Department of Earth and Environmental Sciences
University of Waterloo

Course EARTH652: Reactive Transport Modelling

Instructors: Philippe Van Cappellen and Fereidoun Rezanezhad

Lecture: Two-week intensive course (Spring term, May 14-25, 2018)

Course Description:

This course will review the unifying concepts and mathematical models underlying the quantitative description of reactive transport systems. The focus will be on the coupling of biogeochemical reactions to transport processes in near-surface environments (*e.g.,* soils, sediments, tailings ponds, and shallow aquifer). Examples will range from simple "back of the envelope" mass balance calculations to numerical simulations. Students will learn how to assemble the building blocks of a reactive transport model (RTM). Particular attention will be given to the formulation of biogeochemical reaction networks, the kinetics of abiotic and biotic redox processes, mixed kinetic-equilibrium models, and numerical methods. Some advanced topics, such as bioenergetic models of geomicrobial activity and dual-porosity media, will be covered as special topics as time permits.

Requirements:

This course is designed for graduate students with a background in environmental (geo)chemistry, and a working knowledge of transport processes and partial differential equations. At the start of the course, participants should be familiar with the basic functions of MATLAB and the use of the built-in solvers for ordinary and partial differential equations. Participants should be ready to start right away with MATLAB – no tutorial will be provided. Enrollment is limited to 20 participants.

Course objective:

During this course, students will develop an understanding of coupled hydrological and biogeochemical processes in subsurface environments and explore theoretical approaches to quantitatively analyze these processes. After completing this course, students will be able to 1) interpret chemical distributions in terms of coupled hydrological and biogeochemical processes, 2) derive and manipulate equations governing saturated/unsaturated flow and reactive transport, and 3) apply reactive transport models to real-world situations.

Format:

A typical day will consist of a lecture and exercises in the morning, while the afternoon is reserved for computer practicals. Note that practicals will include creating your own MATLAB scripts and running simulations. You will need to bring your PC with a valid licence of MATLAB. Written reports of the daily assignments are due the next day unless specified otherwise. Two full afternoons will be reserved for group projects (4-5 participants per project). The project will be presented on the last day of the course.

Evaluation:

Class Participation	10%
Assignments	60%
Project and Presentation	30%

Course Outline:

Day 1: General Introduction

- **AM:** Time and spatial scales of reactive transport. Mass conservation. Characteristic time scales. Equilibrium versus steady state.
- **PM:** Solving ODEs in MATLAB: Box models. Assignment 1: PCBs in the Laurentian Great Lakes

Day 2: Reactive Transport Systems

- **AM:** Forcings, processes and properties. Continuum hypothesis. Representative elementary volume. Mass conservation equations. Diffusion and advection. Porous media. Tortuosity. Advection-diffusion-reaction.
- **PM:** Solving PDEs in MATLAB. Assignment 2: Steady state oxygen profiles in sediments. Group projects (forming of the teams).

Day 3: Numerical Methods

- **AM:** Analytical solutions. Taylor series. Forward differencing. Backward differencing. Central difference. Accuracy. Second order derivatives. Crank-Nicolson. Assignment 3: Comparison forward and backward methods.
- **PM:** Solving PDEs in MATLAB. Assignment 4: Non-steady state oxygen profiles in sediments.

Day 4: Coupling Reaction and Transport

- **AM:** Boundary conditions. Damköhler and Péclet numbers. Reaction fronts. Length scales. Reaction types. Mixed equilibrium-kinetic systems. Groundwater carbonate geochemistry. Assignment 5: Boundary conditions. Assignment 6: Quartz dissolution: equilibration length scale.
- **PM:** Newton-Raphson method. Assignment 7: Groundwater pH.

Day 5: Special Topics I: Uranium in the Environment

- **AM:** Uranium: mobility, speciation, bioremediation, toxicity. Microbial uranium reduction. Experimental data. Kinetic models. Key role of chemical speciation.
- **PM:** Reserved for group project.

Day 6: Special Topics II: Transport in Porous Media

- **AM:** Saturated and unsaturated flow. Solute transport. Dual porosity systems. Breakthrough curves: analytical and numerical solutions. Gas transport. Multicomponent diffusion. Travel time distributions.
- **PM:** Introduction to HYDRUS and HP1 (Coupled Hydrus-PHREEQC-1D).

Day 7: Special Topics III: Soil Processes

- **AM:** Soil pore structure. Soil aggregates. Soil respiration. Water table fluctuations. Freeze-thaw cycles. Nutrient transport. Greenhouse gas exchanges. Contaminated soils (hydrocarbons).
- **PM:** Transport with HYDRUS & HP1.

Day 8: Special Topics IV: Geomicrobiology

- **AM:** Microbial growth. Microbial ecology. Bioenergetics. Biofilms. Microbial transport. Bioavailability. Biodegradation.
- **PM:** Reactive Transport with HYDRUS & HP1. Assignment 8: Sulfate reduction in peat soils

Day 9: Special Topics V: TBD

- **AM:** TBD
- **PM:** Finalize group projects and presentations.

Day 10: Group Presentations

- **AM:** Group presentations and discussion
- **PM:** Group presentations and discussion