



# **FAE3009 Geochemical Modelling with Visual MINTEQ 5.0 credits**

**Geokemisk modellering med Visual MINTEQ**

This is a translation of the Swedish, legally binding, course syllabus.

## **Establishment**

Course syllabus for FAE3009 valid from Spring 2012

## **Grading scale**

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## **Education cycle**

Third cycle

## **Specific prerequisites**

At least 5 ECTS credits in soil chemistry, water chemistry, or equivalent.

## **Language of instruction**

The language of instruction is specified in the course offering information in the course catalogue.

## **Intended learning outcomes**

After the course, the PhD student should know the principles of what can be done (and also what cannot be done) with geochemical software such as Visual MINTEQ. Moreover, PhD students should acquire experience in solution strategies for solving equilibrium problems in soil and water chemistry.

## Course contents

Introduction to chemical equilibrium software, thermodynamic databases, simulation of element speciation in waters (inorganic complexes, 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 to organic matter in solution and in the solid phase, surface complexation models (DLM, CD-MUSIC) for simulation of ion binding onto (hydr)oxide surfaces (in particular ferrihydrite and goethite), definition and use of multisurface geochemical models for simulation of metal chemistry in soils.

## Disposition

Exercises and lectures are held during one intensive week at KTH. Participants work with individual project assignments after the course and should complete the assignments no later than three months after the end of the course.

## Course literature

Book chapters, scientific papers on models and on the use of the models. Exercise compendium with problems that are solved during the course.

## Examination

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

## Other requirements for final grade

Active participation and correctly solved problems (3.0 credits), individual project in which Visual MINTEQ is used in own research (2.0 credits).

## Ethical approach

- All members of a group are responsible for the group's work.

- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.