

PhD programme in Earth, Environmental and Resources Sciences

| | |
|-----------------------|--|
| Instructor(s) | Prof. Linda Daniele, University of Chile (UCHILE) |
| Course Title | Hydrogeochemical Interpretation and Modeling using PHREEQC and CrunchFLOW |
| Total Number of Hours | 8 hours (2 CFU) |
| Registration | Registration (also for DiSTAR PhD students) https://forms.office.com/e/F7cF6QO8Ad |

Course Description

This intensive course provides doctoral students with advanced tools for interpreting and modeling hydrogeochemical data. It focuses on integrating field data analysis, geochemical speciation, and reactive transport modeling using PHREEQC and CrunchFLOW. Students will learn to assess data quality, perform charge-balance calculations, and interpret water-rock interactions using equilibrium and kinetic approaches. The course includes practical applications such as mixing models, adsorption processes, inverse modeling, and reactive transport simulation. Case studies and hands-on exercises support the development of problem-solving skills and the ability to interpret hydrogeochemical systems at different scales.

Course Contents

1. Hydrogeochemical interpretation and data quality: charge balance, analytical errors, and speciation.
2. PHREEQC applications: speciation, mixing models, adsorption, and inverse modeling.
3. Kinetic processes: dissolution/precipitation and limitations of equilibrium approaches.
4. Reactive transport modeling with CrunchFLOW: flow, transport, and water-rock interaction.
5. Case studies and synthesis: scaling, numerical issues, and integrated interpretation.

Learning Outcomes

By the end of the course, doctoral students will be able to:

- Understand hydrogeochemical data quality and interpretation challenges
- Apply PHREEQC for speciation, mixing, and inverse modeling
- Simulate kinetic reactions in geochemical systems



- Understand principles of reactive transport modeling
- Interpret complex hydrogeochemical systems using integrated approaches

Teaching Format

Lectures, hands-on modeling exercises, and case study discussions.

Essential Bibliography

PHREEQC and CrunchFLOW documentation and selected scientific papers

Assessment Method

Active participation and practical exercises