



# SOCIETÀ GEOCHIMICA ITALIANA




*Course on*

## **Geochemical Modelling Applied to Natural Fluid-Rock systems**

**Firenze  
9-12 February 2026**

# Geochemical Modelling Applied to Natural Fluid-Rock systems



Geochemistry is a fundamental tool for investigating subaerial systems, hydrothermal–volcanic systems, ore deposits, and mineral alteration processes. Through geochemical analysis, scientists can trace the origin, migration, and evolution of fluids responsible for mineralization, reconstruct the thermal and chemical gradients of ancient systems, and identify the mechanisms driving element transport and deposition. In hydrothermal systems, for instance, geochemistry helps reveal how temperature, pressure, and fluid composition influence the solubility of metals and the formation of ore minerals. Isotope geochemistry can help distinguish between magmatic, meteoric, and metamorphic fluid sources, while trace element distributions shed light on reaction pathways and alteration zoning. Similarly, in the context of ore deposit exploration, geochemical mapping and mineral–fluid equilibrium modeling provide critical insights into the spatial and temporal evolution of mineralizing systems. Understanding these processes not only aids in resource discovery but also in the development of sustainable mining strategies and post-mining environmental management. Ultimately, geochemistry bridges the gap between environmental science, mineral exploration, and planetary processes, offering a unified framework to interpret how Earth’s surface and interior systems interact through time. Understanding, and modeling, are the ultimate tools for an accurate interpretation.

## Motivation for this workshop

Environmental legislation often provides a simplified approach to the analysis of natural materials (water, soils, sediments and rocks), which does not take into account the complexity of the geochemical processes that govern their chemical composition. When laboratory- acquired elemental concentrations of soils or natural waters are simply compared with legal threshold values, the information that is used tends to create more issues than solutions. Additionally, legal exclusions of certain elements from analytical protocols limit the scope of understanding, making it difficult to fully characterize the processes that control the chemical evolution of natural fluids and the distribution of elements at the Earth’s surface. In the study of natural waters, in particular, the absence of labile in situ parameters like redox state, alkalinity, and sometimes pH in analytical reports prevents a proper evaluation of the balance or imbalance of aqueous solutions, thus hindering the understanding and prediction of their potential evolutionary pathways. As a consequence, the available compositional data are frequently used to generate classification diagrams that show correlation trends, but do not reveal the complex interactions between aqueous solutions, mineral phases and gases at the origin of the examined compositions. Overcoming these limitations is crucial to advance the study of geochemistry of aqueous solutions, both technically and in regulatory terms and, thus, to understand and predict the fate and distribution of elements in both natural and anthropized environments.

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## Aims and Scope

The course aims to address these issues by answering the following questions:

- Can we expand the data provided by analytical sets to move from classification schemes to predictive modeling?
- Is it possible to create alternative numerical models to describe conceptual models and test different scenarios in the testing phase?
- How can we derive fundamental thermodynamic parameters that describe the behavior of certain elements within a given system?
- Can we design laboratory experiments and simulate their results to optimize boundary conditions and calibrate our models to obtain more accurate results?
- Can we establish a universal theoretical framework to explain trends observed in laboratory experiments and in natural systems?



## Why PHREEQC?

The course bridges theory and fieldwork through computational methods, focusing on geochemical modeling. It introduces participants to **PHREEQC-based open-source geochemical modelling codes** such as **PhreePlot**, **PHAST**, **PhreeqcRM** and **PhreeSQL** showing their capabilities through coding examples. PHREEQC is one of the most popular software packages for simulating a wide range of processes using a variety of modelling forms. It allows the users to examine a number of topics using the modelling approach as the main investigation technique or as supporting tool in the interpretation of data and processes.

## The Course

The course will at first provide the **thermodynamic principles and theoretical framework** that are at the base of geochemical codes and are necessary for their correct use. The instructors will cover **aqueous solution speciation**, the **numerical methods** used to solve gas-water-rock equilibrium systems, and the role of **thermodynamic databases** in understanding the data and affecting the model results. Participants will learn how to **process large datasets** (including thousands of data points) and **present results through graphs** derived from speciation and solubility calculations. They will also learn the importance of time (through **kinetic modeling**) and temperature on geochemical reactions. The final part of the course will focus on **inverse models**, enhancing participants' skills in **transport and reactivity modeling**.

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## The Program

**DB** – Prof. Donato Belmonte; **GM** – Dr. Giordano Montegrossi; **GS** – Prof. Giuseppe Saldi;  
**MZ** – Prof. Marino Vetuschi Zuccolini

### Monday February 9 – Room 3, via G. Capponi 9

14:00 – 15:00	Geochemical thermodynamics and modelling of a fluid-rock system : basic principles and applications	<b>DB</b>
15:00 – 16:00	The solid phase - Thermodynamic properties, equation of state and mixing models of mineral phases (with practical exercises)	<b>DB</b>
16:00 – 16:30	Coffee break	
16:30 – 17:30	The aqueous phase: thermodynamic properties, aqueous speciation, activity models	<b>GM</b>
17:30 – 18:30	Equation of state and gas/water interaction	<b>GM</b>

### Tuesday February 10 – Room 3, via G. Capponi 9

08:00 – 10:30	Phase equilibrium calculations in simple and complex systems - 1) Use and misuse of thermodynamic databases, 2) Gibbs free energy minimization, 3) Practicals and hands-on tutorial	<b>DB</b>
10:30 – 11:00	Coffee break	
11:00 – 13:00	Redox state, Pressure and Temperature effects in different geological context	<b>GM</b>
13:00 – 14:00	Lunch break	
14:00 – 16:00	Introduction to PHREEQC-based codes: from field to computer, PHREEQC features, implementations and programming rules	<b>MZ</b>
16:00 – 16:30	Coffee break	
16:30 – 18:30	Examples: reproducing diagrams from literature, tips & tricks, odd results, useful approach	<b>MZ</b>

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### Wednesday February 11 – Room A, via G. La Pira 4

<b>08:00 – 10:00</b>	Introduction to kinetic including with stable isotopes	<b>GM</b>
<b>10:00 – 10:30</b>	Coffee break	
<b>10:30 – 12:30</b>	Examples – PHREEQC, Phreeplot: toward complex diagrams	<b>MZ</b>
<b>12:30 – 14:00</b>	Lunch break	
<b>14:00 – 16:00</b>	Examples - PHREEQC, PHAST: transport and reaction	<b>MZ</b>
<b>16:00 – 16:30</b>	Coffee break	
<b>16:30 – 18:30</b>	Examples - iPHREEQC and PhreeSQL: parallel computation on big data and post-processing	<b>MZ</b>

### Thursday February 12 – Room 14, via G. Capponi 9

<b>08:00 – 10:30</b>	Experiment-computation integration, illustrated with examples of kinetic reaction models using PHREEQC	<b>GS</b>
<b>10:30 – 11:00</b>	Coffee break	
<b>11:00 – 12:30</b>	Experiment-computation integration, illustrated with examples of kinetic reaction models using PHREEQC	<b>GS</b>
<b>12:30 – 13:30</b>	Discussion and Closing Remarks	

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## Where?

The course will be held in the historic center of Florence at the University of Florence:

- 9, 10 and 12 February 2026: via G. Capponi 9
- 11 February 2026: via G. La Pira 4

## Organizing Committee

Donato Belmonte  
Giordano Montegrossi  
Giuseppe Saldi  
Orlando Vaselli  
Stefania Venturi  
Marino Vetuschì Zuccolini

## Registration fee

The school is reserved to **2026 SoGel members**.  
(<http://www.societageochimica.it/iscriviti>)

The **registration fee** is **50 €**. Travel, accommodation and meals are charged by students.

The maximum number of students is 30.

To register and for more information, send an e-mail to **segreteria@societageochimica.it**