REDUPP
Reducing Uncertainty in Performance Prediction

EURATOM

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Latest News in Short

First Annual Report available

The First Annual Report of the REDUPP project is now available as Posiva Working Report 2012-28 at the Posiva web page: *www.posiva.fi*

Lecture Series continued

On September 13, in conjunction with the 2nd informal workshop, held in Uppsala (see below and overleaf) the REDUPP Lecture Series continued with two lectures:

*David Shoesmith held REDUPP Lecture #2 entitled: "The Influence of In-reactor Irradiation on the Chemical/Electro-chemical Reactivity of Uranium Dioxide"

*Peter Oppeneer held REDUPP Lecture #3 entitled: "Modeling of nuclear fuel materials using first-principles calculations"

The Lectures were attended by project members and 15 project-external people, from various locations (eg Uppsala, KTH, SKB, Studsvik). Thank you David and Peter!

Second Informal Workshop

The Second Informal Workshop was held in Uppsala on Friday 14 September. The workshop was visited by Dave Shoesmith, Kastriot Spahiu and José Godinho.

A short report from the workshop is found overleaf.

General Progress

The project is now at the end of the first period (first 18 months), and all Deliverables planned for this period are submitted. The two milestones of the first period have been reached – Samples ready and delivered, First Annual Meeting held – and we will summarise the progress in the upcoming Periodic Report to the EC. The second workshop in Uppsala in September 2012 proved fruitful for discussions and collaborations which has aided the progress, as well as for outreach in connection with the REDUPP Lectures.

The REDUPP project has been presented at the Goldschmidt meeting (Montréal, June 2012), where both Claire Corkhill (USFD) and José Godinho (SU) went to present their work, on CeO_2 and CaF_2 . A paper on the experimental work on CeO_2 is *In Press* at the Journal of Nuclear Materials (Stennett et al). Pablo Maldonado and Peter Oppeneer (UU), in collaboration with José Godinho plan submission of a paper to The Journal of Physical Chemistry, concerning surface energies of CaF_2 and CeO_2.

Lena Z Evins and Neil Hyatt will attend 'The Euratom Disposal Programme Dissemination Workshop' (EURADISS) in October to present the REDUPP project.

See www.skb.se/REDUPP for more information on the project.

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Short report: The Second Informal Workshop, Uppsala, Sept. 2012

The Second Informal Workshop of the REDUPP project, held in Uppsala, 14 September 2012 was attended by WP representatives and 3 guests associated with the project: José Godinho (SU), Kastriot Spahiu (SKB) and David Shoesmith (Western University, Ontario).

Claire Corkhill presented the work on CeO_2 dissolution (WP2 and WP5), where the experiments explore the effects of grain size, pH and temperature. Time for the static batch experiments is now up to ~220 days. For 90°C and 0.01 M HNO_3, the smallest size fraction (25-50 µm) is showing a fairly steady rate, while the medium size fraction appears to have reached a very slow rate close to zero. Higher dissolution rates are observed for pH 2 while in neutral and alkaline conditions there is very slow net dissolution. Precipitation of $Ce(OH)_4$ is indicated for the test run at pH 8.5 and pH 11.7, and is also suggested by PHREEQC modelling. The set-up of the single pass flow through and the micro-channel flow through experiments were discussed, and examples of materials used were passed around.

The results presented by José Godinho in Godinho et al (2012; GCA 86 392–403) were discussed at this workshop in light of two different modelling approaches. The first-principles calculations together with Uppsala, are further presented below. The experimental results have also been used for the 2D ELLE modelling, to explore the possibilities to simulate the dissolution using this tool. A manuscript is planned for submission during the autumn.

After lunch, Emmi Myllykylä presented the progress in WP 3 concerning ThO_2. The pre-tests for dissolution of 2-4 mm

Figure 1. Fragments of the ThO2 pellet made in Sheffield. Note the bright orange colour.

fragments have now been carried out to 115 days, and ended. PHREEQC modelling has been performed for the pre-test conditions. Efforts have been made to solve the problems which arose during the pre-tests: The mystery of orange colour of the ThO_2 pellet surfaces (see Figure. 1) , presented in April, and the difficulties in grinding due to hardness of ThO_2. Also, the requisition for Th-229 tracer is now ready, and an order will be placed to Oak Ridge National Lab. The solubility as a function of pH will be investigated by using the tracer.

Ab initio modelling of fluorite surfaces (WP 6), presented by Pablo Maldonado, show that surfaces are grouped together in 'families' following a linear relation. This allows the surface formation energy of any plane to be calculated. It is possible to use the same equation for CeO_2 as for CaF_2, using a scaling factor of ~2.38. An article is being prepared, in collaboration with José Godinho (Stockholm University), for submission later in the autumn.

Kaija Ollila presented the latest results from the WP4 experiments with alpha-doped UO_2 in natural groundwater. In short, there is now a suggestion that the dissolution rate is slightly higher in natural vs. synthetic groundwater.

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