

Geochemical Modelling Workshop

Using PHREEQC for laboratory and industrial applications

When:	Saturday 11 August - Sunday 12 August 2018
Where:	Boston University, Room TBC
Price:	\$350 per person
Presenters:	Julien Declercq and Rob Bowell, SRK Consulting (UK) Limited



Abstract

This two day workshop will provide an introduction to geochemical modelling and the USGS geochemical / thermodynamic modelling code PHREEQC (PH, REdox, EQUilibrium, Code). PHREEQC is a free, well-supported software code and one of the most, if not the most, widely used code amongst academia and industry for thermodynamic modelling applications.

During the two day workshop, we will present the different geochemical modelling steps, from the definition of a conceptual model to the geochemical calculations within PHREEQC. We will also present exercises drawn from the presenters' experiences, both in a laboratory setting and applied industrial setting.

The workshop will take place in four sessions split over the two days. The first day will provide an introduction to geochemical models, the conceptualisation of the problems, and an overview of the thermodynamics that govern PHREEQC and the definitions within the databases. We will make a point of discussing the thermodynamic databases available within PHREEQC, their issues and the possible ways to overcome these. We will also provide the basic skills needed to use PHREEQC, including the definition of inputs and outputs, of solid and aqueous solutions, and of the reactions and equilibrium calculations.

The second day will provide a more in-depth look at the possibilities offered by PHREEQC in terms of kinetic, transport, and sorption calculations. The aim is to develop an understanding of how to extract the equations defining the reactivity of mineralogical phases from the literature or experimental data and integrate these into PHREEQC. We will then show you how to use sorption experiments to define attenuation equations and sorption blocks in the program and provide an introduction to transport simulations. The workshop will finish with a general discussion.

Intended Audience

This course is intended for students, researchers, and professionals using or planning to use PHREEQC to model and predict the results of geochemical operations, from simulation of laboratory experiments to natural settings (such as groundwater interaction with bedrock, simulating field data and predicting water quality).

Attendees are encouraged to bring with them their own examples of natural or laboratory systems that they wish to model for discussion with the session tutors.

Presenter biography:

Julien Declercq, MSc., PhD

Julien is a senior consultant with five years' experience in environmental geochemistry, applied primarily to environmental mine impact assessment. Julien's PhD and subsequent postdoctoral research focused on using PHREEQC to define the reactivity of minerals (mainly forsterite) in the conditions necessary for CO₂ storage in aquifers, predict the conditions of the experiments and to model the experimental results. Julien has also undertaken the revision of the Minteq database and established a mineral dissolution kinetics database for PHREEQC.

Rob Howell, Ph.D., C. Chem. MRSC, Eur. Geol., C. Geol. FGS FIMMM

Rob is a corporate consultant with 30 years of experience specialist in the application of chemistry, geochemistry and mineralogy to solve engineering problems. Rob has a background in applied geology in tropical and deeply weathered terrain's and mining consulting in the fields of due diligence, financial and technical audits, process chemistry, environmental geochemistry, environmental engineering and mineralogy. Rob regularly publishes in the field of mineralogy, process chemistry, and applied geochemistry, ARD, contaminated land and water treatment. Co-author of technical publications on gold mineralogy and processing (CRC); water management in the mining industry (UK-EA); and arsenic stabilization (MIRO). Senior Editor Reviews in Mineralogy & Geochemistry v79 on Arsenic geochemistry. Contributor to Encyclopaedia of Geochemistry v.13 (Economic Geology) and to IAEA Geochemistry of Uranium.

Materials Provided:

Each participant will receive: (1) paper and electronic versions of the hand-outs used for the lecture part of the workshop; and (2) an electronic copy of the model inputs used during the course of the workshop.

Materials Required:

Laptop equipped with a version of Microsoft windows with PHREEQC interactive (current build: 3.4.0-12927.msi) downloaded and installed. The latest version can be found at:

http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

Useful links:

SRK Consulting (UK) Ltd

<http://www.srk.co.uk/>

PHREEQC abstract

<http://pubs.usgs.gov/tm/06/a43/>

PHREEQC manual

ftp://brrftp.cr.usgs.gov/pub/charlton/phreeqc/Phreeqc_3_2013_manual.pdf

Tony Appelo's web page for introductory exercises

<http://www.hydrochemistry.eu/>

PHREEQC frequently asked questions

http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/faq.html

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