

Geochemical Modelling of Natural and Contaminated Groundwaters

Last Updated Wednesday, 25 June 2008

Held: 15 - 19th March, 2004 - University of Bern, Switzerland

organised by

ITC School of Underground Waste Storage and Disposal

and

Rock-Water Interaction Group

Institute of Geological Sciences

University of Bern

Modelling geochemical interactions in groundwaters is an essential aspect of assessing the long-term behaviour of underground waste repositories and of contaminated natural environments. Not only does groundwater chemistry affect the behaviour of wastes and engineered materials, it is also of central importance in the transport of contaminants through rocks and soils. Because groundwater chemistry is transient over the long periods of concern in waste disposal, the ability to model rock-water interactions and evaluate palaeo-flow systems is also important. This course provides an in depth introduction and practical training in the key areas of groundwater geochemical modelling: thermodynamics, kinetics, isotope behaviour, groundwater mixing and reactive transport.

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). Students: from 6. Semester upwards.

Course outline

Hours

Monday, March 15 (8:45 - 12:00 & 13:30 - 17:00)

1.5

Introduction to modelling: Equilibrium approach, inverse modelling, forward modelling, kinetic effects, testing of models, introduction to isotope hydrogeology.

2.0

Thermodynamics: Equilibrium constant, solubility product, activity of aqueous species / gases / solids, speciation, thermodynamic data bases

1.5

Kinetics: Fundamental equations, mineral dissolution rates

2.0

Exercise 1: Modelling of speciation and mineral saturation (PHREEQC)

Hours

Tuesday, March 16 (8:45 - 12:00 & 13:30 - 17:00)

2.0

Carbonate groundwaters: Governing equilibria, speciation, pH buffering

2.0

Exercise 2: Geochemical modelling of carbonate system (PHREEQC)

1.5

Overview of dominant species in groundwater: Species predominance diagrams, identification of contaminants

1.5

Redox: Redox half cells, redox equilibria, balancing redox equilibria, redox of a system, electrochemical potential, Eh-pH (pe, fO₂) relationship, measurement of Eh, case studies

Hours

Wednesday, March 17 (8:45 - 12:00 & 13:30 - 17:00)

1.0

Redox: continued

1.0

Exercise 3: Redox computer exercises (PHREEQC)

2.0

Ion exchange and sorption: Theory, examples, computation of ion exchange and sorption

3.0

Exercise 4: Ion exchange and sorption (PHREEQC)

Hours

Thursday, March 18 (8:45 - 12:00 & 13:30 - 17:00)

2.0

Isotopes in groundwater: Theory, application (residence time, groundwater flow paths, redox)

1.0

Exercise 5: Isotopes

2.5

Silicate reactions and weathering: Theory (governing equilibria, speciation, pH buffering, activity- activity ratio diagrams)

1.5

Exercise 6: Silicate reactions (PHREEQC)

Hours

Friday, March 19 (8:45 - 12:00 & 13:30 - 17:00)

2.0

Reactive transport modeling

2.5

Exercise 7: Reactive transport modelling (CRUNCH, PHREEQC)

2.0

Exercise 8: From sampling to interpretation

0.5

Overview of other topics and course summary

Course tutors

Dr. Urs Mäder

Dr. Nick Waber

Course credits = 2.5 ECTS points
Course material provided

lecture notes

problem sets

some parts of manuals for computer programs (or PDF files)

contact addresses for obtaining computer codes
Course fees (Excluding travel, accommodation and subsistence)

Professional: 2500 CHF

Postdoctoral Researches: 1200 CHF

Postgraduates: A limited number of cost free places* will be available

Course registration and payment.

Closed
Working language

This course will be taught in English. There will be a pre-course problem set in order to form a common basis, and to "condition" participants to a rapid pace of presentation of new material.

Contact person

Hideki Sakuma (ITC Course Director)

Information links

- University of Bern (Institute of Geological Sciences, Rock Water Interactions Group)

<http://www.geo.unibe.ch/rwi/rwi.htm>

- Hotels recommended

Hotel Isola Garni Bern

Hotel Arabelle