EXHIBITORS

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EXHIBITORS

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www.fluitec.ch

GAS
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Global Analyser Solutions is the unique branding Interscience uses for its turnkey products for the Energy market. GAS offers custom configured GC analysers for complex separations and data processing. Online analysers are available for various applications, like fast monitoring of chemical processes, catalyst screening, reactor analysis and air monitoring. The efficient configurations are based on proven GC technology, resulting in robust instruments with an optimal return on investment.

www.gassite.com

magritek

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www.magritek.com

EXHIBITORS



Microinnova is an industry leader in flow chemistry and an expert in continuous manufacturing solutions and modular plant design. We provide process development and realize plants for efficient, continuous processes in the fields of synthesis, workup, and formulation. Based on nearly 20 years of experience in process intensification and more than 200 successfully completed projects, we are the partner of choice for your continuous manufacturing program.

<https://microinnova.com>



For over 60 years Micromeritics Instrument Corporation (Georgia, USA) is a global provider of advanced solutions for material characterization with market-leading instrumentation and application expertise in the core areas: density; surface area and porosity; particle size; powder and catalyst characterization and process development as well as net-zero technologies. Contract testing is offered via the Particle Testing Authority located in Norcross (USA), Munich (Germany) and Shanghai (China).

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- » Life Science and Biotechnology
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EXHIBITORS/SUPPORTER



Parr Instrument (Deutschland) GmbH was founded in 1993. We are worldwide the only subsidiary of Parr Instrument Company, IL, USA. Parr designs and manufactures pressure reactors and tubular reactors in a variety of special alloys and sizes for the study of catalytic and non-catalytic reactions in batch, continuous-flow, and multiple/parallel operation for the chemical, polymer, biofuels, hydrometallurgical, pharmaceutical, petroleum, and petrochemical industries. Parr has an extensive line of sample preparation vessels and is also specialized in Combustion Calorimeters.

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SUPPORTER



The Royal Society of Chemistry (RSC) is a global, not-for-profit publisher with over 50 transformative and open access journals. We recently committed to publishing our fully-owned journals 100% Open Access by 2028.

Our key titles include *Reaction Chemistry & Engineering* reporting cutting-edge chemical engineering and chemistry research towards enhancing the understanding and efficiency of reactions, and *RSC Sustainability*, dedicated to solving sustainability challenges for a greener future.

RSC.org

PROGRAMME AT A GLANCE

Monday, 15 May 2023	
12:00	Registration & Lunch Max Buchner Hall
13:00	Welcome Address Jörg Sauer
13:05	PLENARY LECTURE C. Franklin Goldsmith
Chair:	Kai Ehrhardt
13:50	Bjarne Kreitz
14:15	Christof Hamel
14:40	COFFEE BREAK IN EXHIBITION AREA
Chair:	Marion Börnhorst
15:10	David Kellermann
15:35	Carlos Alvarado-Camacho
16:00	Martin Kutscherauer
16:25	Short Presentations of the Exhibitors
16:45	Short Introduction of Poster Programme
17:00	Poster Party (17:00 – 19:00)

PROGRAMME AT A GLANCE

Tuesday, 16 May 2023	
	Max Buchner Hall
Chair:	Stefan Palkovits
09:00	PLENARY LECTURE Olaf Deutschmann, Stephan Schunk
10:00	Aleksandr Fedorov
10:25	Martin Votsmeier
10:50	COFFEE BREAK IN EXHIBITION AREA
Chair:	Jens Friedland
11:20	Lukas Wehrle
11:45	Inga Dorner
12:10	Fridolin Röder
12:35	LUNCH BREAK IN EXHIBITION AREA
Chair:	Gregor Wehinger
13:35	Theresa Overbeck
14:00	Leon Rousseau
14:25	Hans-Jörg Zander
14:50	Luisa Peterson
15:15	COFFEE BREAK AND POSTER DISCUSSIONS IN EXHIBITION AREA
16:30	General Assembly of the Subject Section „Chemical Reaction Engineering“ (open to all interested attendees) (16:30 – 17:45)
18:30	Conference Dinner (18:30 – 22:30)

Wednesday, 17 May 2023	
	Max Buchner Hall
Chair:	Horst Zanthoff
09:00	Asem Al-Shabani
09:25	Thomas Cholewa
09:50	Dorela Dhamo
10:15	Hendrik Held
10:40	Andres Aquino
11:05	COFFEE BREAK IN EXHIBITION AREA
Chair:	Markus Busch
11:35	Leonard Both
12:00	Jakob Albert
12:25	Poster Awards & Young Talent Award
Chair:	Jonathan Bloh
12:45	PLENARY LECTURE Henning Marckmann
13:30	Closing Olaf Wachsen
13:35	End of Meeting and Lunch

PROGRAMME

Monday, 15 May 2023

- 12:00 Registration & Lunch
- 13:00 **WELCOME ADDRESS**
J. Sauer, KIT, Eggenstein-Leopoldshafen
Chair: J. Sauer, KIT, Eggenstein-Leopoldshafen
- 13:05 **PLENARY LECTURE**
Adventures in computer generated microkinetic mechanisms
F. Goldsmith¹; ¹ Brown University, Providence/USA
Chair: K. Ehrhardt, BASF, Ludwigshafen
- 13:50 **Automated Generation of Reaction Mechanisms for the Fischer-Tropsch Synthesis**
B. Kreitz¹; F. Goldsmith¹; ¹ Brown University, Providence/USA
- 14:15 **Mechanistic Kinetic Modelling in Homogeneous and Bio Catalysis – Potential and Application**
M. Gerlach¹; S. Kirschtowski¹; W. Kortuz¹; I. Müller²; I. Potratz²; C. Hamel³; ¹ Otto von Guericke University Magdeburg, Magdeburg/D; ² Hochschule Anhalt, Köthen/D; ³ Otto von Guericke University / Anhalt University of Applied Sciences, Magdeburg/D
- 14:40 **Coffee Break in Exhibition Area**
Chair: M. Börnhorst, TU Dortmund
- 15:10 **Dynamically Operated Fixed Bed Reactors for CO₂ Methanation: Strategies to Mitigate Catalyst Deactivation**
D. Kellermann¹; M. Langer¹; H. Freund¹; ¹ Technische Universität Dortmund, Dortmund/D
- 15:35 **Propylene oligomerization over an sPA catalyst: industrial reactor modelling**
C. Alvarado-Camacho¹; J. Poissonnier¹; M. Herrero-Manzano¹; J. W. Thybaut¹; ¹ Ghent University, Ghent/B
- 16:00 **Improvement of pseudo-continuum reactor models for maleic anhydride production based on particle resolved CFD simulations**
M. Kutscherauer¹; S. Anderson¹; G. Mestl²; S. Böcklein²; T. Turek¹; G. Wehinger¹; ¹ Clausthal University of Technology, Clausthal-Zellerfeld/D; ² Clariant AG, Heufeld/D
- 16:25 **Short Presentations of the Exhibitors**
- 16:45 **Short Introduction of Poster Programme**
E. Moioli, Hitachi Zosen Inova, Zurich
- 17:00 **POSTER PARTY** (17:00 – 19:00)

PROGRAMME

Tuesday, 16 May 2023

Chair: S. Palkovits, RWTH Aachen

- 09:00 **Digitalization in Catalysis and Reaction Engineering: More than just a Buzzword**
O. Deutschmann¹; S. Schunk²; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D; ² hte GmbH, Heidelberg/D
- 10:00 **Machine learning for small data: Accelerated kinetic model development for CO₂ hydrogenation into hydrocarbons**
A. Fedorov¹; A. Perechodnik¹; D. Linke¹; ¹ Leibniz-Institut für Katalyse e.V., Rostock/D
- 10:25 **Physics-informed Neural Networks for Reactor Simulations**
K. Wilhelm¹; F. Döppel¹; M. Votsmeier²; ¹ Technical University of Darmstadt, Darmstadt/D; ² Technical University of Darmstadt; Umicore AG & Co. KG, Darmstadt/D
- 10:50 **Coffee Break in Exhibition Area**
Chair: J. Friedland, University of Ulm
- 11:20 **Evaluating high power density direct ammonia SOFC/GT hybrid systems as a pathway to decarbonize the mobility sector**
L. Wehrle¹; A. Ashar²; O. Deutschmann¹; R. Braun²; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D; ² Colorado School of Mines, Golden/USA
- 11:45 **Critical Role of Flooding Degree in Silver Gas Diffusion Electrodes for Electrochemical CO₂ Reduction**
I. Dorner¹; P. Röse¹; J. Osiewacz²; B. Ellendorff²; T. Turek²; U. Kremer¹; ¹ Karlsruhe Institute of Technology; ² Clausthal University of Technology
- 12:10 **Novel methods to accelerate the identification of degradation models for batteries**
F. Röder¹; F. Schomburg¹; S. Ramasubramanian¹; ¹ University of Bayreuth, Bayreuth/D
- 12:35 **Lunch Break in Exhibition Area**
Chair: G. Wehinger, TU Clausthal
- 13:35 **Three-dimensional single pellet model for the reaction-diffusion mechanisms during reduction and carburization of iron oxide**
T. Overbeck¹; M. Hensmann¹; G. Wehinger²; ¹ VDEh Betriebsforschungsinstitut GmbH, Düsseldorf/D; ² Clausthal University of Technology, Clausthal-Zellerfeld/D
- 14:00 **Enhanced heat management in 3D printed catalyst structures: from CFD modelling to experimental demonstration**
L. Rousseau¹; I. Roghair¹; M. van Sint Annaland¹; ¹ Eindhoven University of Technology/NL
- 14:25 **Linde Engineering 3D Furnace Model for Reformer and Cracker Applications**
H. Zander¹; K. Nicholson²; ¹ Linde GmbH, Linde Engineering, Pullach/D; ² Linde Engineering North America LCC, Tonawanda (NY)/USA
- 14:50 **Hybrid modeling of the catalytic CO₂ methanation using process data and mechanistic knowledge**
L. Peterson¹; J. Bremer²; K. Sundmacher³; ¹ Max Planck Institute of Complex Technical Systems, Magdeburg/D; ² Clausthal University of Technology, Clausthal-Zellerfeld/D; ³ Otto von Guericke University Magdeburg; Max Planck Institute for Dynamics of Complex, Magdeburg/D
- 15:15 **Coffee Break and Poster Discussions in Exhibition Area**
- 16:30 **General Assembly of the Working Group Reaction Engineering**
open to all interested attendees (16:30 – 17:45)

PROGRAMME



Wednesday, 17 May 2023

Chair: H. Zanthoff, Evonik Operations GmbH, Marl

- 09:00 Rh-catalyzed but-1-ene hydroformylation in a continuously operated gas-phase membrane reactor
A. Al-Shabani¹; M. Schörner¹; L. Arsenjuk²; R. Franke³; M. Haumann¹; ¹Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen/D; ² Evonik Operations GmbH, Marl/D; ³ Evonik Operations GmbH | Ruhr-Universität Bochum, Marl | Bochum/D
- 09:25 Kinetic investigation of ruthenium catalyst for ammonia synthesis using an in situ adsorption enhanced process
T. Cholewa¹; O. Salem²; A. Schaadt²; R. Güttel³; ¹Fraunhofer Institut für Solare Energiesysteme ISE, Freiburg im Breisgau/D; ²Fraunhofer Institute for Solar Energy Systems ISE, Freiburg/D; ³Universität Ulm, Ulm/D
- 09:50 Sustainable Aviation Gasoline via Power-to-Liquid Route: Coupling of High-Temperature Fischer-Tropsch Synthesis and Isomerization Reaction
D. Dhamo¹; S. Lüttin¹; M. Rubin¹; R. Dittmeyer¹; ¹Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
- 10:15 A Comprehensive Approach for Bottleneck Identification in Trickle Bed Reactors for the Liquid Phase Hydrogenation of Viscous Aromatic Derivatives on Egg-Shell Catalysts
H. Heldt¹; H. Freundt¹; ¹Technische Universität Dortmund, Lehrstuhl Reaction Engineering and Catalysis, Dortmund/D
- 10:40 Liquid Phase Epoxidation of Propylene to Propylene Oxide with Hydrogen Peroxide on Titanium Silicalite-1: Spatially Resolved Measurements and Numerical Simulations
A. Aquino¹; R. Horn¹; O. Korup¹; ¹Hamburg University of Technology, Hamburg/D
- 11:05 Coffee Break in Exhibition Area
Chair: M. Busch, TU Darmstadt
- 11:35 Depolymerization of synthetic fibres and recovery of terephthalic acid
L. Both¹; ¹RITTEC Umwelttechnik GmbH / TU Braunschweig, Braunschweig/D
- 12:00 Sensitivity analysis and parameter optimisation for the fractionative catalytic conversion of lignocellulosic biomass
J. Albert¹; A. Bukowski¹; K. Schnepf²; S. Wesinger¹; A. Brandt-Talbot³; ¹Universität Hamburg (UHH), Hamburg/D; ²FAU Erlangen-Nürnberg, Erlangen/D; ³Imperial College, London/UK
- 12:25 POSTER AWARDS & YOUNG TALENT AWARD
Chair: J. Sauer, O. Wachsen
- 12:45 PLenary Lecture
Cellulosic Ethanol a Key Intermediate for Sustainable Mobility and Chemical Production
H. Marckmann¹; ¹CLARIANT, Planegg/D
- 13:30 Closing
Chair: O. Wachsen
- 13:35 End of Meeting and Lunch (13:35 – 14:30)

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Fundamental questions
Elemental answers

POSTER

POSTER

DIGITISATION IN REACTION ENGINEERING

- P 1.01 **Digitalization in Electrochemical Reaction Engineering: Accelerated Workflow for Simulation of Solid Oxide Cells (SOCs)**
P. Jägerfeld¹; J. Riedel¹; H. Gossler²; L. Wehrle¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D; ² omegadot software & consulting, Limburgerhof/D
- P 1.02 **Exploration of the chemical reaction space through selectively accelerated reactive molecular dynamics without prior knowledge**
M. Papusha¹; C. Huang¹; J. Kiecherer²; K. Leonhard¹; ¹ RWTH Aachen University, Aachen/D; ² Covestro Deutschland AG, Leverkusen/D
- P 1.03 **Experiment & Modelling in a Digital Twin Approach for Re-initiated Oxygen inhibited RAFT Polymerisation**
E. Pashayev¹; F. Kandelhard¹; P. Georgopanos¹; ¹ Helmholtz-Zentrum Hereon, Geesthacht/D
- P 1.04 **Machine learning methods for the classification and prediction of gas-liquid flow regimes in micro reactors**
S. Haase¹; H. May¹; A. Hiller¹; M. Schubert¹; ¹ Technische Universität Dresden/D

MODELL DEVELOPMENT FOR COMPLEX REACTION KINETICS

- P 2.01 **Identification of Kinetic Parameters for Microkinetic Models by Chemical Reaction Neural Networks (CRNNs)**
H. Stagge¹; ¹ Universität Ulm, Ulm/D

PROCESSES FOR THE USE OF NEW, SUSTAINABLE RAW MATERIALS

- P 3.01 **Catalyst Testing for Methanol Production using Alternative Synthesis Gases generated from Steel-Mill-Gases**
K. Girod¹; S. Kaluza²; H. Lohmann¹; S. Schlüter¹; ¹ Fraunhofer UMSICHT, Oberhausen/D; ² Hochschule Düsseldorf, Düsseldorf/D
- P 3.02 **Life Cycle Assessment of the production of Vanillin from Lignin by homogeneous oxidative depolymerization (POMLig)**
S. Wesinger¹; M. Papajewski¹; J. Albert¹; ¹ Universität Hamburg (UHH), Hamburg/D
- P 3.03 **Continuous flow synthesis of the alternative platform molecule 5-chloromethyl furfural**
F. Schael¹; B. Steup¹; P. Rojahn¹; K. Nigam²; ¹ Hochschule Darmstadt, Darmstadt/D; ² Indian Institute of Technology, New Delhi/IND
- P 3.04 **Electrochemical Ethanol Oxidation using RuO₂-based Catalysts**
I. Kohlhaas¹; N. Kurig¹; R. Palkovits¹; ¹ RWTH Aachen University, Aachen/D
- P 3.05 **CO₂-free Hydrogen Production by Pyrolysis of Methane: A comparative experimental study**
A. Celik¹; I. Ben Othman¹; H. Müller¹; P. Lott¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology, Karlsruhe/D
- P 3.06 **Selective ethanol to Acetaldehyde oxidation through nitrogen doped polymer derived carbon**
O. Leubner¹; F. Herold²; J. Gläsel¹; A. Drochner¹; B. Etzold¹; ¹ Technische Universität Darmstadt/D; ² Norwegian University of Science and Technology, Trondheim/N

ELECTROCHEMICAL REACTION ENGINEERING

- P 4.01 **Revealing Kinetic Limitations of Electrocatalytic CO₂ Reduction in Aprotic Electrolytes by Dynamic Modeling**
N. Oppel¹; P. Röse¹; U. Kreuer¹; ¹ Karlsruhe Institute of Technology, Karlsruhe/D
- P 4.02 **Systematic determination of optimal design-points of fully integrated Power-to-SNG process chains via detailed simulation of SOEC stacks**
O. Furst¹; L. Wehrle¹; D. Schmidler²; J. Dailly²; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D; ² European Institute for Energy Research (EIFER), Karlsruhe/D
- P 4.03 **Spectroelectrochemical Exploration of Biogenic Substrates**
N. Kurig¹; R. Palkovits¹; ¹ RWTH Aachen University, Aachen/D
- P 4.04 **Microfluidic Electrochemical Sensor in Comparison with Screen-Printed Carbon-Based Electrode Based on N-Doped Carbon Nanoonions/Nafion for Sensing of Cd₂⁺**
M. Ghanbari¹; B. Etzold¹; ¹ Technische Universität Darmstadt/D
- P 4.05 **Investigation of the gas permeation stream through GDEs in electrochemical CO₂ reduction**
M. Römer¹; N. Näser¹; B. Etzold¹; ¹ Technische Universität Darmstadt/D
- P 4.06 **High-throughput Experimentation in Electrochemistry for Alkaline Water Electrolysis**
G. Wasserschaff¹; A. Müller¹; S. Sahehmahamad¹; F. Huber¹; B. Hecker²; D. Dogan²; H. Tempel²; R-A. Eichel²; C. Hofmann³; P. Löb³; H-J. Kost³; A. Ziogas³; ¹ hte GmbH, Heidelberg/D; ² Institute of Energy and Climate Research, Fundamental Electrochemistry, Forschungszentrum Jülich GmbH, Jülich/D; ³ Fraunhofer Institute for Microengineering and Microsystems, Mainz/D
- P 4.07 **Preparation of highly active electrodes for alkaline water electrolysis by electrodeposition of high surface area NiFeOOH on Nickel mesh substrates with varying geometry**
J. Hoffmann¹, N. Schmitt¹, A. Wiser², B. Etzold¹; ¹ TU Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie, Darmstadt/D; ² Umicore AG & Co KG, Hanau-Wolfgang/D

EXPERIMENTAL REACTOR DIAGNOSTICS

- P 5.01 **Exploring Carbon Deposition on Methane Dry Reforming by Laser-Induced Breakdown Spectroscopy and Species Concentration Profiles**
D. Espinoza¹; H. Appala¹; O. Korup²; R. Horn²; ¹ TUHH, Hamburg/D; ² TUHH / REACNOSTICS GmbH, Hamburg/D
- P 5.02 **In-situ study of NO reduction and CO oxidation on Pt by using planar laser-induced fluorescence**
S. Wan¹; T. Häberl¹; P. Lott²; R. Suntz²; O. Deutschmann²; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Karlsruhe Institute of Technology (KIT), Karlsruhe/D
- P 5.03 **Forced Dynamic Operation of Methanol Synthesis – Quantification of fluctuating volumetric outlet flowrates**
L. Kaps¹; W. Kortuz¹; A. Seidel-Morgenstern¹; ¹ Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D

POSTER

P 5.04 Isopotential Spectroscopy – A New Concept for Operando Studies of Catalysts in Catalytic Reactors

B. Wollak¹; K. Bharatula¹; S. Stahl²; S. Sichert¹; O. Korup³; R. Horn³; ¹ Hamburg University of Technology, Hamburg/D; ² REACNOSTICS GmbH, Hamburg/D; ³ TUHH / REACNOSTICS GmbH, Hamburg/D

P 5.05 Flow Calorimetry as a Tool for Fast Reactions

D. Kirschneck¹; M. Maier¹; ¹ Microinnova Engineering GmbH, Allerheiligen bei Wildon/A

P 5.06 Operando multi-spectroscopic correlation analysis of electronic and structural changes during homogeneous catalytic activity

A. Koba¹; S. Klingler²; B. Mizaihoff²; D. Ziegenbalg¹; ¹ Ulm University - Institute of Chemical Engineering, Ulm/D; ² Ulm University, Ulm/D

P 5.07 Numerical model based workflow for the correction of measured temperature profiles in slender fixed beds

P. Reinold¹; M. Kutscherauer¹; G. Mestl²; S. Böcklein²; T. Turek¹; G. Wehinger¹; ¹ Clausthal University of Technology, Clausthal-Zellerfeld/D; ² Clariant AG, Heufeld/D

P 5.08 Influence of Different Initiators and Mixing on Temperature Gradients in High-Pressure LDPE Autoclaves

L. Schmidt¹; M. Busch¹; ¹ Technische Universität Darmstadt/D

REACTION KINETICS AND REACTOR MODELLING & SIMULATION**P 6.01 Automated Kinetic Parameter Optimization of Catalytic Reactions using Basin-Hopping:**

CH_4 Oxidation over PdO/ZrO_2
R. Chacko¹; K. Keller¹; S. Tischer¹; A. Shirasath¹; P. Lott¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D

P 6.02 Automated reduction of large reaction mechanisms: Modeling methane pyrolysis in the gas-phase

A. Shirasath¹; M. Mokashi¹; F. Kleuker¹; S. Tischer¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D

P 6.03 Flow calorimetry evaluation software

F. Steinemann¹; D. Rütti²; M. Moser¹; A. Georg¹; D. Meier²; ¹ Fluitec mixing + reaction solutions AG, Neftenbach/CH; ² ZHAW Zurich University of Applied Sciences, Winterthur/CH

P 6.04 Microkinetic Model for High Temperature Oxidative Coupling of Methane over Monoliths coated with $\text{Pt}/\text{Al}_2\text{O}_3$

J. Chawla¹; S. Schardt¹; S. Angelis¹; P. Lott¹; L. Maier¹; S. Tischer¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D

P 6.05 Numerical simulation study of biogas pyrolysis and comparison with experiments

M. Mokashi¹; P. Lott¹; A. Celik¹; I. Othman¹; A. Shirasath¹; H. Müller¹; S. Tischer¹; L. Maier¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D

P 6.06 In-situ investigation of the morphological development of a soot layer during combustion

A. Raiolo¹; U. Tuttles¹; U. Nieken¹; ¹ University of Stuttgart, Stuttgart/D



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POSTER

- P 6.07 **Development and validation of kinetic model for low temperature methanol steam reforming and water-gas shift reactor design in Aspen Plus**
A. Rehman¹; D. Neu¹; P. Wolf¹; C. Schwarz¹; M. Haumann¹; ¹ Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen/D
- P 6.08 **Synergy of Kinetic and Process Modelling – A Case Study**
M. Feigel¹; J. Breitsameter¹; B. Rieger¹; O. Hinrichsen¹; ¹ Technische Universität München, Garching/D
- P 6.09 **Experimental study and comprehensive kinetic modeling of direct dimethyl ether synthesis with novel catalytic system**
G. Rodrigues Niquini¹; B. Lacerda de Oliveira Campos¹; K. Herrera Delgado¹; S. Pitter¹; J. Sauer¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
- P 6.10 **Reactive CFD Modelling of Single Pellet String Reactors with Different Levels of Detail**
C. Bauer¹; T. Gros¹; H. Bui¹; O. Hinrichsen¹; ¹ Technische Universität München, Garching bei München/D
- P 6.11 **Model-based Investigation of Sustained Ring-Opening Polymerization of Lactide with non-toxic Zinc Guanidine Catalysts**
N. Conen¹; A. Jupke¹; ¹ RWTH Aachen University, Aachen/D
- P 6.12 **Optimal Design of Experiments for the determination of the Kinetics of the homogeneous rhodium-catalyzed Hydroaminomethylation**
S. Kirschtowski¹; W. Kortuz²; K. Rätze¹; K. Sundmacher²; C. Hamel¹; ¹ Otto von Guericke University Magdeburg, Magdeburg/D; ² Otto von Guericke University Magdeburg and Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg/D
- P 6.13 **Elucidating the influence of intercalated anions in NiFe LDH on the oxygen evolution reaction through a mechanistic study**
M. Berger¹; I. Popa²; R. Palkovits²; ¹ RWTH Aachen University, Aachen/D; ² RWTH Aachen University Institut für Technische und Makromolekulare Chemie (ITMC), Aachen/D
- P 6.14 **Equilibrium Study of Formic Acid-Amine Adducts with Isothermal Titration Calorimetry**
C. Kabatnik¹; C. Krekel¹; A. Jupke¹; ¹ RWTH Aachen University, Aachen/D
- P 6.15 **Determination and evaluation of selectivity and yield limits in reaction networks using the Feinberg Equivalence Principle**
A. Brune¹; A. Seidel-Morgenstern¹; C. Hamel¹; ¹ Otto von Guericke University Magdeburg/D
- P 6.16 **Selective Oxidation of Green Methanol to Oxygenates - Comparison of Empirical and Mechanistic Kinetic Approaches**
J. Walter¹; C. Hamel¹; ¹ Otto von Guericke University Magdeburg, Magdeburg/D
- P 6.17 **Efficient Implementation of Detailed Surface Kinetics by Neural Network Representations of the Rate-determining Steps**
F. Döppel¹; M. Votsmeier²; ¹ Technical University of Darmstadt, Darmstadt/D; ² Technical University of Darmstadt; Umicore AG & Co. KG, Darmstadt/D
- P 6.18 **Two-layered Vectorial Kernel Models for Detailed Surface Kinetics using a Goal-Oriented Approach**
F. Döppel¹; T. Wenzel²; R. Herkert²; B. Haasdronk²; M. Votsmeier³; ¹ Technical University of Darmstadt, Darmstadt/D; ² University of Stuttgart, Stuttgart/D; ³ Technical University of Darmstadt; Umicore AG & Co. KG, Darmstadt/D

POSTER

- P 6.19 **Model Based Reactor Optimization for a Heterogeneously Catalyzed Fast Highly Endothermal Reaction**
M. Zallmann¹; S. Walter²; I. Gummin²; H. Freund¹; ¹ Technische Universität Dortmund, Dortmund/D; ² DSM Nutritional Products Ltd., Sisseln/CH
- P 6.20 **Polypropylene process modelling: From lab to industry – Challenges and opportunities**
A. Konopka¹; J. Fernengel²; R. Fischer²; O. Hinrichsen¹; ¹ Technical University of Munich, Garching/D; ² Clariant Produkte (Deutschland) GmbH, Munich/D
- P 6.21 **Validation of a Reaction Kinetic and Heat Balance Model for Anionic Polymerization in Batch Reactors**
F. Kandelhard¹; P. Georgopoulos¹; ¹ Helmholtz-Zentrum Hereon, Geesthacht/D
- P 6.22 **Digitalization of Up-Scaled Block Copolymer Syntheses via RAFT Polymerization**
F. Kandelhard¹; E. Pashayev¹; J. Schymura¹; P. Georgopoulos¹; ¹ Helmholtz-Zentrum Hereon, Geesthacht/D
- P 6.23 **Simulation based approach for rational Core-Shell tandem catalyst design**
G. Brösigke¹; J. Repke¹; ¹ Technische Universität Berlin, Berlin/D
- P 6.24 **Egg-White' Catalyst Pellet Preparation by Fluidized-Bed Coating**
R. Zimmermann¹; J. Bremer²; K. Sundmacher³; ¹ Otto-von-Guericke Universität Magdeburg/D; ² Clausthal University of Technology, Clausthal/D; ³ Max Planck Institut for Dynamics of Complex Technical Systems, Magdeburg/D
- P 6.25 **Applicability and validity of CFD-based compartment models for one to multiple operating points**
S. Schwarz¹; M. Grünewald¹; ¹ Ruhr-Universität Bochum, Lehrstuhl für Fluidverfahrenstechnik, Bochum/D
- P 6.26 **Temperature Influence of the Transfer Activity of Alcohols in the LDPE Polymerization**
L. Euler Bueno¹; M. Busch¹; ¹ Technische Universität Darmstadt/D
- P 6.27 **Towards assessing kinetics of ammonia oxidation at conditions of the Ostwald process**
F. Kornemann¹, L.-C. Stoltenberg¹, F. Biermann¹, A. Wiser², S. Pinnow³, A. Drochner¹, M. Votsmeier^{1,2}, B. Etzold¹; ¹ Technische Universität Darmstadt, Ernst-Berl-Institut für Technische und Makromolekulare Chemie, Darmstadt/D; ² Umicore AG & Co. KG, Hanau-Wolfgang/D; ³ Thyssenkrupp Industrial Solutions AG, Dortmund/D
- P 6.28 **An ab-initio study of the reaction mechanism of the catalyzed phosgenation**
B. Grandke¹, R. Ahmed¹; K. Leonhard¹; ¹ RWTH Aachen University, Aachen/D
- P 6.29 **Influence of the reactor design on the suitability for the kinetic analysis of thermal runaway reactions**
P. Desel¹, M. Ulbricht², A. Roppert^{1,2}; ¹ Hochschule Niederrhein University of Applied Sciences, Krefeld/D; ² University Duisburg-Essen, Essen/D
- P 6.30 **Physics-informed Neural Networks for Reactor Simulations**
K. Wilhelm¹; F. Döppel¹; M. Votsmeier^{1,2}; ¹ Technical University of Darmstadt/D; ² Technical University of Darmstadt; Umicore AG & Co. KG, Darmstadt/D
- P 6.31 **Learning kinetic models from experimental data using neural ODEs**
T. Kircher¹; F. Döppel¹; M. Votsmeier^{1,2}; ¹ Technical University of Darmstadt/D; ² Umicore AG & Co. KG, Hanau/D

POSTER

REACTION ENGINEERING OF CATALYZED REACTIONS

- P 7.01 **Reaction engineering at work: the scale up of a plate-type methanation reactor**
E. Moiol¹; ¹ Hitachi Zosen Inova, Zurich/CH
- P 7.02 **Core-Shell-Nanoreactors for Fischer-Tropsch Synthesis: Effect of Active Particle Size and Support Activity on Product Distribution**
K. Wein¹; G. Baade¹; R. Güttel¹; ¹ University of Ulm, Ulm/D
- P 7.03 **Photocatalytic nitrate reduction under sunlight over TiO₂ layers on glass rings generated by dip-coating**
L. Becker¹; M. Guci¹; M. Schwidder¹; ¹ Otto von Guericke Universität Magdeburg/D
- P 7.04 **Loop photoreactor to study mass transfer effect on photocatalytic hydrogen generation using UV LEDs**
P. Li¹; D. Kowalczyk¹; D. Ziegenbalg¹; ¹ Universität Ulm, Ulm/D
- P 7.05 **Spray Polymerization of ε-Caprolactone**
A. Frankowski¹; M. Müller¹; W. Pauer¹; G. Luinstra¹; ¹ Universität Hamburg (UHH), Hamburg/D
- P 7.07 **Catalytic hydrogenation and dehydrogenation of the liquid organic hydrogen carrier (LOHC) benzyltoluene**
B. Bong¹; C. Mebrahtu¹; R. Palkovits¹; ¹ RWTH Aachen University Institut für Technische und Makromolekulare Chemie (ITMC), Aachen/D
- P 7.08 **Investigation of short-chain Fischer-Tropsch product formation under dynamic conditions using the periodic transient kinetics method**
M. Gäßler¹; S. Hermann¹; R. Güttel¹; ¹ University of Ulm, Ulm/D
- P 7.09 **Acetylene Formation over Pt-based Monolithic Catalysts: Influence of Rare Earth Oxides on Oxidative Coupling of Methane**
S. Schardt¹; F. Ehrlich¹; J. Chawla¹; P. Lott¹; O. Deutschmann¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D
- P 7.10 **Bimetallic Ni-Co catalysts for Dry Reforming of Methane in inductively heated reactor systems**
G. Küchen¹; V. Olszok¹; B. Kreitz²; T. Turek¹; A. Weber¹; G. Wehinger¹; ¹ Clausthal University of Technology, Clausthal-Zellerfeld/D; ² Brown University, Providence/USA
- P 7.11 **Identification of significant parameter in the Ostwald process using statistically optimized experimental designs**
L. Stoltenberg¹; F. Kornemann¹; F. Biermann¹; A. Wiser²; C. Renk³; A. Orth⁴; M. Votsmeier⁵; A. Drochner¹; B. Etzold¹; ¹ Technische Universität Darmstadt, Darmstadt/D; ² Umicore AG & CO. KG, Hanau-Wolfgang/D; ³ Thyssenkrupp Industrial Solutions AG, Dortmund/D; ⁴ Umesoft GmbH, Eschborn/D; ⁵ Technical University of Darmstadt; Umicore AG & Co. KG, Darmstadt; Hanau/D
- P 7.12 **Spatially and temporally resolved operando investigations on CO₂ methanation under dynamic reaction conditions**
T. Eng¹; D. Weber²; T. Franken²; M. Rubin¹; R. Dittmeyer¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D; ² Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen/D

POSTER

- P 7.13 **Model-based optimization of enzymatic cascades immobilized in porous particles**
L. Paschalidis¹; J. Burger¹; ¹ Technical University of Munich, Straubing/D
- P 7.14 **Biogas conversion in electrically heated catalytic reforming reactors**
M. Ebrahim¹; E. Klemm¹; ¹ University of Stuttgart, Stuttgart/D
- P 7.15 **Enabling Load-Flexible Ammonia Synthesis using Polytropic Fixed-Bed Reactors**
L. Gottheil¹; J. Bremer¹; ¹ Clausthal University of Technology, Clausthal-Zellerfeld/D
- P 7.16 **Sustainable Processes for synthetic fuel production**
F. Vogelsang¹; A. Roth¹; ¹ Fraunhofer IGB, Stuttgart/D
- P 7.17 **Tackling catalyst deactivation with spectroscopy in molecularly catalyzed reactions for constant product quality**
N. Wessel¹; S. Obst¹; K. Köhnke¹; A. Vorholt¹; W. Leitner¹; ¹ Max Planck Institute for Chemical Energy Conversion, Mülheim a.d. Ruhr/D; RWTH Aachen, Aachen/D
- P 7.18 **Design of a Counter-Flow Reactor for Ammonia Synthesis: Optimizing the Temperature Profile by utilizing Additive Manufactured Fluid Guiding Elements**
L. Bifarr¹; W. Benzinger¹; P. Pfeifer¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
- P 7.19 **Direct activation of CO₂ to hydrocarbons in Fischer-Tropsch Synthesis over iron catalyst**
M. Kirarslan¹; O. Görke¹; P. Pfeifer¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D
- P 7.20 **Spherical polymer-based carbons as catalyst support**
J. Schmidpeter¹; N. Fleck²; C. Wetzel²; L. Peña³; O. Shimelis³; J. Abrahamson³; J. Gläsel¹; M. Schulz⁴; B. Etzold¹; ¹ Technical University of Darmstadt, Ernst-Berl-Institute for Technical Chemistry and Macromolecular Science, Darmstadt/D; ² Merck Electronics KGaA, Darmstadt/D; ³ MilliporeSigma, Bellefonte/USA; ⁴ Merck Life Science KGaA, Darmstadt/D

NEW REACTOR CONCEPTS

- P 8.01 **Experimental analysis of inductive heating of catalytic beds**
D. Kleschew¹; U. Nieken¹; ¹ University of Stuttgart, Stuttgart/D
- P 8.02 **Monolith based pore-through-flow membrane bioreactors in pilot scale for the use of prebiotic production**
I. Pottratz¹; C. Hamel²; ¹ Hochschule Anhalt, Köthen/D; ² Otto-von-Guericke-Universität Magdeburg, Magdeburg/D
- P 8.03 **Making Photocatalyst Screening Accessible using a Milli Scale Multi-Batch Screening Photoreactor**
D. Kowalczyk¹; D. Ziegenbalg¹; ¹ Universität Ulm, Institut für Chemieingenieurwesen, Ulm/D
- P 8.04 **A Tool for Scaling-Up Photoreactors – the MISCOP System**
F. Guba¹; F. Gaulhofer²; D. Ziegenbalg²; ¹ Universität Ulm, Ulm/D; ² Ulm University - Institute of Chemical Engineering, Ulm/D
- P 8.05 **Application of a new electrochemical cell for hydrogen peroxide generation**
M. Enstrup¹; U. Kunz¹; ¹ Clausthal University of Technology, Clausthal-Zellerfeld/D

POSTER

NOTES

P 8.06 Polymeric reactor materials for catalytic reactions beyond earthJ. Friedland¹; M. Merk¹; R. Gütte¹; ¹ Ulm University, Ulm/D**P 8.07 Mimicking industrial alkaline water electrolysis on a laboratory scale using a cost-effective beaker cell approach**N. Thissen¹; D. Vogel¹; J. Thoede¹; A. Mechler¹; ¹ RWTH Aachen University, Aachen/D**P 8.08 A Berty reactor for kinetic measurements on thin films and plates**L. Thuma²; G. von der Waydbrink¹; E. Strotz¹; C. Marshall¹; K. Skorupska¹; R. Schlägl¹;¹ Fritz Haber Institute of the Max Planck Society, Berlin/D; ² Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin/D**NOVEL PROCESSES****P 9.01 Thermodynamic analysis of the effect of in situ product absorption in sorption-enhanced ammonia synthesis**T. Kunz¹; R. Gütte¹; ¹ University of Ulm, Ulm/D**P 9.03 Direct reduction of mineral iron carbonate ore with hydrogen combined with methane and methanol synthesis**S. Kleiber¹; A. Loder¹; M. Siebenhofer¹; S. Lux¹; ¹ Graz University of Technology, Graz/A**P 9.04 Reaction kinetics of liquid phase DME synthesis in reactive distillation columns**M. Semmel¹; O. Salem¹; A. Schaadt¹; J. Sauer²; ¹ Fraunhofer Institute for Solar Energy Systems ISE, Freiburg/D; ² Karlsruhe Institute of Technology (KIT), Karlsruhe/D**P 9.05 Techno-Economic Evaluation of Directly Coupled CH₂O / CH₃OH Synthesis Based on CO₂**P. Münzer¹; U. Arnold¹; J. Sauer¹; ¹ Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen/D**P 9.06 Dry reforming of steelworks off-gases in a pilot plant integrated into a steel mill: a study on the influence of operating parameters**P. Blanck¹; ¹ Karlsruhe Institute of Technology (KIT), Karlsruhe/D**P 9.07 Novel Downstream Process Concepts for Cyclic Acetal Synthesis**M. Haas¹; A. Jupke¹; ¹ RWTH Aachen University, Aachen/D**P 9.08 Iron as energy carrier: Oxidation of iron particles and the effect of cyclization**C. Kuhn¹, A. Knapp¹, M. Deutschmann², H. Nirschl², S. Tischer¹, O. Deutschmann¹;¹ Institute for Chemical Technology and Polymer Chemistry; ² Institute of Mechanical Process Engineering and Mechanics, Karlsruhe Institute of Technology, Karlsruhe/D**MISCELLANEOUS****P 10.01 Slow aging mechanisms in non-oxidative propane dehydrogenation on Pt-ZSM5 catalysts**J. Matthies¹; D. Dittmann¹; M. Dyballa¹; U. Nieken¹; ¹ Universität Stuttgart/D

NOTES

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