001-2-5068 Aqueous Chemistry Modeling with PHREEQC

Number of credits: 2 credit hours

Number of meetings: 2 hours per week

Prior requirements: Chemistry of Water S2 (001-2-0003) or an equivalent course, Computer programing course (C, MATLAB or Python), or knowledge in coding.

Registration Limitation: limited to 12 participants

Course goal:

Providing theoretical and practical knowledge for advanced modeling of chemical processes in various aqueous systems using the PHREEQC computer program.

Course objectives:

- Understanding the complexity of chemical-equilibrium modeling in real aqueous environments and introduction to different thermochemical databases and ion activity models.
- Introduction to advanced modeling of chemical-equilibrium systems using computer programs.
- Hands-on experience in using PHREEQC to determine aqueous speciation and perform multiphase chemical-equilibrium calculations.
- Learning how to couple PHREEQC to a general programming language for unlimited modeling
- Hands-on experience in modeling reaction-transport processes and kinetics in natural, polluted and industrial aqueous environments

Introduction:

Chemical equilibrium processes are central in most aqueous systems. It determines the speciation of metals and acid-base reactive species, thus determine their reactivity and mobility. It also determines interaction with gas phase such as the atmosphere and solid phases such as different minerals in soils and aquifers. In real systems, including natural, polluted and engineered, hundreds or more equilibrium reactions occur simultaneously. In addition, the chemical activity of the dissolved constituents depends on the composition, which depends on equilibrium speciation, leading to complex systems of equations which can be only (realistically) solved by computer codes. PHREEQC, developed by the United States Geological Survey, is the leading software for chemical equilibrium modeling. It has numerous modeling capabilities, it is free and open sourced. PHREEQC can also be used within other programing platforms resulting in almost unlimited modeling flexibility. It is therefore a relevant and useful tool to many water professionals in a variety of fields

Course Contents:

Apart from the first lecture, every meeting will accompanied by hands-on practicing in modeling with PHREEQC

- Short repetition on basic water-chemistry concepts and introduction to real-life water chemistry problems.
- Activity coefficient models for complex aqueous systems such as high salinity brines: Extended Debyie-Huckel, SIT, Pitzer. Ion Association models.
- Thermochemical databases – Source of data, activity model and self-consistency. Adding species and phases to the database and performing complex aqueous phase speciation
- Modeling irreversible reactions together with multiphase chemical equilibrium in PHREEQC, including modeling of multistage processes
- Handling outputs in PHREEQC and export to excel
- Adsorption and ion-exchange modeling in PHREEQC
- Short introduction to Python programing language and using PHREEQC in Python
- Modeling kinetic processes and chemical equilibrium with Python-PHREEQC
- Modeling reactive-transport processes with Python-PHREEQC

Course requirements:

- Attendance in the meetings and guiding one classwork session (40%)
- Final project submission (60%)