

Short Courses

Modelling and prediction of speciation in solution and at solid/solution interfaces

Place

Chimie ParisTech Engineer School
Paris (France)

Dates

May 15th-18th 2017

Lecturers

A. Hofmann (Univ. Lille 1 – CNRS, France)
G. Lefèvre (Chimie ParisTech – CNRS, France)
J. Lützenkirchen (KIT/INE, Germany)
R. Marsac (Univ. Rennes – CNRS, France)

Relevant audience and requirements

Researchers and PhD students who want learn or progress in speciation modelling and simulation. Basics of solution chemistry are required.

Objectives

The various modules are intended to introduce the use of scientific software for modelling the speciation of elements in solution or adsorbed to a mineral surface. The course consists of three parts:

- (1) a 1-day introduction to the use of the PHREEQC software to simulate speciation of ions and solids,
- (2) a 1-day introduction to reactive transport with PHREEQC,
- (3) a 2-day lecture on the different surface complexation models and their limitations with examples in PHREEQC.

Lectures are given in a computer room to allow parallel hands-on practical sessions with PHREEQC.

Program

Day 1: Introduction to PHREEQC

Thermodynamic data and databases. Use of PHREEQC: input and output files, equilibria in solution, precipitation/dissolution, ion exchange.

Day 2: Introduction to reactive transport

Transport equations and critical parameters. Coupling between reaction and transport. Modelling in PHREEQC and examples.

Day 3: Introduction to surface complexation

Basics of surface charge/potential, reactive surface groups in 2-pK model, electrostatic double layer, zeta potential, DLVO theory.

Day 4: Advanced courses on surface complexation

Approaches to inverse modelling of solid/solution systems. Multisite Complexation (MUSIC) Model.

Contact

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Registration deadline: March 15th 2017

Form to send to *gregory.lefevre@chimie-paristech.fr*

Given name:

Surname/Family name:

Phone:

E-mail address:

Address:

Contact details of the person in charge of the payment:

Fees (including lunches): €1400 (incl. VAT)

Schedule: 8:30 – 16:00