

Hydrogeochemical Transport Modeling *Course*

Instructor: Dr. Boris M. van Breukelen

Hosted by the Freie Universität Berlin, Germany, 8-11 October, 2013

OVERVIEW

This 4-day course introduces participants to the modelling of hydrochemical, isotope geochemical, and microbial processes with the popular PHREEQC and related software. Simulation of all major biogeochemical processes will be explained and practiced step-by-step starting from simple systems and going towards more complex integrated case studies in the end. The course is designed for people who want to refresh their knowledge on (isotope) hydrochemistry and learn how to construct (isotope) biogeochemical models for their own studies. The course focuses on applications in environmental chemistry and contaminant hydrogeology in groundwater and soils. Exercises cover both organic and inorganic (metal) biogeochemistry.



"Groundwater acidification: Nickel mobilization and Al cation-exchange"

COURSE CONTENTS AND GOALS

- Learn to make a conceptual hydrochemical model: which processes and model parameters are relevant, extent of complexity
- How to program a conceptual model in a PHREEQC input file, extend the database file, and inspect the model outcome (PfW, Phreeqc3, Excel, Python)
- How to simulate the main hydrogeochemical processes: complexation, mineral dissolution/precipitation, cation exchange, surface complexation, redox processes and biodegradation
- When and how to formulate reactions as kinetic instead of equilibrium
- How to simulate microbial growth following various approaches
- How to simulate isotope fractionation processes in geochemical models
- Which cases require batch, mixing, inverse, 1-D flow path, and 3-D flow models (with PHAST). All these model types will be applied
- Model calibration, sensitivity, and uncertainty analysis with PEST

Two thirds of the course time is devoted to computer exercises, one third to lectures. Computer exercises will be introduced by short lectures and explained afterwards. Besides Phreeqc for Windows, other useful and freely available open source software will be instructed: PHAST (PHREEQC coupled to HST3D for 3-D modelling), PEST (for Parameter Estimation), and Python (open source alternative to MATLAB for making graphs; see examples in this flyer).

COURSE INSTRUCTOR

The course will be presented by the international expert **Dr. Boris van Breukelen,** Assistant Professor Hydrochemistry at the VU University Amsterdam and specialist for modelling of biogeochemical processes and associated isotope fractionation in (polluted) groundwater environments. This course will be given for the sixth time.



"3-D PHREEQC modelling with PHAST: Aerobic benzene degradation"

COURSE AUDIENCE

The course is aimed at researchers, PhD-students, consultants, and engineers who (plan to) undertake hydrochemical modelling as part of their work or studies. The use of PHREEQC both as research instrument and practical tool will be shown.

PREREQUISITES

Participants will benefit the most from this course if they have a basic knowledge and understanding of groundwater (flow/transport) and hydrochemical processes. Prior modelling experience is not required.

ENROLLMENT & REGISTRATION

The fee for the 4-day course is € 1100. Each day 6½ hours of instruction will be given excluding three breaks of in total 2 hours. The number of participants is limited to 14. The fee covers instruction, desktop computers to work on, the course material printed and on USB flash drive, lunch and refreshments on all days, and a certificate of participation.



"Microbial As(V) respiration: Microbial growth at thermodynamic limits"

COURSE LOCATION, TRANSPORTATION, AND LODGING

The course will be held at the Freie Universität Berlin, Institute for Geological Sciences, Workgroup Hydrogeology. Detailed information regarding transportation, parking, and lodging will be sent upon registration.

FURTHER INFORMATION & REGISTRATION

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