Water quality modeling

<table>
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<th>Cursus</th>
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<tr>
<td>Energie et durabilité</td>
<td>MA1, MA3</td>
<td>Opt.</td>
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<tr>
<td>Science et ing. computationelles</td>
<td>MA1, MA3</td>
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<tr>
<td>Sciences et ingénierie de l'environnement</td>
<td>MA1, MA3</td>
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Remarque
donnée une année sur deux, les années paires

Summary
This course builds on environmental chemistry and microbiology taken in previous courses. The emphasis is on quantification using the public domain package, PHREEQC, which is an excellent computation tool. Numerous applications are investigated during the course.

Content
Overview of principles and modelling for water quality in water bodies and the subsurface
Topics to be covered will be selected from the following: water phase equilibrium reactions, reaction kinetics, precipitation and dissolution, (mineral) subsurface reactions, cation exchange, bioremediation and contamination degradation, redox reactions, inverse reaction path modelling.

Modelling for prediction, diagnosis and design
The public domain geochemical modelling package, PHREEQC (https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/) will be used extensively for a variety of modelling scenarios and applications based on the reaction processes described above.

Keywords
Biogeochemical modelling, PHREEQC, microbial degradation, carbonate chemistry, aqueous speciation, kinetics, thermodynamics, cation exchange, reactive transport, redox

Learning Prerequisites

Recommended courses
Microbiology for the engineer
Sites remediation
Environmental chemistry

Important concepts to start the course
Basic concepts of chemical modeling (e.g., law of mass action, Monod kinetics) as well as fundamentals of chemical thermodynamics.
Some familiarity with nonlinear algebraic equations and first-order ordinary differential equations.
Students are expected to bring their own laptop to exercise classes (and install PHREEQC).

Learning Outcomes
By the end of the course, the student must be able to:
• Propose solutions to water quality problems
• Formulate mathematical models describing transport processes
• Justify approximations used in approaches to remediation of groundwater
• Assess / Evaluate quantitative results pertaining to changes in water quality
• Choose different methods to solve water quality problems
• Illustrate analyze and plot data explaining outcomes of modeling of water quality problems
• Modify existing PHREEQC models
• Implement concepts taught and illustrated in class and tutorials

Transversal skills

• Assess one’s own level of skill acquisition, and plan their on-going learning goals.
• Manage priorities.
• Make an oral presentation.
• Access and evaluate appropriate sources of information.

Teaching methods
Ex cathedra teaching, exercises

Expected student activities
Attend classes
Present homework solution to class
Complete exercises

Assessment methods
Homework assignments: 10%, mid-term exam: 20%, final written exam (120 min) in the post-semester exam period: 70%.

Supervision
Office hours No
Assistant No
Forum No

Resources
Bibliography
Class notes

Bibliography en bibliothèque
• Geochemistry, Groundwater and Pollution / Appelo

Websites
• https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

Moodle Link
• http://moodle.epfl.ch/course/view.php?id=1121