

# Geochemical Modelling Workshop

## Using PHREEQC for laboratory and industrial applications

**When:** Saturday 12 August - Sunday 13 August 2017  
**Where:** TBC  
**Price:** €350 per person  
**Presenters:** **Julien Declercq and David Tait, SRK Consulting (UK) Limited**



# GOLDSCHMIDT<sup>®</sup>

## PARIS 2017 | AUGUST 13-18

### 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 has four years' experience as a consultant 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 CO<sub>2</sub> 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.

### David Tait, FGS, MSc.

David has 10 years of experience working as a hydrogeological and geochemical consultant working on mining, landfill and contaminated land projects. Before that David spent 4 years working in public and private-sector analytical laboratories. David specialises in water quality risk assessments for industrial sites and his geochemical modelling experience predominantly involves the use of Phreeqc for assessing the evolution of water quality and mine water impacts. David has also conducted geochemical transport modelling within PHREEQC, PHAST and PHT3D within Visual Modflow.

## 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: v3.3.5-10806) downloaded and installed. The latest version can be found at:

[http://wwwbrr.cr.usgs.gov/projects/GWC\\_coupled/phreeqc/](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](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](http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/faq.html)

## Contact

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