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# Evaluation of Fluorapatite as a Waste-Form Material: Third Quarter Report, March 1 - May 31 2003

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# Third Quarter Report

## Evaluation of Fluorapatite as a Waste-Form Material

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### Personnel

The current project participants are listed below.


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**Project Description**

Fluorapatite, fluorinated calcium phosphate, has been identified as a potential matrix for the entombment of the zirconium fluoride fission product waste stream from the proposed FLEX process. If the efficacy of fluorapatite-based waste-storage can be demonstrated, then new and potentially more-efficient options for handling and separating high-level wastes, based on fluoride-salt extraction, will become feasible. This proposal will develop a dual-path research project to develop a process to fabricate a synthetic fluorapatite waste form for the $ZrF_4$, FP waste stream, characterize the waste form, examine its performance under environmental conditions, and correlate the behavior of the waste form with natural analogs. Characterization of the material will be accomplished through probing the molecular-scale electronic and geometric structure of the materials in order to relate them to macroscopic properties, with the goal of developing techniques to evaluate and predict the performance of different waste-form materials. Time and funding permitting, other waste forms for the zirconium fluoride, fission product salt waste stream will be examined and benchmarked against the fluorapatite matrix baseline.

**Highlights of Accomplishments**

1. Baseline spectroscopic measurements have been obtained for commercial hydroxyapatite and natural fluorapatite using a wide variety of techniques (*e.g.*, Raman, XPS, FT-IR) useful for probing the chemical and physical properties of materials.

2. Detailed SEM images of natural fluorapatite crystals indicate the presence of naturally included minerals (*e.g.*, Ni), offering the possibility of studying natural analogs to waste-loaded apatite materials.

**Technical progress**

The primary efforts by the two Chemistry M.S. students on this project have been to obtain baseline spectroscopic and imaging data (see Highlights) on pure samples of commercial hydroxyapatite and natural fluorapatite. The goals of these efforts are two-fold: (1) to have fundamental data with which to compare physically and chemically modified materials relevant to waste-storage issues; and (2) to provide substantial training opportunities for the graduate students. A detailed analyses of the measured data also was begun during the reporting period.

In March, co-PI Dale Perry visited UNLV. Discussions held at that time led to plans for physically and chemically preparing samples of hydroxyapatite and fluorapatite "loaded" with surrogate waste materials, such as transition metals and compounds. These plans were developed with the goal of initiating efforts along these lines during summer 2003.

**Management Issues**

1. *Are you spending according to your proposed schedule?* Yes.
2. *How are your completion goals tracking with your proposed timeline?* Reasonably well.
3. *What problems have you encountered? Do you need assistance from the UNLV program management on any of these issues? From the national program?* We have been unable to get any information from Jim Laidler about the most common waste materials targeted for apatite-based storage.
4. *Has the proposed schedule/timeline changed?* We have not begun any joint efforts with the Russian collaborators, partly because their funding was delayed for many months.
5. *What do you expect to accomplish in the next quarter?* Chemical and physical modifications of the baseline materials to include surrogate wastes, followed by spectroscopic and microscopic studies to compare with the pure apatite samples. First detailed measurements using modern x-ray spectroscopy at the ALS.