

Numerical Modeling of Water-Rock-Gas Interactions and Natural Hydrogen Generation (G584)



Tutor

[Dr. Eric C. Gaucher](#): Lavoisier H2 Geoconsult

Overview

In the rapidly evolving field of natural hydrogen, mastering geochemical modeling is a critical asset for any technical team. This course will give participants the skills to undertake the numerical modeling of water-rock-gas systems and become familiar with the widely-used PHREEQC software package. You will receive debugged and optimized PHREEQC scripts and the specific LH₂G methodology for water chemistry quality control. This allows your team to save weeks of in-house development and avoid costly modeling errors.

Duration and Logistics

Classroom version: A 4-day course including case studies, exercises, and practical work on a variety of waters and H₂ generation systems. The exercises become more complex to allow for a step-by-step approach. The course can be given at your office, or for those wanting an out-of-office experience in Europe, the course can be delivered in Chamonix, France.

Level and Audience

Intermediate. The course is largely aimed at geoscientists, hydro-geochemists, hydrogeologists or process engineers wishing to acquire skills in geochemical numerical modeling. You will be required to have a basic knowledge of chemistry, geochemistry and fundamental notions of thermodynamics.

Objectives

You will learn to:

1. Evaluate water chemistry and correction of the chemical composition.
2. Calculate the speciation of an aqueous solution and simulate water/rock/gas interactions in open or closed batch systems.
3. Model the evolution of fluid composition as a function of temperature, pressure and salinity.
4. Assess the chemical composition of a fluid during dissolution/precipitation of solid phases.
5. Characterize how hydrogen is generated from various rock types.

Course Content

Overview

This is a unique course developed to explore the simulation of hydrogen-generation in selected geological environments.

Day 1

Introduction to Phreeqc

- Phreeqc Program History
- Main keywords
- Databases (Phreeqc, LLNL, Thermoddem, etc)

Case study: Water-rock interaction in the context of a French sparkling mineral water, Badoit.

- Hydrogen production from granite

Day 2

Case study: Petroleum and geothermal waters (carbonate and clastic systems)

- LH₂G Method for verifying and correcting reservoir water analyses with PHREEQC
- Temperature correction, regasification, mineral equilibrium

Day 3

Case study: Caprock Complex Systems Minerals and Clay surface

- Equilibrium with complex mineral assemblage
- Ion exchange

Day 4

Case study: Source rock H₂ generation system

- Hydrothermal systems
- Serpentinization

Day 5: Optional custom course day

Develop your own model.