

Geochemical modelling with ORCHESTRA



12-13 August Institut de physique du globe de Paris - Université Paris Diderot (IPGP)

Short description of the course

This two-day course will teach the participants to set up geochemical modelling cases using the software-package ORCHESTRA. Special attention will be given to modelling using advanced adsorption models i.e. the NICA-Donnan for metal binding to organic matter; the Generalized Two Layer Model for ion binding to (hydrated) oxides (Al,Fe,Mn) and the CD-MUSIC model for ion binding to (hydrated) ferric oxide. The optimisation of model parameters using ORCHESTRA in combination with PEST will be demonstrated with a case to optimise proton and metal binding parameters for the NICA-Donnan model based on experimental data. We will discuss the multi-surface approach to model metal partitioning and speciation in soils, sediments and surface water systems and the possibility to combine this with reactive transport modelling. The course includes introductions to the topics and practical sessions to work with the model. Other topics that will be briefly addressed in the course include applications of ORCHESTRA with reactive transport, kinetics, radio-active decay and a biotic ligand model.

About ORCHESTRA

ORCHESTRA, Objects Representing CHEmical Speciation and TRANsport, is a freeware chemical speciation and transport code developed and maintained by Hans Meeussen (Meeussen 2003). Orchestra is programmed in Java and therefore independent of the operating system and runs on Microsoft-Windows, OS-X (Mac) and LINUX. In contrast with other model platforms, the model equations are not part of the model code itself but are described as objects in text format and read by the ORCHESTRA calculation kernel during runtime. This allows users to modify and add new models, which makes ORCHESTRA a very flexible tool. The present object database includes objects to enable the calculation of chemical equilibria (law mass action), mineral equilibria including solid solutions, radio-active decay and transport (convection, diffusion). Several advanced adsorption models are implemented in ORCHESTRA including the NICA-Donnan model for ion binding to humic substances, the Generalized Two Layer Model of Dzombak and Morel and the CD-MUSIC model for ion binding to ferrous oxides and an electrostatic Donnan model for sorption to permanent charge surfaces. Databases with default model parameters are provided for the NICA-Donnan model, GTLM (HFO and MnO), inorganic speciation and mineral equilibria. The model has a graphical user interface to select the desired elements and models. Model parameters can be fitted in combination with the parameter optimization software PEST.

Web pages: ORCHESTRA <http://orchestra.meeussen.nl/>

PEST-ORCHESTRA <http://ressources21.univ-lorraine.fr/content/research-tools/>

Course material: The course includes a tutorial and exercises for the practical sessions. Registered participants can download the course material together with instructions to install the models. The models PEST and ORCHESTRA can be downloaded free of charge from the above mentioned websites.

Practical things: participants should bring their own laptops. ORCHESTRA runs on Windows, Linux and Apple OSX. Pest runs on Windows and Linux.

About the lecturers

Marc F. Benedetti is professor at Université Paris Diderot. He is one of the developers of the NICA-Donnan model has started to address the mechanisms regulating the formation of complexes between trace elements and natural organic colloids. Through a fruitful combination of potentiometric techniques, new ion exchange approaches (Donnan effect), the studies so far have provided a conceptual framework to decipher how major physico-chemical parameters affect the binding of trace elements to organic ligands. These studies also contribute for our general understanding of how different elements compete to binding macromolecules and how the later control the fate of metals in the environment

<http://www.researcherid.com/rid/A-5463-2011>

Bert-Jan (J.E.) Groenenberg is senior researcher/lecturer at Wageningen University and Research and LIEC/Université de Lorraine. He is a specialist in the modelling of geochemical processes and reactive transport in soils and teaches geochemical modelling and environmental risk assessment at the undergraduate and graduate level.

Noémie Janot is a postdoctoral scholar at LIEC/Université de Lorraine. Her research interests include contaminant biogeochemistry and their speciation in ternary metal/OM/mineral systems. She has experience with potentiometric and spectroscopic techniques as well as with thermodynamic speciation models.

Hans (J.C.L.) Meeussen is senior researcher/ consultant with NRG (Nuclear research and consultancy Group, Petten The Netherlands) and guest lecturer at Wageningen University. He is the developer of the ORCHESTRA framework and expert in modelling geochemical processes and reactive transport.

José-Paulo Pinheiro is a professor at ENSG/LIEC/Université de Lorraine. He is specialist in trace metal speciation and bioavailability, interested in developing new experimental methodologies suitable for application in the field and the theoretical aspects, both dynamic and thermodynamic in order to be able to understand the behaviour of trace metals in natural systems.

Booking

Book your course at: <https://goldschmidt.info/2017/eventTypeView?type=323>