

European Federation of Chemical Engineering  
**2<sup>nd</sup> Working Party on Polymer Reaction Engineering**  
Hamburg, May 24<sup>th</sup> to 26<sup>th</sup> 2013



**Invitation**

Dear company representatives, professors and PhD-students,

the 2<sup>nd</sup> Working Party on Polymer Reaction Engineering to be held in **Hamburg from May 24<sup>th</sup> to 26<sup>th</sup>** presents a platform for young and motivated scientists to exchange and discuss recent research and to get into contact with interesting companies and possible employers.

After the successful kick-off in Lyon, we were able to extend the scope of research fields, participating universities and industry representatives. Over 30 PhDs will present their research results in oral presentations and poster contributions covering all fields of Polymer Reaction Engineering:

- Emulsion polymerization
- Polymerization kinetics
- Modeling of polymerizations
- Reaction-plants
- Gas-phase polymerizations
- Polymer morphology

We are looking forward to seeing you in Hamburg

The organizing committee

**Sponsors**

**SULZER**

سابك  
**sebic**

**BASF**  
The Chemical Company

 **WILEY-VCH**

**Organizing Committee**

Markus Busch (Chair of WPPRE, TU Darmstadt)  
Werner Pauer (Secretary of WPPRE, University Hamburg)  
Annelie Halfar (University Hamburg)  
Claudia Schwartzkopff (TU Darmstadt)  
Isabel Kadel (TU Darmstadt)

**Contact**

For further information please contact:  
[wppre@chemie.tu-darmstadt.de](mailto:wppre@chemie.tu-darmstadt.de)

**Homepage**

<http://events.dechema.de/pre2013>



TECHNISCHE  
UNIVERSITÄT  
DARMSTADT



Universität Hamburg  
DER FORSCHUNG | DER LEHRE | DER BILDUNG

Program

**Friday, 24<sup>th</sup> May**

13:00-14:00 **Registration at the conference site**  
**Poster wall preparation**

Session I

Chair: Annelie Halfar (University of Hamburg)

14:00-14:20 **Stefano Lazzari** (ETH Zürich)  
*Modeling Multiradicals in Bulk Crosslinking Copolymerisation*

14:20-14:40 **Calista Preusser** (Queen's University)  
*Developing a Model for the Aqueous Phase Copolymerisation of Acrylic Acid and Acrylamide*

14:40-15:00 **David Eckes** (TU Darmstadt)  
*Modelling the Microstructure of Ethylene Vinyl Acetate Copolymers considering Different Types of Short Chain Branches*

15:00-15:20 **Shaghayegh Hamzehlou** (University of Basque Country)  
*Copolymerization of N-Butyl Acrylate and Styrene: Terminal vs. Penultimate Model and the Effect of Backbiting*

15:20-16:30 **Coffee Break and Poster Session**

Session II

Chair: Thomas Kröner (University of Halle)

16:30-16:50 **Paul H. M. Van Steenberge** (Ghent University)  
*Efficient Stochastic Calculation of the Chemical Composition – Chain Length Distribution accounting for Possible Diffusional Limitations*

16:50-17:10 **Nazila Yaghini** (University of Amsterdam)  
*2-D-Molecular Weight Distribution Modeling for Topological Scission*

17:10-17:30 **Ágnes Bárkányi** (University of Pannonia)  
*Effects of Droplet Interactions on Polymer Properties in Suspension Polymerization of Vinyl Chloride. A Simulation Study.*

17:30-17:50 **Arash Alizadeh** (University of Lyon I)  
*Modeling of Time Scale for Vaporization of Liquid Droplets during Condensed Mode Operation of Ethylene Polymerization in FBRs*

19:00 **Dinner**  
Ristorante Terzetto

*The dinner is kindly sponsored by*

Program

**Saturday, 25<sup>th</sup> May**

**Session III**

Chair: Tom Jansen (Eindhoven University of Technology)

08:00-08:20 **Kevin A. Payne** (Queen's University)  
*ARGET ATRP: A Systematic Investigation of Limitations at Low Copper Levels*

08:20-08:40 **Dambarudhar Parida** (University of Strasbourg)  
*Effect of Microreactor Geometry and Operating Parameters on ATRP Processes*

08:40-09:00 **Thomas Kröner** (University of Halle)  
*Model-based Transfer of Free Radical Copolymerisation from Batch to Continuous Operation*

09:00-09:20 **Dhiraj K. Garg** (University of Strasbourg)  
*Analytical Solution of FPR for Constant Volume, Isothermal, Well-mixed Batch Reactor and its Application*

09:20-10:30 **Coffee Break and Poster Session**

**Session IV**

Chair: Michal Vonka (Institute of Chemical Technology Prague)

10:30-10:50 **Jone Urrutia** (University of the Basque Country)  
*Fouling in Emulsion Polymerization Reactors*

10:50-11:10 **Amaia Agirre** (University of the Basque Country)  
*Continuous Production of Vinyl-Acetate – Veova 10*

11:10-11:30 **Tom Jansen** (Eindhoven University of Technology)  
*Mass Transfer and Particle Size Conservation in Miniemulsion Polymerization*

11:30-11:50 **Barthélémy Brunier** (University of Lyon)  
*Evaluation of Laponite Partitioning in Pickering Emulsion Polymerization*

12:00-13:30 **Lunch**  
Café SternChance

*The lunch is kindly sponsored by*

**SULZER**

European Federation of Chemical Engineering  
**2<sup>nd</sup> Working Party on Polymer Reaction Engineering**  
Hamburg, May 24<sup>th</sup> to 26<sup>th</sup> 2013



**Program**

**Saturday, 25<sup>th</sup> May**

**Session V**

Chair: Amaia Agirre (University of the Basque Country)

13:30-13:50 **Alexandr Zubov** (Institute of Chemical Technology Prague)  
*Meso-scale Modeling of Transport and Reaction in Reconstructed Porous Polyolefin Particles*

13:50-14:10 **Richard Pokorný** (Institute of Chemical Technology Prague)  
*Mathematical Modelling of Heat Transfer in Polymer Foams: Morphology Optimization*

14:10-14:30 **Andra Nistor** (Institute of Chemical Technology Prague)  
*Systematic Investigation of Micro-Cellular Polystyrene Foams Prepared with High-pressure CO<sub>2</sub>*

14:30-15:00 **Coffee Break and Poster Session**

**Session VI**

Chair: Claudia Schwartzkopff (TU Darmstadt)

15:00-15:20 **Joana Kettner** (University of Halle)  
*Influence of Temperature and Catalyst Injection Procedure on Gas-Phase Polymerization of Propylene*

15:20-15:40 **Leonhard Mayrhofer** (Johannes Kepler University)  
*Investigation of Single Particle Gas-Phase Ethylene Homo-Polymerization with Ziegler-Natta Catalyst*

15:40-16:00 **Thomas Hoechfurtner** (Johannes Kepler University)  
*Kinetic Studies of the Influence of Different Al-Alkyls on the Polymerization of Ethene with Ziegler-Natta catalyst*

16:00-16:30 **Coffee Break and Poster Session**

16:30-16:40 **Wiley prize for best contribution**

16:40-17:15 **Miran Milosevic** (Sabic Europe)  
*Entering SABIC with Education in Chemical Engineering*

17:15-18:15 **Labtour (optional)**

18:30 **Barbecue at the Institute**

*The best contribution prize is kindly sponsored by*



European Federation of Chemical Engineering  
**2<sup>nd</sup> Working Party on Polymer Reaction Engineering**  
Hamburg, May 24<sup>th</sup> to 26<sup>th</sup> 2013



Program

**Sunday, 26<sup>th</sup> May**

**Meeting Point** 10:45 at St. Pauli Landungsbrücken, Bridge 2

11:00-13:00 **Boat trip through Hamburg**

13:00-14:30 **Lunch**  
*Fischrestaurant Hoppe*

14:30 **Departure / Free time**



*Boat trip and lunch are kindly sponsored by*

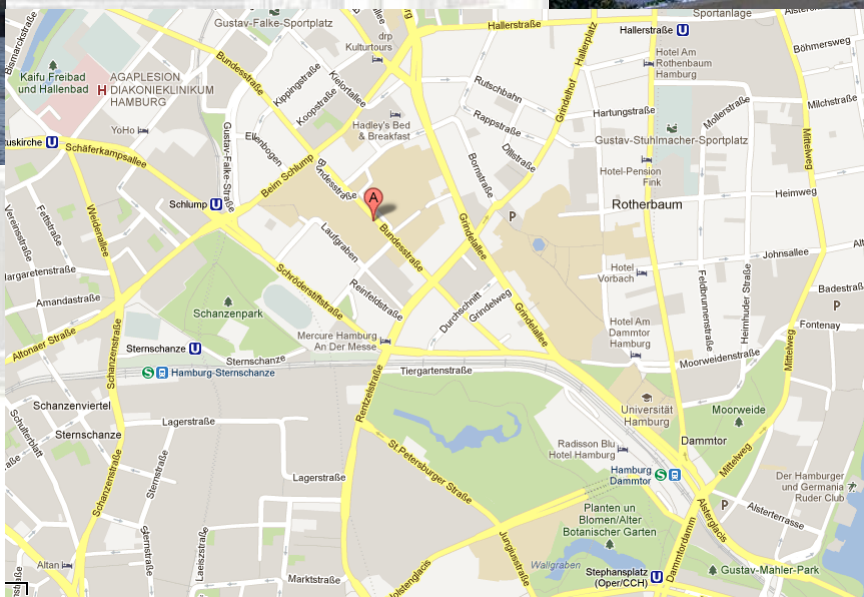


Conference site

**Institut für Technische und  
Makromolekulare Chemie**

Room 39  
Bundesstr. 45  
20146 Hamburg

From Hamburg central station, take the subway line U2 to Schlump. From there, it is about 5 minutes to walk.



**Posterlist:**

- 1. Advantages of Milli-Structured PTFE-Tubular Reactors for Continuous Emulsion Polymerization Reactors**  
Fabian Lüth, University Hamburg
- 2. Suspension polymerization modelled by coupled CFD and population balances**  
Michal Vonka, Institute of Chemical Technology Prague
- 3. Modeling of compartmentalization effects in technical high-pressure autoclaves**  
Sebastian Fries, TU Darmstadt
- 4. A realistic model of topological scission in LDPE molecular weight distribution**  
Nazila Yaghini, University of Amsterdam
- 5. Meso-scale Modeling of Transport and Reaction in Reconstructed Porous Polyolefin Particles**  
Alexandr Zubov, Institute of Chemical Technology Prague,
- 6. A kinetic Monte Carlo methodology for tracking monomer sequences in copolymers**  
Paul H. M. Van Steenberge, Ghent University
- 7. Modelling the Microstructure of Ethylene Vinyl Acetate Copolymers considering Different Types of Short Chain Branches**  
David Eckes, TU Darmstadt
- 8. Modeling of Time Scale for Vaporization of Liquid Droplets during Condensed Mode Operation of Ethylene Polymerization in FBRs**  
Arash Alizadeh, University of Lyon I
- 9. Modelling and Simulation of Droplet Interactions in Suspension Polymerization of Vinyl Chloride Using Population Balance Model**  
Ágnes Bárkányi, University of Pannonia, Hungary
- 10. Micro- and nano-cellular polymer foams: preparation and heat transport modelling**  
Richard Pokorný and Andra Nistor, Institute of Chemical Technology Prague
- 11. Developing a Model for the Aqueous Phase Copolymerisation of Acrylic Acid and Acrylamide**  
Calista Preusser, Queen's University, Canada
- 12. Model-based Transfer of Free Radical Copolymerisation from Batch to Continuous Operation**  
Thomas Kröner, University of Halle, Germany

**Posterlist:**

13. **Crosslinking Copolymerization by Monte Carlo Simulation: Multiradical Consideration**  
Shaghayegh Hamzehlou, University of the Basque Country, Spain
14. **Influence of Temperature and Catalyst Injection Procedure on Gas-Phase Polymerization of Propylene**  
Joana Kettner, University of Halle, Germany
15. **Fouling in Emulsion Polymerization Reactors**  
Jone Urrutia, University of the Basque Country, Spain
16. **Kinetic Studies of the Influence of different Al-Alkyls on the Polymerization of Ethene with Ziegler-Natta catalyst**  
Thomas Höchfurtner, Johannes Kepler University, Austria
17. **Kinetic study of single particle gas-phase ethylene homo-polymerization with Ziegler- Natta catalyst**  
Leonhard Mayrhofer, Johannes Kepler University, Austria
18. **Kinetics of Free-Radical Crosslinking Polymerization: a Comparative Experimental and Numerical Study**  
Stefano Lazzari, ETH Zürich, Switzerland
19. **Analytical solution of FRP for constant volume, isothermal, well mixed batch reactor and its applications**  
Dhiraj K. Garg, University of Strasbourg, France
20. **A Clean Synthetic Route to Medical Grade Biodegradable Polymers - Enzymatic Polymerization using Supercritical Dioxide as Reaction Medium**  
Christian Schmidt, Clausthal University of Technology, Germany
21. **Continuous production of Vinyl Acetate-Veova 10**  
Amaia Agirre, University of the Basque Country, Spain