



LEISTUNGSZENTRUM  
SIMULATIONS- UND  
SOFTWARE-BASIERTE  
INNOVATION



INTERNATIONAL WORKSHOP  
5<sup>TH</sup> MATHEMATICAL METHODS  
IN PROCESS ENGINEERING –  
MODELING, SIMULATION,  
OPTIMIZATION

October 10 to 11, 2024  
Fraunhofer ITWM, Kaiserslautern  
Germany

INVITED SPEAKERS

– Academic Speakers

- **Prof. Dr.-Ing. Jakob Burger**  
TUM, München, DE
- **Prof. Marianthi G. Ierapetritou**  
University of Delaware, US
- **Prof. John Bagterp Jørgensen**  
Technical University of Denmark, Lyngby, DK
- **Prof. Flavio Manenti**  
Politecnico di Milano, IT
- **Prof. Miguel Ángel Rodríguez Pérez**  
University of Valladolid, ES
- **Prof. Qi Zhang**  
University of Minnesota, US

– Industrial Speakers

- **Dr. Norbert Asprien**  
BASF SE, Ludwigshafen a. R., DE
- **Dr. Lorenz Fleitmann**  
Evonik Operations GmbH, Marl, DE
- **Dr. Ikenna Ireka**  
Covestro Deutschland AG, Leverkusen, DE
- **Dr. Robert Lee**  
BASF SE, Ludwigshafen a. R., DE
- **Dr. Jochen Steimel**  
AVEVA GmbH, Frankfurt a. M., DE
- **Dr. Bernd Wunderlich**  
Linde GmbH, Pullach, DE

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GENERAL INFORMATION

– Entry Fee

- **Industry: 750 EUR\***  
(VAT is not charged according to § 4 No. 22a UStG)  
Invoicing takes place after the event.
- **Research staff: free of charge**

\*During the event, coffee, refreshments and lunch will be offered.  
Registered participants will receive workshop materials and can attend the networking dinner on October 10, 2024.

– Registration

Please register online by  
September 27, 2024:  
<https://s.fhg.de/mmipe-2024>



– Contact with Regard to Scientific Program

**Prof. Dr. Michael Bortz**  
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– Contact with Regard to Organization

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– Conference Venue

**Fraunhofer Institute for Industrial Mathematics ITWM**  
Fraunhofer-Platz 1  
67663 Kaiserslautern  
[www.itwm.fraunhofer.de](http://www.itwm.fraunhofer.de)

Directions: [www.itwm.fraunhofer.de/contact](http://www.itwm.fraunhofer.de/contact)



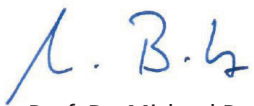
## PREFACE

Model-based simulation and optimization is seen as an essential part of unlocking the potential for increased energy and resource efficiency and maintaining high levels of value creation. Mathematical models, algorithms and data science are in the core of this development.

On October 10 to 11, 2024, the Fraunhofer High Performance Center Simulation and Software Based Innovation will organize the international workshop »Mathematical Methods in Process Engineering« with 6 internationally outstanding invited speakers and 12 short contributions from researchers of the center and from industry.

All lectures are invited, and also attendance will require invitation. The number of invited participants is limited to about 80, including selected partners from the process industry.

The workshop will provide a unique opportunity for scientific discussions and personal networking between scientists from academia and industrial practice to reflect and shape the topics of future process engineering.



Prof. Dr. Michael Bortz  
Fraunhofer ITWM



Prof. Dr.-Ing. Hans Hasse  
RPTU Kaiserslautern

## PROGRAM – THURSDAY, OCTOBER 10, 2024

9:45	Registration open, welcome coffee
10:00	<b>Opening</b> Prof. Dr. Michael Bortz, Prof. Dr.-Ing. Hans Hasse
10:15	<b>Keynote</b> Dr. Andreas Fuessler, Vice President Materials Research, BASF SE, Ludwigshafen a. R., DE
<b>S1</b>	<b>SESSION 1: MSO IN PROCESS ENGINEERING I</b> Session Chair: Prof. Dr. Karl-Heinz Küfer
10:45	<b>Towards a Circular Economy: Leveraging Process Systems Engineering Tools for Sustainable Solutions</b> Prof. Marianthi G. Ierapetritou, University of Delaware, US
11:35	<b>How to Account for Uncertainties in Chemical Process Design?</b> Dr. Norbert Asprion, BASF SE, Ludwigshafen a. R., DE
12:00	<b>Tools to Realistically Assess the Cost of Robustness in Chemical Plant Design</b> Dr. Katrin Teichert, Fraunhofer ITWM, Kaiserslautern, DE
12:25	Lunch (foyer)
<b>S2</b>	<b>SESSION 2: NUMERICAL MODELS AND CHALLENGES</b> Session Chair: Dr. Dietmar Hietel
13:30	<b>Data-Driven Decision-Focused Surrogate Modeling for Fast Online Optimization</b> Prof. Qi Zhang, University of Minnesota, US
14:20	<b>Numerical Optimization in Process Design and Operations – Industrial Challenges</b> Dr. Bernd Wunderlich, Linde GmbH, Pullach, DE
14:45	<b>MESHFREE Simulations in Chemical Engineering: Homogenization and Foaming Processes as Key-Challenges for the Numerical Model</b> Dr. Jörg Kuhnert, Fraunhofer ITWM, Kaiserslautern, DE
15:10	Coffee break (foyer)
<b>S3</b>	<b>SESSION 3: DATA AND MODELS</b> Session Chair: Prof. Dr.-Ing. Hans Hasse
15:50	<b>Multi-Complexity and Multi-Scale PSE Tools to Handle Transitions in Practical Process Engineering</b> Prof. Flavio Manenti, Politecnico di Milano, IT
16:40	<b>Autonomous Research Machines and Self-Driving Labs: Challenges and Progress</b> Dr. Robert Lee, BASF SE, Ludwigshafen a. R., DE
17:05	<b>Hard-Coding of Physical Constraints in Neural Networks</b> Dr. Thomas Specht, RPTU Kaiserslautern, DE
18:00	Transfer by bus to diner location for speakers and external industrial participants: <b>Round table discussions and networking dinner</b>

## PROGRAM – FRIDAY, OCTOBER 11, 2024

8:30	Arrival of participants, welcome coffee
<b>S4</b>	<b>SESSION 4: MODELLING, SIMULATION AND OPTIMIZATION OF FOAMS</b> Session Chair: Dr. Jörg Kuhnert
8:40	<b>Understanding the Foaming Mechanisms in Polyurethane Foams: Development of Foams With Improved Structure and Properties</b> Prof. Miguel Ángel Rodríguez Pérez, University of Valladolid, ES
9:30	<b>Virtual Polymeric Foam Development and Processing: Challenges and Prospects</b> Dr. Ikenna Ireka, Covestro Deutschland AG, Leverkusen, DE
9:55	<b>Simulations of Polyurethane Foam Expansion Processes: Benefits and Challenges</b> Dr. Dariusz Niedziela, Fraunhofer ITWM, Kaiserslautern, DE
10:20	Coffee break (foyer)
<b>S5</b>	<b>SESSION 5: ADVANCED SIMULATION APPROACHES</b> Session Chair: Dr. Konrad Steiner
10:50	<b>Model Predictive Control and Optimization for Industrial Power and Chemical Process Systems</b> Prof. John Bagterp Jørgensen, Technical University of Denmark, Lyngby, DK
11:40	<b>From Derivatives to Directions: Using Mathematics to Drive Next-Generation Simulation Model Troubleshooting</b> Dr. Jochen Steimel, AVEVA GmbH, Frankfurt a. M., DE
12:05	<b>Uncertainty Propagation for Nonlinear Regression Models</b> Martin Bubel, Fraunhofer ITWM, Kaiserslautern, DE
12:30	Lunch (foyer)
<b>S6</b>	<b>SESSION 6: MSO IN PROCESS ENGINEERING II</b> Session Chair: Prof. Dr. Michael Bortz
13:30	<b>Automated Design of Fluid Separation Processes by Reinforcement Machine Learning</b> Prof. Dr.-Ing. Jakob Burger, TU München, DE
14:20	<b>Performance Monitoring: Challenges and Chances for Simulation-Based Soft Sensors</b> Dr. Lorenz Fleitmann, Evonik Operations GmbH, Marl, DE
14:45	<b>Filtering Pareto Fronts: a New Kind of Decision Support for Process Design</b> Dr. Philipp Süß, Fraunhofer ITWM, Kaiserslautern, DE
15:10	Wrap up/closing
15:30	End of the workshop