

We help you navigate
in chemical space.

GTT-Technologies

Users' Meeting 2025



www.gtt-technologies.de

Wednesday afternoon (June 4, 14:00-18:00 CEST)

From theory to application: Let equilibrium work for you.

- 14:00 Welcome & introduction
Moritz to Baben, Stephan Petersen (GTT-Technologies)
- 14:20 Exergy for solution phases
Klaus Hack (GTT-Technologies)
- 14:40 Use of FactSage for the production of supplementary cementitious materials from slags and tailings
Michiel Giels (KU Leuven)
- 15:00 Fission product speciation under nuclear reactor operating conditions
Morgane Rochedy (CEA IRESNE)
- 15:20 Break
- 15:40 A path towards semantically correct and information rich databases
- 16:00 Effects of Fe/Al on P compounds in municipal sewage sludge derived biochars and impacts of adding K compounds
Naeimeh Vali (University of Borås)
- 16:20 Uncovering one of the last unknowns in the steel industry, i.e, slag carryover through FactSage simulations
Ashok Kamaraj (Indian Institute of Technology Hyderabad)
- 16:40 Break
- 17:00 Introducing **FactSage 8.4**: From Equilib to FactFlow, FactProSim & ChemApp for Python
Moritz to Baben, (GTT-Technologies)
- 18:00 End of day

Demo

Thursday morning (June 5, 9:00-13:00 CEST)

Beyond theory: How EERZ advances process modeling.

- 09:00 Introducing **FactFlow**: Flowsheeting made easy
Shivani Gonde, Moritz to Baben, (GTT-Technologies)
- 09:40 Introducing **FactProSim**: EERZ made easy
Ömer Büyükuslu, Shivani Gonde (GTT-Technologies)
- 10:30 Break
- 11:00 **ChemApp for Python**: Exploring the chemical space
Bruno Reis, Ömer Büyükuslu (GTT-Technologies)
- 11:50 Exploring thermochemical effects of hydrogen in blister copper deoxidation with ChemApp for Python and machine learning optimization
Alberto Rivera Romero (CENIM-CSIC)
- 12:10 How ChemApp for Python is used to simulate Me_2H_2 : Storage and transport of H_2 using redox reactions
Ahmed Mansy (TU Clausthal)
- 12:30 Lunchbreak

Demo

Demo

Demo

Thursday afternoon (June 5, 14:00-18:00 CEST)

Predicting green transformation: Next-gen process models.

- 14:00 Simulation of open bath furnace process for hot metal production with ChemApp for Python
Viktor Büttner (HKM)
- 14:20 Accelerating equilibrium calculations for large-scale DRI smelting furnace models – progress with RapidThermo
Johan Zietsman (Ex Mente)
- 14:40 Using FactSage for the prediction of powder pack diffusion coatings as protection against attack in high temperature electrolyser environments
Alexander Donchev (DECHEMA)
- 15:00 Break
- 15:20 **KilnSimu**: Discovering rotary kiln insights
Cassie Früh (GTT-Technologies), Karri Penttilä (VTT)
- 16:20 Break
- 16:40 Our next-gen process models integrating heat, mass & reaction kinetics
Anna Ravensburg (GTT-Technologies)
- 18:00 End of day
- 19:30 Group dinner
Living im Magellan (Pontstraße 78)

Friday morning (June 6, 9:00-12:00 CEST)

No data? No problem! Tackling missing thermochemical information.

- 09:00 Development of high-Mn steel database
Min-Kyu Paek (TU Clausthal)
- 09:20 CALPHAD modelling of oxide materials for energy conversion and storage
Ming Chen (Technical University of Denmark)
- 09:40 Break
- 10:00 Database development on molten salt reactors (MSR)
Ondrej Benes (European comission ERC)
- 10:20 From structure to thermodynamic and thermophysical properties of molten salt nuclear fuels: experimental and computational studies at the TU Delft
Anna Smith (TU Delft)
- 10:40 Overview of database development at FZJ
Rhys Jacob (Forschungszentrum Jülich)
- 11:00 Break
- 11:20 Outlook for **Calphad Optimizer 3.0**
Bruno Reis, Florian Tang (GTT-Technologies)
- 11:50 Farewell
Moritz to Baben, Stephan Petersen (GTT-Technologies)
- 12:00 End of day

Locations

Venue: Forum M

Buchkremerstraße 1-7, 52062 Aachen

WLAN: Forum Gast

Password: F0rum4AC

↪ Zero

Group dinner: Living im Magellan

Pontstr. 78, 52062 Aachen, 5.6., 19:30

Program

Program, speaker list, and abstracts

All available on our [Users' Meeting 2025](#) website.

On-site Info

Practical info

Find directions, food options and more on our [On-site Info](#) website.

The GTT-Café

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