Post-doctoral position
Development of COMPass-PhreeqC coupling

Location: BRGM Orléans, France

Scientific fields: Hydrothermal, Geochemistry, Reactive transport modelling

Keywords: Scientific computing, Reactive transport modelling, lithium, mineral resources

Duration: 18 months

Supervisors: Simon Lopez, Arnault Lassin, Laurent André

Application deadline: 31/01/2025

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Context:

Lithium is a critical chemical element that plays a key role in the energy transition. It is one of the main components of batteries for electric vehicles, for which global demand continues to grow. According to the French Ministry of Ecological Transition, the supply of critical metals, and lithium in particular, will be increasingly strategic for the French economy of tomorrow. Among the potential sources of lithium identified in France, those from geothermal brines circulating in the deep reservoirs of the Upper Rhine Graben (URG) appear particularly promising.

BRGM, the French geological survey, and Lithium de France, France's leading independent operator of geothermal heat and lithium, are combining their expertise in a scientific study of geothermal lithium resources in Northern Alsace. Our research project focuses on gaining a better understanding of the mechanisms of natural lithium enrichment in geological reservoirs and in the thermal waters they contain, particularly in the URG area. The goal is to optimize prospecting methods and define the conditions for sustainable management of the geothermal lithium resource.

Thanks to an experimental laboratory approach coupled with 0D to 3D numerical simulations, this project will contribute to a better understanding of the natural lithium cycle and assess how this resource could be developed in a sustainable way.

By the end, this collaboration between BRGM and Lithium de France aims to preserve the natural environment of geothermal lithium, thereby securing a sovereign resource essential to the energy transition.

Description of the post-doctoral work:

The exploitation of deep geothermal reservoirs involves hydrodynamic, thermal and chemical disturbances that need to be predicted to insure the long-term lifespan of these reservoirs. Numerical modelling is a powerful tool to assess these perturbations with non-linear effects. The 3D coupled thermo-hydrodynamic-geochemical simulations envisaged in the project will aim to account for the reciprocal effects of thermal, hydrodynamic and geochemical processes in the reservoir during its exploitation like, for instance, porosity/permeability changes due to dissolution/precipitation reactions whose kinetics are promoted by temperature.

In the specific geological context of the Upper Rhine Graben, such simulations will be done by means of the development of a coupling between a thermo-hydrodynamic code adapted to fractured media, namely the ComPASS software[1], and a geochemical code, namely PhreeqC. ComPASS is based on recent developments to simulate multiphase and multicomponent hydrothermal transfers. Simulations can be carried out on unstructured meshes including complex fracture networks, in which the flow is two-dimensional, coupled to the three-dimensional flow in the porous matrix (hybrid model). For the geochemical code PhreeqC, modules (i.e., IPhreeqC and PhreeqC-RM[2]) have been specifically developed to facilitate its coupling with hydraulic and transport codes. Both ComPASS and PhreeqC codes have been developed to enable parallel calculations.

The post-doctoral work consist in implementing a sequential non-iterative approach (SNIA) coupling of ComPASS and PhreeqC relying on PhreeqC-RM. In addition to managing the balance of materials, charges and heat during information exchange, the coupling must consider that changes in fluid chemistry can induce dissolution/precipitation reactions affecting rock porosity and permeability, and consequently fluid circulation.

Profile:

The applicant will mobilize the following skills and qualities:

- teamwork,
- writing skills,
- good Python programming skills (knowledge of C++ will be a plus)
- experience in modelling of coupled processes (experience in reactive transport modelling and/or hydrothermal modelling will be a plus)

[1] https://brgm.hal.science/hal-04246471
[2] http://dx.doi.org/10.1016/j.advwatres.2015.06.001