Title: Numerical modelling of the formation of clay minerals under hydrothermal conditions.

Laboratoire d'Hydrologie et de Géochimie de Strasbourg (LHYGES) - UMR 7517 (Université de Strasbourg et CNRS)

Advisors : Bertrand Fritz, Damien Daval (LHYGES, Strasbourg)

e-mail address : bfritz@unistra.fr
tél.: 03 68 85 04 12

In the context of the Soultz-sous-Forêts enhanced geothermal system (Alsace, France), the circulation of fluid in the reservoir may favor the dissolution of the main rock-forming minerals of the reservoir (K-spar), while promoting the precipitation of secondary phases (Al-oxides and clays minerals). Laboratory experiments are underway to reproduce and study these dissolution/precipitation processes which occurred in hydrothermal systems.

The aim of this internship is to apply the NANOKIN code to model the reactions observed in laboratory. The major objective is to build a predictive model which would enable us to foresee the nature (Al oxides or clay minerals) and the size of secondary particles formed during our experiments depending on the chemical composition of the solution. Ultimately, such simulations will be compared with the mineralogical composition of the reacted powders to evaluate the predicting ability of the simulations and better design future dissolution/precipitation experiments.

Duration of the stage: 5 months (February to June 2015).

Expected skills:

- numerical modelling,
- mineralogical background,
- aqueous chemistry (thermodynamics, kinetics of water-rock interaction)

Recent publications related to the code NANOKIN :

- Noguera C., Fritz B., Clément A. et Baronnet A (2006) - Nucleation, growth and ageing in closed systems II : dynamics of formation of a new phase. *J. of Crystal Growth,* 297, 187-198.
- Fritz B., Clément A., Amal Y., Noguera C.(2009) Simulation of the nucleation and growth of simple clay minerals in weathering processes : the NANOKIN Code. G*eochimica et Cosmochim. Acta*. 73, 1340-1358. Doi : 10.1016/j.gca.2008.11.043
- Noguera C., Fritz B. and Clément A. (2011) - Simulation of the nucleation and growth of clay minerals coupled with cation exchange. *Geochim. et Cosmochim. Acta,* 75, Issue 12, 3402-3418.
- Fritz B., Clément A., Montes-Hernandes G. and Noguera C. (2013) - Calcite formation by hydrothermal carbonation of portlandite: complementary insights from experiment and simulation. *CRYSTENGCOMM,* 15, 3392-3401, DOI:10.1039/C3CE26969H.