

**STATEMENT OF WORK FOR DR. JEFFERY GREATHOUSE:****Background and Task Description:**

The work to be accomplished under this consulting arrangement will consist of molecular mechanics and molecular dynamics simulations of radionuclide sorption related to technical assistance provided as part of the Radionuclide Transport Key Technical Issue (RT KTI). Goals of this work are to provide a detailed understanding of the processes controlling radionuclide sorption on minerals present in the alluvial aquifer of the Yucca Mountain area, and to provide support for detailed process models currently being used in Total-System Performance Assessment (TPA) abstractions. The simulations will study the sorption behavior of uranium, neptunium, and other actinides on a variety of mineral sorbents and under varying geochemical conditions.

The consultant will be working with CNWRA researchers, but should be able to work independently. Specific activities are anticipated to include: (1) review of current literature on molecular simulations of sorption processes; (2) use of the computer codes Cerius-2, MOLDY, MONTE, DL-POLY or other codes to conduct molecular simulations of radionuclide sorption; and (3) preparation of abstracts or manuscripts describing the results of the study. In the course of this work, other related tasks may be identified.

**Estimated Utilization (hours):**

250 hours

**Milestones and Deliverable Dates**

The following deliverable and date are expected:

Progress report on molecular simulation study of radionuclide sorption — May 31, 2004.

The content of this report will be determined in consultation with the CNWRA PI. A copy of Dr. Greathouse's electronic scientific notebook needs to be provided to the CNWRA.