

November9, 2001

Dr. English C. Pearcy, Manager
Geohydrology & Geochemistry
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road
Building 189
San Antonio, Texas 78228-0510

SUBJECT: REVIEW AND APPROVAL OF INTERMEDIATE MILESTONE 1402-871-200:
"MOLECULAR DYNAMICS STUDY OF AQUEOUS URANYL INTERACTIONS
WITH QUARTZ (010) - JOURNAL PAPER" DATED OCTOBER 23, 2001

Dear Dr. Pearcy:

The Intermediate Milestone entitled "Molecular Dynamics Study of Aqueous Uranyl Interactions with Quartz (010)" (IM1402-871-200) submitted to the U.S. Nuclear Regulatory Commission on October 23, 2001, has been reviewed by the NRC staff. This product is programmatically and technically acceptable.

This paper is exceptionally well written, describing a state-of-the-art approach for characterizing aqueous uranium speciation, and sorption on quartz. Molecular dynamics (MD) simulations of the uranium-quartz-water-carbonate system help explain spectroscopic as well as batch sorption studies, strengthening the technical basis for parameters used in performance assessment. The molecular simulation technique provides a mechanistic view of the speciation and sorption processes.

It is my understanding that the decision to study the uranium-quartz system using this technique as opposed to other radionuclide-bearing systems was driving by the extent to which this system has already been characterized. The MD approach allowed for the integration of different lines of evidence, demonstrating the viability of the technique. In the report, there is mention of uranium sorption on calcite. Can this technique be applied to the neptunium-calcite system, to help explain processes involving that key radionuclide? Although the DOE has stated that it does not intend to use process models in performance assessment, situations when studies help provide mechanistic bases to the empirical results of sorption tests will most likely be referenced. This study serves to convey to the public the technical bases for the NRC work in the area of radionuclide transport and contributes to the NRC strategic goal of increasing public confidence.

If you have any questions concerning this review, please contact me at (301) 415-6597.

Sincerely,

/RA/

John W. Bradbury
Program Element Manager
High-Level Waste Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

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