SUPPORT FOR CONSULTANT REQUEST

February 13, 1998

CONSULTANT: F. Paul Bertetti

RATIONALE FOR USING AND PROGRAMMATIC IMPACT OF NOT USING SUBCONTRACTOR:

This subcontract is established to support the Radionuclide Transport KTI (20-1402-871). The subcontractor will use existing surface complexation models and parameters derived from previous CNWRA sorption research to develop response surfaces suitable for use in PA calculations.

STATEMENT OF WORK:

Preparation of Sorption Modules for PA - Demonstration of Approach

Task Description

The current TPA performance assessment code uses constant sorption coefficients to simulate radionuclide retardation. Sorption, however, is a complex function of system chemistry which is likely to vary throughout the system. This type of chemical dependence for sorption is included in the current TPA code. Detailed process models such as surface complexation models (SCMs) exist for sorption, but these tend to be too cumbersome for direct incorporation into the existing code. One approach to including chemical dependence while maintaining computational efficiency is to use the more detailed modeling to develop response surfaces or look-up tables that can be interpolated to provide sorption coefficients ("smart" K_Ds) for PA analysis that have a more firm geochemical basis.

This task calls for demonstration of the feasibility of this approach to sorption modeling for PA. The consultant is to use geochemical models provided by CNWRA to apply existing SCMs with parameters derived from previous CNWRA sorption research to develop a response surface suitable for use in PA. The consultant will be working with CNWRA researchers, but should be able to work independently. Specific aspects of the work are expected to include:

- A demonstration of approach will initially be focused on Np sorption, with the potential for additional work on U using existing CNWRA data.
- Independent geochemical variables would include, but not necessarily be limited to, pH and $P(CO_2)$.
- The dependent variable to be calculated would be a sorption coefficient (K_D) normalized to surface area ($K_A = K_D/SA$). It is anticipated that surface area could be used as a sampled parameter in PA to extract K_D values from the response surface for use in the transport calculations.

Milestones and Deliverable Dates

The following deliverables and dates are expected:

- Report on preliminary results on development of a sorption module for Np (04/01/98)
- Interim report on demonstration of approach (05/04/98)
- Final report on development of a sorption module for PA (06/30/98)

5/4/98 ECP 4/1/98

The content of these reports will be determined in consultation with the CNWRA PI.

LIST OF ELIGIBLE CONSULTANTS CONSIDERED:

None.

RATIONALE FOR SOLE/SINGLE SOURCE SELECTION:

F. Paul Bertetti conducted sorption research at CNWRA until he left in 1995. He also conducted sorption modeling for CNWRA and was responsible for developing some of the parameters that are an essential part of this proposed subcontract. Because of his prior experience with CNWRA research in areas integrally related to the proposed subcontract, Mr. Bertetti is uniquely able to conduct the proposed scope of work.

RATIONALE FOR NOT USING SwRI RESOURCES:

No resources exist at SwRI for conducting this scope of work.

PROGRAMMATIC IMPACT ON CNWRA WORK:

This will support deliverables for the Radionuclide Transport KTI, including: Preliminary Fracture Sorption Module for TPA 3.2 - Letter Report (IM 1402-871-810) and Preliminary Alluvium Sorption Module for TPA 3.2 - Letter Report (IM 1402-871-830).

RATIONALE FOR RATE:

Estimated duration/hours: 320 hours

Estimated rate/hour: [illegible]our

WORK BREAKDOWN STRUCTURE NUMBERS:

20-1402-871