ENG-400

Water quality modeling

Cursus	Sem.	Type
Computational science and Engineering	MA1, MA3	Opt.
Energy Management and Sustainability	MA1, MA3	Opt.
Environmental Sciences and Engineering	MA1, MA3	Opt.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	Written
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	2 weekly
Exercises	2 weekly
Number of positions	

Remark

Pas donné en 2021-22 - donné 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 qualtiy 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
Assistants	No
Forum	No

Resources

Bibliography

Class notes
Appelo, C. A. J., and D. Postma. 2005. Geochemistry, Groundwater and Pollution, 2nd Edition. A. A. Balkema Publishers, Leiden, The Netherlands.

Ressources 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