PhD position

Theoretical study of the fission products remobilisation on primary circuit surfaces for the evaluation of the differed source term

Keywords: theoretical chemistry, surface chemistry, nuclear chemistry

In a severe nuclear accident in a pressurized water reactor, a part of the fission products (FPs) is released from the core and transported via the primary circuit to the confinement vessel, and in some cases to the environment, in variable proportions according to the scenario. During such transport, an important fraction of the FPs is deposited on the different compartments visited and constitutes a potential reservoir for a differed remobilization. The evaluation of the source term needs a fine modelling of the physico-chemical phenomena related with the FPs in the transport (gas-phase reactivity, interface, nucleation…)

The goal of the present PhD project is to improve our capacity to account for the surface effects, in particular non congruent condensation, in the calculation tool developed at IRSN used for severe accident, ASTEC/SOPHAEROS. The condensed phases MoO_3, MoO_2 and RuO_2 and their reaction with the species present in the primary circuit, will be characterized. The PhD candidate will:

(i) investigate, with ab initio calculations, the reactions adsorbate-substrate, and obtain their corresponding $\Delta_f G^{\circ}_{adsorb}(T)$

(ii) implement the values of $\Delta_f G^{\circ}_{adsorb}(T)$ in the code chemical transport ASTEC/SOPHAEROS to model a series of experiments where Ru and Mo are involved

This PhD project will allow the candidate to master theoretical tools to model physico-chemical processes for interest in nuclear processes, and surface chemistry-related phenomena, in close contact with experimental groups.

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Dates, place : Sept/Oct 2021- Sep 2024. The thesis will be mainly conducted at IRSN/LETR in Cadarache (France), with registration and regular visits at LCT (Sorbonne Université in Paris, France).

Salary : IRSN full-time PhD contract of ~ 1600€/month neto, 36 months

Background required : Master degree in Chemistry, Physics or equivalent, with a research internship in theoretical chemistry, materials modelling or related. He/she must know materials modelling codes (VASP, QE, others) and Unix environment. Basic programming skills (python, fortran, c) script level is highly appreciated. Fluent in English oral/written, French recommended.

Contact : CV + motivation letter + recommendation letter

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