



KTH Land and Water  
Resources Engineering

## Geochemical modelling with Visual MINTEQ

*4 days Tuesday-Friday + individual project assignment.*

### Course outline

The aim of this course is to provide course participants with general knowledge on what can be done (and also what cannot be done) with a geochemical code such as Visual MINTEQ. Although we will concentrate on Visual MINTEQ, we will also briefly bring up related software codes such as PHREEQC, Orchestra, Ecosat and WHAM. An advantage with Visual MINTEQ is that it is easy to get started with it. However, some advanced functions, such as coupled chemical transport modeling, need to be done with other programs such as PHREEQC.

Topics covered during this four-day course:

- Introduction to chemical equilibrium programs and thermodynamic databases.
- Modelling speciation in water (inorganic complexes, including different redox species)
- Precipitation and dissolution of mineral phases at equilibrium
- Models for organic complexation (SHM, NICA-Donnan) and their use for simulation of metal complexation in water and in the solid phase
- Use of surface complexation models for simulation of metal ion binding to (hydr)oxides (in particular ferrihydrite and goethite).
- Multisurface models: combination of surface complexation models and organic complexation models for simulation of metal geochemistry in soils.

The course consists of a number of lectures and exercises, plus one individual project assignment to be solved afterwards. The general format is that a lecture is scheduled before lunch each day from Tuesday to Thursday; these lectures will present theory and a number of examples. Exercise time is scheduled for the afternoons and for Friday morning. The exercises consist of a number of problems to be solved; these problems illustrate a number of different typical questions that are normally encountered when using a geochemical model. To pass the course, the participant needs to:

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- Follow the course actively (i.e. be present at the lectures and exercises)
- Solve the problems given during the exercises
- Solve an individual project assignment that makes use of own data, if possible

There is no special textbook for the course, but the participants will have access to the following course material:

- pdf files from the lecture presentations
- a small exercise compendium (containing the problems to be solved during the exercises)
- copies of book chapters and papers that present organic complexation models and surface complexation models
- between 10 and 20 papers showing various examples of modelling applications (to be distributed electronically)

**Schedule** (standard format, can be different depending on participants' interests)

Tuesday (day 1)

9.30-10	Introduction
10-12	Speciation in water; inorganic complexes, redox, thermodynamic databases
12-13	Lunch
13-17	<b>Exercise:</b> Overview of Visual MINTEQ. Modelling speciation (inorganic complexes, redox), managing thermodynamic databases

Wednesday (day 2)

9.30-12	Models for organic complexation. Principles (NICA-Donnan, SHM). Biotic ligand model (BLM).
12-13	Lunch
13-17	<b>Exercise:</b> Speciation modelling that accounts for organic complexation in solution and in the solid phase. Simulation of ecotoxicity with the BLM.

Thursday (day 3)

9.30-12	Surface complexation models. Thermodynamic principles, interface models, examples of applications. Multisurface models, combination of speciation and binding to two or more solid surfaces.
12-13	Lunch

13-17      **Exercise:** Simulation of the binding of metals and anions to (hydr)oxides.

Friday (day 4)

9.15-11.30    **Exercise:** Multisurface models.

11.30-12.00    Final words.

**Miscellaneous**

Course prerequisites: Documented knowledge in basic water chemistry

Computers: Either participants are expected to bring their own laptops, or the course has access to a computer room. The operating system should be Windows (preferably XP or 7).

Course size: The number of participants should preferably be between 10 and 20.

The course described above has previously been held in Luleå (twice), in Kalmar and in Hanoi. Contact us for more information regarding costs etc. if you are interested in asking us to arrange the course at your university or company.

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