

Master Internship

« Modelling retention of radionuclides - Benchmarking of ThermoChimie Database »

DES-Service d'Étude du Comportement des Radionucléides, Paris-Saclay University, CEA, F-91191 Gif-sur-Yvette.

The fate of chemicals in the environment is of importance in many industrial fields. In the context of radioactive waste management, the behaviour of radionuclides and non-radiological contaminants is assessed using geochemical and migration models. These models are usually relying on thermodynamic data, accounting for stability of phases, speciation in solution, surface complexation, etc. In this context, the Thermochimie consortium (Andra, Ondraf-NIRAS, NWS) is developing further a robust thermodynamic database: "Thermochimie" [1,2].

"ThermoChimie-DB" is under constant development to broaden the ranges of conditions to which it can be applied (pH, T°C, Eh, Compounds). This study aims to model retention with several systems and databases, including Thermochimie, in order to evaluate its performances and limitations. The systems include various radionuclides (Zn/Ni(II), Am/Eu(III), Th(IV)), with a focus on the effect of organic compounds on retention [3]. This benchmarking exercise will help to assess the sensitivity of models to specific thermodynamic data and evidence eventual systems of interest for further studies (lack of data, significant decrease of retention).

The internship will be hosted in the French Alternative Energies and Atomic Energy Commission **(CEA)**. It will be linked to a larger international program, "ThermoChimie project Phase III", including several partners (Andra, Ondraf, NWS, CEA, Amphos²¹).

[1] <u>https://www.thermochimie-tdb.com/</u>

[2] Giffaut et al., 2014. Andra thermodynamic database for performance assessment: ThermoChimie. Applied Geochem. 49, 225-236.

[3] Fralova et al. 2021. Effect of organic compounds on the retention of radionuclides in clay rocks: mechanisms and specificities of Eu(III), Th(IV), and U(VI). *Applied Geochemistry*, 104859.

Applicant profile: Master student in Chemistry, with a focus on nuclear fuel cycle. Practice of PhreeqC and or Thermodynamic databases would be a plus. Curious and motivated by the main topics of our Institute: Energy, Environment, Waste management. Fluent in English.

Workplace / Location: CEA, Saclay Center, 91191 Gif-sur-Yvette, FRANCE. Availability / duration: 4 to 6 months, 1st semester of 2023

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