

Short Course in Multicomponent Reactive Flow and Transport

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Held: 18th - 21st October, 2005 - University of Bern, Switzerland

ITC School of Underground Waste Storage and Disposal

and

Rock-Water Interaction Group

Institute of Geological Sciences

University of Bern
Course outline

This 4 day short course will present the fundamentals of reactive flow and transport in porous media through a combination of lectures and hands-on computer exercises based on the reactive flow and transport code Crunch (See below for technical details on the Crunch code).

Lectures will focus on fundamental issues regarding the analysis and understanding of reactive transport in porous media, with applications to both earth and environmental science. This includes the theoretical and practical considerations in modeling reactive transport, but also issues concerning conceptual model development and parameter estimation. Wherever possible, linkages are made between computer simulations and laboratory and/or field investigations of the relevant reactive transport phenomena.

Computer laboratory exercises will make use of the code Crunch to investigate some of the essential mathematical and numerical aspects of modeling reactive transport, for example, the treatment of (bio)geochemical reactions as equilibrium versus kinetically-controlled, the role of different transport processes like advection and diffusion, sources of error in the numerical implementation of reactions and transport, and the effect of coupling between reactions and transport on the porosity and permeability of natural media. Laboratory exercises will draw on examples from reactive contaminant transport, chemical weathering, non-isothermal flow and reaction, microbially-mediated oxidation-reduction reactions, as well as other topics.

It is recommended for all those working on the hydrogeological and geochemical aspects of site characterization and performance and safety assessment.

Course prerequisite

University-level inorganic chemistry. Introductory thermodynamics or physical chemistry. Introductory mineralogy, or mineral chemistry, or clay mineralogy. Basic knowledge of the mineral chemistry of rock forming silicates and carbonates. Advanced course in aqueous geochemistry, or thermodynamics, or petrology, or sedimentary geochemistry. Computer literacy (Mac or PC).

Lecture Topics

October 18

- Review of multicomponent aqueous geochemistry
 - a. Aqueous and surface complexation
 - b. Multicomponent ion exchange
 - c. Kinetics of mineral precipitation and dissolution
 - d. Microbially-mediated reaction networks and the control of redox

- Mathematical and numerical implementation of mixed equilibrium and kinetic reaction networks

October 19

- Introduction to groundwater flow
- Variable density flow
- Heat transfer and its effect on flow
- Fundamental transport processes in porous media
- Numerical treatment of transport

October 20

- Reactive flow and transport in one dimension
 - a. Non-dimensional groups that control system behavior (Damköhler and Peclet numbers)
 - b. Types of numerical error associated with reactive transport simulation
- Topics in multi-dimensional reactive flow and transport

October 21

- Advanced topics in reactive transport
 - a. Reaction-induced porosity and permeability change
 - b. Scale dependence of reactive transport
 - c. High performance computing and reactive transport

Course tutors

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Rock-Water Interaction / University of Bern

APPENDIX A: A Computer Program for Multicomponent Reactive Transport in Porous Media

CRUNCH is a computer program for simulating multicomponent multi-dimensional reactive transport in porous media. The code is written entirely in FORTRAN 90 and incorporates into a single code most of the features previously found in the GIMRT/OS3D package (Steefel and Yabusaki, 1996; Steefel, 2001) along with a large number of new features. The use of the FORTRAN 90 language allows for runtime allocation of memory for arrays, thus minimizing the memory requirements while maximizing the number of options which can be selected at runtime. Using an automatic read of a

thermodynamic and kinetic database, the code can be used for reactive transport problems of arbitrary complexity and size (i.e., there is no a priori restriction on the number of species or reactions considered).

The main features of the code include:

- simulation of advective, dispersive, and diffusive transport transport in up to two dimension using the global implicit (GIMRT) option or three dimensions using time-splitting of transport and reaction (OS3D);
- non-isothermal transport and reaction;
- 2D and 3D variable density flow under fully saturated conditions, coupled at every time step to the reactive transport calculations;
- reaction-induced porosity and permeability feedback to both diffusion and flow;
- unsaturated (gas-liquid) transport with equilibrium gas-aqueous phase exchange;
- multicomponent aqueous complexation;
- kinetically-controlled mineral precipitation and dissolution;
 - multicomponent ion exchange on multiple sites;
- multicomponent surface complexation on multiple sites with or without an electrostatic correction based on the double layer model (Dzombak and Morel, 1990). Site densities are linked to mineral concentrations which may evolve;
- biologically-mediated reactions based on Monod-type formulations;
- radioactive decay chains;
- burial, erosion, and compaction of porous medium, with explicit treatment of spatially variable solid phase advection;
- multicomponent diffusion with an electrochemical migration term to correct for electroneutrality where diffusion coefficients of charged species differ;
- automatic read of a reformatted version of the EQ3/EQ6 database augmented with a kinetic database;
- multiple options (equilibration with a gas or mineral phase, total concentration, fixed activity) for initialization of boundary and initial conditions.

Features now under development include:

- Calculation of heat transfer and coupling to the flow;
- Treatment of activity corrections at high ionic strength with the Pitzer approach, with an automatic read of the EQ3/6 Pitzer database;
- Extension to three dimensions for the GIMRT option.

The code uses an integrated finite volume approach currently restricted to orthogonal grids. Advective transport may be simulated with the standard upwind method or with a third order accurate TVD method when using the OS3D runtime option.