STATEMENT OF WORK

Frederick Glasser

RATIONALE

Large amounts of cementitious materials are anticipated to be used during repository construction. The groundwater contacting the cement will undergo reactions that will increase the pH significantly. The resultant alkalinization will affect container materials (for example, shift corrosion mode from unifom to localized), waste foms (for example, increase glass leach rate), and radionuclide transport (for example, alter sorption). It is necessary to model the reactions of cement with groundwater of varying compositions at the anticipated near-field temperatures close to boiling point of water. Preliminary survey of the literature indicates that there is a paucity of high temperature themodynamic data. However, a more thorough review of the literature is needed to assist the modeling activities. Based on the literature survey, recommendations may be made for model conceptualization as well as experimental investigations.

ANTICIPATED ACTIVITIES

Initial activity will involve a thorough review of existing literature to determine the type of data available for extrapolation of room temperature chemistry calculations to high temperatures and high ionic strengths. The second part of the activity will be to collaborate with CNWRA staff in a preliminary exercise of appropriate models to determine the possible range of near-field environments as a result of cement-water interactions. Depending upon the extent of the data available and the environmental ranges calculated, recommendations may be made for further experimental/modeling activities.

The work shall be perfomed in FY96 and a final report to the CNWRA submitted before September 20, 1996. Depending upon the results of the survey and preliminary calculations, and the funding constraints, further work may be perfomed in FY97.

SUPPORT FOR CONSULTANT REQUEST

March 2, 1998

CONSULTANT: Frederick P. Glasser

RATIONALE FOR USING AND PROGRAMMATIC IMPACT OF NOT USING CONSULTANT:

This consultancy is established to support the Evolution of the Near-Field Environment KTI (20-1402-561) by reviewing DOE and NRC documents related to the effects of cementitious materials on repository performance. The results of these reviews will be used to support development of the ENFE IRSR.

STATEMENT OF WORK:

Documents to be reviewed (no particular order):

1. "TSPA-VA Methods & Assumptions Report" - Sections 6.3 "Near Field Geochemical Environment" and 6.6 "Engineered Barrier Transport System"

2. DOE Site Characterization Plan (SCP) Progress Report #16 - pg. 4-7 through 4-8, 5-17 through 5-18, 5-22, 5-43 through 5-46, 5-61 through 5-64, 6-8, 6-32 through 6-34, and 6-37.

3. "Near-Field and Altered-Zone Environment Report Volume 1: Technical Basis for EBS Design, Rev. 1," 1997, pg. 46 - 47.

4. TRW, 1996. "Status/Summary Report for Fiscal Year 1996 Activities within the Performance Assessment Overview Study on the Consequences of Cementitious Materials" (total of 186 pages with attachments that include (1) an expert report by Prof. Della Roy entitled "Potential Geochemical Effects of Evolving Cementitious Materials"; (2) an expert report by Prof. Hamlin Jennings entitled "Report on Potential Geological Effects of Evolving Cementitious Materials Used in the Yucca Mountain Waste Disposal Project"; and (3) expert report by Dr. Maria Onofrei entitled Independent Analysis of Issues related to Repository Performance"

5. "Hydrothermal Alteration of Concrete: Yucca Mountain Repository Analogues", Myers and Meike, 1997, UCRL-JC-128948.

6. "Experimental Investigation of Cement, Topopah Spring Tuff, and Water Interactions at 200 °C," Carrol, Alai, and Bruton, 1997.

7. "Hydrothermal Alteration of Cementitious Materials Part II: Second and Third Batch of Samples," Myers and Meike ,1997.

8. "Thermodynamics of Calcium Silicate Hydrates Phase I: Development of a Database Dedicated to Modeling Concrete Dissolution at 25 °C," Clodic and Meike, 1997.

9. "A discussion of the relationship between repository thermal history, water budget and the evolution of cementitious materials," Meike, 1997.

Glasser, Frederik P.

STATEMENT OF WORK FOR UNIVERSITY OF ABERDEEN

Task 1—Compilation and critical assessment of literature data on the preparation, thermodynamic properties, including solubility, of selected phases shown in table 1. Critical evaluation of the literature on the probable stability of phases of the $CaO-SiO_2-H_2O$ system under autoclaved conditions, 100–200 °C.

Task 2—Preparation of cement gels at several molar ratios Ca:Si 1.8, 1.5, 1.2 and 0.8 (approximately) and cured at 100–130 °C in water vapour at 1 bar total pressure for up to several months. Determine polymerisation and/or crystallisation state by x-ray diffraction, transmission electron microscopy and NMR. Determine water content by thermogravimetry and surface area by N_2 sorption. If the samples remain physically coherent, determine porosity by mercury intrusion.

Task 3—Using existing stocks, determine experimentally the 25 °C solubilities and pH conditioning abilities of phases shown in table 1 with Ca:Si mole ratios > 0.83 at 20 °C. Include in the measurements the thermally-altered gels, characterization data for which will be obtained in task 2. Rehydrate at 25 °C the gels that were steam cured at 1 bar pressure and 100–130 °C, determine the reaction products, and measure the solubilities for comparison with data for fresh gels.

Table 1. Hydration products of the $CaO-SiO_2-H_2O$ system believed to be stable in the range 100–200°C at Saturated Steam Pressures.

Approximate Ca:Si ratio	Name or Mineral Name	Typical Constitutional Formula
	Portlandite	$Ca(OH)_2$
2	α-dicalcium silicate hydrate	$Ca_2(HSiO_4)OH$
2	Hillebrandite	$Ca_2SiO_3(OH)_2$
1.5	Afwillite	$Ca_3(SiO_3)_2(OH)_2 \cdot 2H_2O$
1.33	Foshagite	$Ca_4(Si_3O_9)(OH)_2$
1.0	Xonotlite	$Ca_6(Si_6O_{17})(OH)_2$
~0.83	Tobermorite (11Å)	$Ca_5Si_6O_{16}(OH)_2 \cdot 4H_2O$
~0.67	Gyrolite	$NaCa_{16}Si_{23}AlO_{60}(OH)_8 \cdot 14H_2O$

Milestones and Deliverable Dates

The following deliverables and dates are expected:

A report on task 1, discussing the critical assessment of literature data on the preparation and thermodynamic properties of cement phases, will be provided by the University of Aberdeen (8/31/99). A status report providing the details and results of experimental studies conducted under tasks 2 and 3 will also be provided by the University of Aberdeen (12/31/99). One of the two reports will need to include an assessment, based on literature data or task 2 and 3 data, of the probable future state of cement at Yucca Mountain following prolonged elevated temperature cure at1 bar H_2O pressure, the potential pH conditioning impact of cement materials during and subsequent to thermal excursion, the suitability of concrete liners as engineering materials in a heated geologic repository such as Yucca Mountain, and the deficiency of current knowledge regarding cement phase properties.