

International Workshop on

How to integrate geochemistry at affordable costs into reactive transport for large-scale systems



Agenda of the Workshop

Wednesday, February 05th

11:00 – 13:00 **Registration**

13:00 – 13:15 Welcome and introduction to HZDR – *Thorsten Stumpf (HZDR, Germany)*

13:15 – 13:35 Motivation and aims of the workshop – *Madlen Stockmann / Vinzenz Brendler (HZDR, Germany)*

13:35 – 14:10 **Keynote Talk 1:** Reactive Transport at the Crossroads: Progress and New Directions – *Carl Steefel (Lawrence Berkeley National Laboratory, USA)*

14:10 – 17:45 **Working Session 1:** Full coupling of reactive transport programs with geochemical codes (20+5min per oral presentation), *Chair: Mavrik Zavarin (Lawrence Livermore National Laboratory, USA)*

TOUGHREACT, a simulation program embedded in the TOUGH suite of codes used in reactive transport modelling of the geological subsurface – *Dorothee Rebscher (BGR Hannover, Germany)*

Reactive Transport Modeling of Large-Scale Systems for Industrial Applications – *Erika Myers (UIT GmbH Dresden, Germany)*

15:00 – 15:30 *Coffee break*

Bounding Computation and Complexity for Reactive Transport on Supercomputers: A Perspective from Nuclear Waste Repository Performance Assessment – *Glenn Hammond (Sandia National Laboratories, USA)*

Cross-scale understanding and description of mineral precipitation processes in reactive transport models – *Jenna Poonoosamy (FZ Jülich, Germany)*

Hydrogeochemical modeling of mineral precipitation potentials in carbon capture and storage (CCS) – *Ulrich Maier (University of Göttingen, Germany)*

Joint discussion - Session 1

18:00 – 21:00 *Get-together and Poster Session*

21:00 End of day one and bus shuttle from HZDR to "[Gewandhaushotel](#)" in Dresden city

Poster Session:

- P1 THEREDA: Thermodynamic Reference Database – *Frank Bok (HZDR, Germany)*
- P2 Pharmaceuticals attenuation in groundwater bodies – *Laura Ceresa (Politecnico di Milano, Italy)*
- P3 Numerical modelling of contaminant migration experiments in the crystalline single fracture models – *Filip Jankovský (ÚJV Řež, a.s., Czech Republic)*
- P4 Lab-Lysimeter Modelling – *Daniel Jara-Heredia (Friedrich Schiller University Jena, Germany)*
- P5 Determination of multicomponent diffusion transfer parameters in low permeable deposits – *Vladimir Likhov (Lomonosov Moscow State University, Russia)*
- P6 Surrogate Modeling of Spatially Heterogeneous Source Terms for Probabilistic Assessment – *Paul Mariner (Sandia National Laboratories, USA)*
- P7 The Up-scaling of Transport Phenomena in Groundwater and Soil as a Basis for Long-Term Considerations within Radioecological Modeling – *Veronika Ustohalova (Öko-Institut e.V. Darmstadt, Germany)*
- P8 Preliminary safety assessments in the site selection procedure in Germany and the implications on the reactive transport modelling – *Johanna Wolf (Bundesgesellschaft für Endlagerung (BGE), Germany)*
- P9 An efficient approach for modeling the reactive flow and transport processes in fractured porous media – *Tao Yuan (HZDR, Germany)*

Thursday, February 06th

08:15 Bus shuttle from "[Gewandhaushotel](#)" in Dresden city to HZDR

09:00 – 9:35 **Keynote Talk 2:** *OpenGeoSys-6 development of reactive transport modeling with the application for radionuclides sorption processes – Haibing Shao (Helmholtz Centre for Environmental Research - UFZ Leipzig, Germany)*

9:35 – 12:30 **Working Session 2:** *Sorption and diffusion processes in reactive transport simulations (20+5min per oral presentation), Chair: Glenn Hammond (Sandia National Laboratories, USA)*

Estimation of Radionuclide Partitioning in Agricultural Soils - Calculation of K_D for Various Parameter Combinations – *Volker Hormann (University of Bremen)*

A Prediction of Uranium(VI) Diffusion in Montmorillonite at Various Chemical Solution Conditions – *Christophe Tournassat (BRGM, France)*

10:25 – 10:50 *Coffee break*

Modelling Cs migration through Opalinus clay: A benchmark for single- and multi-species sorption-diffusion models – *Vanessa Montoya (UFZ Leipzig, Germany)*

Joint discussion - Session 2

12:00 – 13:00 *Lunch break*

13:00 – 13:35 **Keynote Talk 3:** *Radionuclide transport in fractured rock: overview and applications – Paolo Trinchero (Amphos21, Spain)*

13:35 – 17:30 **Working Session 3:** *Multidimensional look-up tables, surrogate functions and SA/UA exploitation for reactive transport modelling (20+5min per oral presentation), Chair: Gabriel Wittum (G-CSC University Frankfurt, Germany)*

Implementation of the Smart K_d -concept into the transport code d^3f++ and application to PA relevant systems – *Ulrich Noseck (Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH Braunschweig, Germany)*

Smart K_d -concept as efficient approach to improve geochemistry in reactive transport – *Madlen Stockmann (HZDR, Germany)*

Multiple complex reactive transport calculations to estimate the influence of uncertain Cs sorption parameters on Cs diffusion in clay and to construct a "new Cs K_d band" – *Wilfried Pfingsten (Paul Scherrer Institute, Switzerland)*

14:50 – 15:30 *Coffee break*

Advanced methods for sensitivity analysis: a means to improve robustness and reduce complexity of geochemical models – *Elmar Plischke (TU Clausthal, Germany)*

Parameter sensitivity and uncertainty of particle-based reactive transport: numerical analysis of pathogen transport at a riverbank filtration site – *Dustin Knabe (TU Berlin, Germany)*

Speeding up reactive transport simulations using statistical surrogate models and other algorithmical acceleration techniques – *Marco de Lucia (GFZ German Research Centre for Geosciences Potsdam, Germany)*

Joint discussion – Session 3

17:45 End of day two and 18:15 bus shuttle from HZDR to workshop dinner in Dresden city

19:00 Workshop dinner in [Restaurant e-VITRUM](#), Lennéstraße 1, Dresden

Friday, February 07th

- 08:15 Bus shuttle from "[Gewandhaushotel](#)" in Dresden city to HZDR
- 09:00 – 9:35 **Keynote Talk 4:** Accelerating reactive transport simulations with on-demand machine learning – *Allan Leal (ETH Zurich, Switzerland)*
- 9:35 – 11:00 **Working Session 4:** Variable metrics (20+5min per oral presentation), *Chair: Wilfried Pfingsten (Paul Scherrer Institute, Switzerland)*
- Multiscale modelling and simulation of geochemical processes – *Gabriel Wittum (G-CSC University Frankfurt, Germany)*
- Machine learning enhanced process coupling and parameter upscaling in reactive transport simulations – *Mohamed Mahrous (Paul Scherrer Institut / University of Bern, Switzerland)*
- 10:25 – 10:50 *Coffee break*
- Implementation of mineral-water interface reactions in models for use in environmental management and nuclear waste repository performance assessment – *Mavrik Zavarin (Lawrence Livermore National Laboratory, USA)*
- Joint discussion - Session 4**
- 11:40 – 12:30 **Final discussions of the different approaches to integrate geochemistry in reactive transport modelling - Conclusions**
- 12:30 – 13:30 *Lunch break*
- 13:30 End of the workshop**
- 14:00 – 16:00 Opportunity to visit radiochemical laboratories of the Institute of Resource Ecology at HZDR
(Registration until 31.01. required per mail to smartkd@hzdr.de)