

## 7 REPOSITORY DESIGN AND THERMAL-MECHANICAL EFFECTS

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### 7.1 INTRODUCTION

Evaluation of time-dependent thermal-mechanical (TM) coupled response of jointed rock mass is the primary focus of the Repository Design and Thermal-Mechanical Effects (RDTME) Key Technical Issue (KTI). Postclosure performance assessment (PA) requires an understanding of the TM response of the jointed rock mass over the compliance period (thousands of years) as it influences near-field environment and waste package (WP) degradation, performance of seals, and flow; and radionuclide transport mechanisms. Design for the preclosure operation period ( $\approx 100$  y) requires an understanding of the TM response of the jointed rock mass as it influences drift stability and waste retrievability. Study of TM effects in the near-field environment of the proposed high-level waste (HLW) repository has two components: (i) stability of underground excavations for both opening design and input for PA and (ii) change of hydrological properties of rock fractures due to TM perturbation of the rock mass for input to design and PA.

The U.S. Department of Energy (DOE) has formulated several hypotheses that, if confirmed, would demonstrate that waste can be isolated at the proposed Yucca Mountain (YM) site for long periods of time. These hypotheses include: (i) flow of water into the repository will be low and (ii) the engineered barriers, possibly including backfill, will limit migration of radionuclides into the host rock and any sources of groundwater. Testing these hypotheses will necessitate an understanding of time-dependent TM coupled effects of jointed rock mass on design of the proposed repository and WPs, and repository seals program. Study of stability of underground excavations is needed to test the DOE hypothesis that the engineered barriers will limit migration of radionuclides into the host rock and any sources of groundwater. Investigation on changes of hydrological properties of rock fractures due to TM perturbation is needed to test the other DOE hypothesis that the flow of water into the repository will be low. The main issue of the RDTME KTI has been divided into resolvable subissues. Resolution of the subissues will lead to resolution of the main issue.

There are three subissues associated with this KTI: (i) design of the proposed repository to meet preclosure and postclosure performance objectives, (ii) evaluation of thermal effects on design of the underground facility, and (iii) the role of repository seals in meeting performance objectives. The FY96 activities reported herein address two RDTME KTI subissues. Comments on seismic topical report no. 2 (TR2); development of a rock joint model; and reviews of Exploratory Studies Facility (ESF) design and the DOE regulatory compliance review report address several components of the KTI subissue on design of the proposed repository to meet preclosure and postclosure performance objectives. A parametric study of drift stability in a jointed rock mass and a review of the DOE *in situ* heater test address some components of the subissue on evaluation of the thermal effect on design of the underground facility. These activities and results will be discussed to assess the extent to which these subissues have been resolved through FY96.

## **7.2 OBJECTIVES AND SCOPE OF WORK**

During FY96, the primary objective of the RDTME KTI was to address some components of subissues (i) and (ii) discussed in the previous section. The main activities in accomplishing the objective include review of the DOE repository design program with emphasis on technical reviews of the DOE seismic design methodology topical report, ESF design reports, and design control process reports. Other activities included identification of thermal load and site specific rock mechanical and thermal parameters that may significantly affect the emplacement drift stability and waste retrievability through a TM parametric study and review of DOE ESF heater tests. An additional activity was to selectively develop prediction tools for the TM analysis of jointed rock mass under cyclic pseudostatic and seismic loads.

The scope of work for review of the DOE design of the proposed repository included review of the DOE seismic TR2 including participation in two DOE/Nuclear Regulatory Commission (NRC) Appendix 7 meetings, review of ESF design and supporting documents, and review of the DOE regulatory compliance review report. The review of ESF heater tests included an DOE/NRC Appendix 7 meeting and a site visit.

Work performed in regard to independent evaluation of thermal effects on stability of the underground excavations included a parametric study of unbackfilled drifts involving nine thermal, mechanical, and site characteristic parameters, each at two levels, using the Universal Distinct Element Code (UDEC). A 1/8 fractional factorial experimental design approach was used in this parametric study.

The review tools preparation activity included enhancement of the basic rock joint model developed in FY95 and development of methodologies for determination of the parameters associated with the enhanced model.

Significant accomplishments associated with these activities are reported in section 7.3. An assessment of the extent to which the above-mentioned subissues have been resolved through FY96 activities is provided in section 7.4.

## **7.3 SIGNIFICANT TECHNICAL ACCOMPLISHMENTS**

### **7.3.1 Repository Seismic Design**

Due to the long-term performance requirements for the proposed repository, the potential influence of repeated seismic events will need to be addressed by the DOE. Currently available seismic design methodologies may not provide an adequate demonstration that a particular design has appropriately considered seismic effects in the context of repository performance. Consequently, the DOE is attempting to develop a coherent seismic design methodology that is suitable for use in the repository design.

The DOE topical report "Seismic Design Methodology for a Geologic Repository at Yucca Mountain" reviewed by the NRC is the second in a series of three seismic topical reports. Altogether, the reports describe the seismic design process that the DOE plans to implement for the YM Geologic Repository Operations Area (GROA). Seismic topical report no. 1 (TR1) describing the DOE methodology to assess vibratory ground motion and fault displacement hazards has already been reviewed and accepted by the NRC (Nuclear Regulatory Commission, 1996). Seismic TR2 presents the DOE seismic design methodology and criteria for the YM GROA to meet the NRC preclosure safety requirements. The seismic

topical report no. 3 (TR3), scheduled for preparation after completion of TR2, will describe the DOE assessment of seismic hazards for the YM GROA and determination of ground motion and fault displacement values appropriate for design of GROA structures, systems, and components and inputs for postclosure PA objectives. After review and acceptance of TR2 and TR3, it is anticipated the NRC will develop and issue a preclosing evaluation report to address the seismic design process the DOE plans to implement for YM GROA (Nuclear Regulatory Commission, 1996).

A review of TR2 and associated DOE/NRC technical interactions generated eight comments: (i) inadequacy of linkages between the proposed preclosure seismic design methodology and the postclosure performance considerations, (ii) lack of relationship between the DOE proposed four seismic performance categories and the NRC category 1 and category 2 design basis events in the proposed rule change to 10 CFR Part 60, (iii) lack of rationale for choosing mean probabilistic seismic hazards to determine ground motion and fault offset design basis events, (iv) inappropriateness of treatment of repeated seismic loadings as low-probability/low-consequence events, (v) lack of verified or generally accepted methods for the design of underground openings under the loads and time frame of interest for repository performance, (vi) nonconservative safety factors for combining seismic load with *in situ* stress and thermal loads, (vii) lack of details regarding fault-specific investigations needed to define values of set-back distance for fault-avoidance, and (viii) lack of details regarding investigations that the DOE intends to conduct to define the set-back distance for type 1 faults.

Specific recommendations to each of the eight comments were made and transmitted to the DOE. The DOE is currently revising its TR2 addressing these comments. Review of the revised TR2 by the NRC in early FY97 is expected to resolve the concerns related to seismic design methodology.

## **7.3.2 Design Control Process**

### **7.3.2.1 Background**

As a result of past DOE/NRC interactions in the area of ESF/GROA design and associated quality assurance issues, the NRC identified deficiencies in the DOE design control process. It has long been recognized by the NRC that it is impossible for the NRC and Center for Nuclear Waste Regulatory Analyses (CNWRA) staffs to conduct a thorough review of all the DOE design documents given the limited resources at NRC disposal. Consequently, the NRC has used a vertical slice approach in which the NRC and CNWRA staffs would selectively review some important aspects of the DOE ESF/GROA design packages and observe the DOE internal reviews looking for trends that can be used as examples to provide feedback and guidance to the DOE. The NRC has paid particular attention to design of the ESF because it will eventually become a part of the GROA if the YM site is found to be suitable and, therefore, many regulatory requirements applicable to the GROA would also be applicable to the ESF. The DOE found it difficult to demonstrate to the NRC the traceability of regulatory requirements and provide necessary documentary evidence to clearly show that all applicable requirements were indeed being applied to various design components. To thoroughly examine this issue, the NRC conducted a phased in-field verification to evaluate the DOE design control process (Nuclear Regulatory Commission, 1996). There are a number of open items (OI) that resulted from this in-field verification, past DOE/NRC interactions, and the NRC review of the DOE ESF/GROA design documents related to this issue. All of these OI are being monitored by the RDTME KTI and a number of them have been closed during FY96 as a result of staff reviews and interactions with the DOE. Some of the main FY96 activities conducted to help resolve the remaining OI and subissues are reported in this section.

### 7.3.2.2 Regulatory Compliance

To address the NRC concerns on the design control process, the DOE submitted a regulatory compliance review report (U.S. Department of Energy, 1995a; 1995b) to the NRC. The report attempts to provide the NRC staff a description of steps taken by the DOE and criteria used by the Civilian Radioactive Waste Management System Management and Operating Contractor to identify, evaluate, and minimize potential impacts to the proposed site as a result of the ongoing site characterization program. Also included in the report is the description of how 10 CFR Part 60 requirements applicable to the ESF Design Package 2C have been incorporated into the current design. The regulatory compliance review report presents an evaluation of 42 selected requirements for their allocation and traceability into the design solutions of the 11 configuration items included in ESF Design Package 2C. On October 22, 1995, the DOE submitted a letter to the NRC further elaborating the steps taken to improve this design control process (U.S. Department of Energy, 1995c).

The regulatory compliance review report was evaluated as a part of the NRC staff Phase 3 In-Field Verification activities using NUREG-1439 (Gupta et al., 1991) as the basis for compliance determination. The review indicated that, in general, the DOE identified 10 CFR Part 60 design requirements applicable to the ESF Design Package 2C. The assessment of 10 CFR Part 60 design requirements included in the report is acceptable.

As a result of this review, the open items in the checklist of the Phase 3 In-Field Verification related to verifying that appropriate regulatory requirements are being applied to ESF Design Package 2C were closed. To complete the Phase 3 In-Field Verification, assertions made by the DOE in its October 25, 1995, letter (U.S. Department of Energy, 1995c) regarding improvement of the design control process will be verified and implementation of the improved design control process in the ESF design packages will be evaluated in FY97.

### 7.3.2.3 Exploratory Studies Facility Design

The DOE Title II design package of ESF Main Drift (Design Package 8A) consists of a series of design analysis documents. These design analysis documents are released by the DOE in installments. The design analysis reports reviewed by the NRC include ESF Alcove Ground Support Analysis (BABEE0000-01717-0200-00001 REV 01C) and ESF Ground Support—Structural Steel Analysis (BABEE0000-01717-1200-00003 REV 00B). In addition to these two design analysis reports, three supporting reports were also reviewed by the NRC: Fracture Analysis and Rock Quality Designation Estimation for the Yucca Mountain Site Characterization Project (Lin et al., 1993), Geotechnical Characterization of the North Ramp of the Exploratory Studies Facility, Volume I of II: Data Summary (Brechtel et al., 1995), and Drift Design Methodology and Preliminary Application for the Yucca Mountain Site Characterization Project (Hardy and Bauer, 1991).

ESF Alcove Ground Support Analysis is a part of the DOE Title II design package of the ESF Main Drift (Design Package 8A). This report deals with analysis of the stability of the Bow Ridge test alcove (Alcove 2) and two radial borehole tests alcoves (Alcoves 3 and 4) using empirical and analytical methods. Both FLAC3D and 3DEC codes were used in the analysis; no support system was considered in the models analyzed. It was concluded that the effect of 80 and 100 kw/acre of thermal loads would not be significant due to the location of the alcoves relative to the repository horizon. Analysis carried out with *in situ* and seismic loads did not include discrete joints in the rock mass. The modeling results given in this report indicated a significant amount of damage (both tensile and shear failures) in the roof, floor,

and sidewalls of the excavations, and in the pillar between the alcoves and the North Ramp. The report on ESF Ground Support—Structural Steel Analysis deals with the analysis, design, and selection of structural steel ground support members and components. The computer program STAAD-III was used for the analysis and American Institute of Steel Construction Specifications (American Institute of Steel Construction, 1989) were used for the design of steel members and components.

Review of the three supporting reports did not raise any major concerns, however, the two design analysis documents resulted in two observations. These observations are helpful to the DOE in its future repository design exercises. The first observation is that the numerical analysis to determine the stability of ESF drifts and Alcoves 2, 3, and 4 is based on continuum modeling and does not consider the effect of existing joint sets in the rock mass. The extensive rock mass damage predicted by this analysis under *in situ* and seismic load is expected to increase significantly if discontinuum analysis is performed. The second observation indicates that the duration of input shear wave used in the dynamic analysis of the stability of ESF drifts and alcoves is unrealistically low.

### **7.3.3 *In Situ* Heater Test**

The First ESF Thermal Test is planned by the DOE to study the effects of thermal load on hydrology, chemistry, and rock mass-ground support interaction, with an ultimate goal of providing information needed for viability assessment of the proposed YM site for permanent disposal of HLW. This test consists of two phases. The first phase—a single heater test—was started on August 26, 1996 and the second phase—a drift-scale heater test—will be initiated next year. The First ESF Thermal Test will be conducted in Alcove 5 (Thermal Testing Facility) located in the Topopah Spring welded unit (TSw2), lithophysae-poor, south of the North Ramp and east of the ESF Main Drift at Station 28+27 m from the portal. An Appendix 7 meeting was held at the site on July 24, 1996, to discuss the First ESF Thermal Test. As a result of the meeting, concerns related to TM coupling were generated and are summarized in the following paragraphs.

One of the objectives of the single heater test is to develop information on rock mass thermal and mechanical properties at elevated temperatures. The rock mass at the instrumentation location for the single heater test appears to be competent with a relatively smaller number of fractures/joints compared to the rock mass conditions at several other locations within the ESF. Therefore, the rock mass thermal and mechanical properties obtained at this location at elevated temperatures may not be transferrable to other repository locations with extensive fractures/joints. Some effort will need to be made to either obtain rock mass thermal and mechanical properties at elevated temperatures at locations with extensive fractures/joints or develop a reasonable approach for data extrapolation. Otherwise, the usefulness of the rock mass thermal and mechanical properties obtained from this single heater test will be somewhat limited. It is not clear how this issue will be addressed by the DOE. There are additional concerns expressed by other KTIs on the single heater test (see sections 4 and 6).

The planned drift-scale heater test includes activities for investigating interactions between the rock mass and ground support systems. Various ground support systems including those used in the North Ramp and ESF Main Drift are planned to be evaluated in a drift about 66 m long. The main focus of the planned test is to identify potential interaction processes that may affect ground support design. It is likely the planned instrumentation drift will be in a competent rock mass, given its proximity to the single heater test. Thus, interaction processes in the relatively less competent rock mass may not be identified. These processes may affect the stability of emplacement drifts during waste emplacement operations and potential

waste retrieval, and therefore deserve attention during site characterization testing. During interaction with the NRC, the DOE expressed confidence that the 66 m long drift will cover the range of rock conditions expected to be encountered in the TSw2 thermo-mechanical unit. This will be verified during FY97.

### **7.3.4 Parametric Study of Drift Stability—Phase I: Discrete Element Thermal-Mechanical Analysis of Unbackfilled Drifts**

Construction of a geological repository in a jointed rock mass at YM will change the state of stress and cause deformation of surrounding rock and joints. Emplacement of radioactive waste in the proposed repository provides a heat source that will be active over an extended period of time and thus complicate the understanding and prediction of rock mass responses. There are two issues that involve TM effects in the near-field environment: stability of underground openings for both design and input for PA and change of hydrological properties of rock fractures due to TM perturbation of the rock mass for input to design and PA. The objectives of the TM parametric study are to understand rock mass response to drift excavation and waste emplacement as a function of time and to identify mechanical, thermal, and site characteristic parameters that would affect the preclosure and postclosure performance of the proposed repository under heated and seismic conditions. The focus of the phase I TM study is to conduct a parametric investigation of emplacement drifts with no backfill, rock support, or seismic load for 100 yr of heating.

#### **7.3.4.1 Study Method and Model Setup**

The study comprised a series of numerical modeling exercises using UDEC (Itasca Consulting Group, Inc., 1993). A total of 74 UDEC calculations were performed, including 10 scoping runs and 64 final runs. The scoping runs were aimed at identifying the effect of joint patterns. The final runs were selected based on a  $2^k$  fractional factorial experiment design methodology to systematically probe the effects of joint patterns and thermal and mechanical parameters [see Ahola et al. (1996) for details of  $2^k$  fractional factorial design and parameter combinations for all UDEC run cases]. The scoping calculations considered five distinct joint patterns, each containing at least two joint sets (subhorizontal and subvertical, except for several cases that contained an additional subvertical or ubiquitous joint set), while thermal and mechanical properties of rock matrix and joints remained fixed at their representative mean values.

Scoping calculations showed that joint patterns did not appear to have a large impact on rock mass response at a distance of more than five diameters away from the drift. Based on the results of scoping analyses, it was decided that for the final UDEC runs only two joint sets would be simulated: one subvertical with varying spacing and orientation and one subhorizontal with fixed spacing and varying orientation. Also, based mostly on engineering judgment and past modeling experience, it was decided the additional parameters considered in the final set of UDEC runs would include joint friction angle, intact rock cohesion, intact rock friction angle, intact rock Young's modulus, and thermal expansion coefficient. The upper and lower values of these parameters are given in table 7-1. Thermal loads considered in both the scoping and final UDEC calculations were selected to encompass the DOE hot and cold repository concepts which included a high (100 MTU/acre) and a low (20 MTU/acre) thermal loading strategy. The heat generation of the spent fuel within the WP was modeled as a simple exponentially decaying thermal flux applied directly to the wall of the circular emplacement drift. The decay constant used was  $3.2197 \times 10^{-10}/s$  and the waste was assumed to be 20 yr old at the time of emplacement. Therefore, a total of nine parameters were considered in the final runs including thermal load, three joint geometric parameters, and five rock and joint thermal and mechanical properties.

**Table 7-1. Upper and lower values for UDEC final analyses**

Parameter	Value		Unit
	Upper	Lower	
Subvertical Joint Inclination	85	70	degree
Subhorizontal Joint Inclination	20	10	degree
Subvertical Joint Spacing	0.5	0.2	m
Joint Friction Angle	38	28	degree
Thermal Load	100	20	MTU/acre
Intact Rock Friction Angle	43	18	MPa
Intact Rock Cohesion	50	20	degree
Intact Rock Young's Modulus	32	16	MPa
Thermal Expansion Coefficient	$12 \times 10^{-6}$	$6 \times 10^{-6}$	$K^{-1}$

The final calculations were evaluated in terms of the effect of each parameter on certain performance measures chosen based on the scoping calculations. These performance measures included maximum and minimum principal stresses around the excavation, maximum joint shear displacement, maximum joint closure and separation, roof-to-floor convergence, and extent of yield zone around the excavation.

The UDEC model included a single drift 5 m in diameter and one unit cell width governed by drift to drift spacing, depending on the areal thermal loading selected. The vertical extent of the UDEC models was determined so that the ambient temperatures applied along the upper and lower boundaries did not artificially impact the results for the total selected simulation time of 100 yr. The vertical boundaries represented lines of symmetry based on the assumption of multiple parallel emplacement drifts, and therefore, were assigned with zero horizontal velocity and zero heat flux boundary conditions. To maintain a reasonable number of blocks and finite difference zones, only a region approximately one drift diameter into the rock mass was modeled as having the specified joint spacings assigned for each case. Beyond this region, the size of the blocks was scaled up accordingly as depicted in figure 7-1.

The modeling procedures consisted of obtaining model equilibrium under the *in situ* stress. The drift was then excavated and a new equilibrium stage was reached. From this stage on, thermal load was applied and coupled TM simulations conducted for 100 yr.

### 7.3.4.2 Discussion of Modeling Results

The scoping analyses considering five joint patterns and two thermal loadings show that, in general, joint pattern does not appear to affect the response of the rock mass at a distance of more than five diameters away from the drift. However, joint pattern affects the magnitude and distribution of stresses in the immediate vicinity of the drift (up to about five diameters into the wall) and, therefore, controls the stability of drifts.

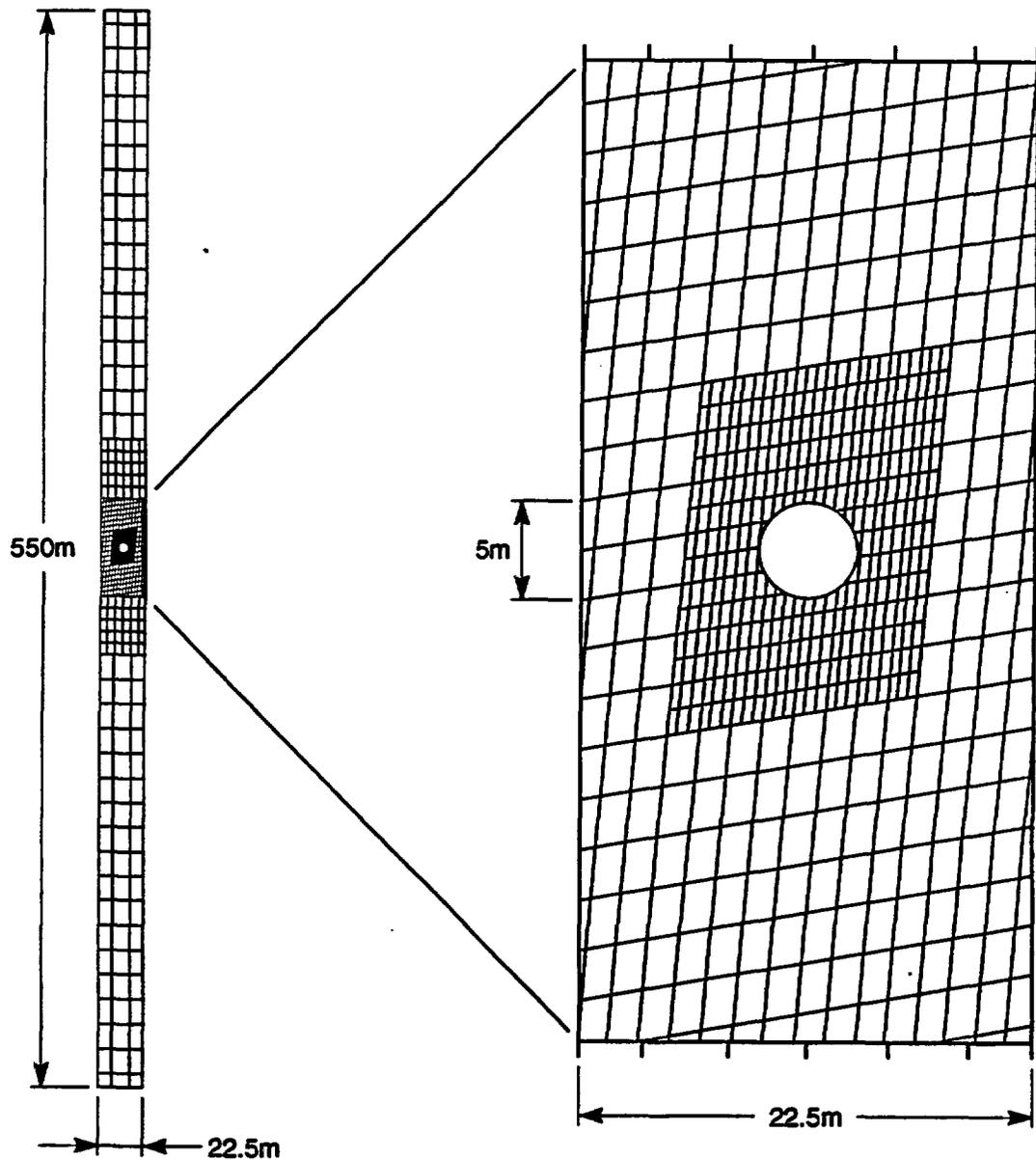


Figure 7-1. UDEC model showing block geometry for one particular joint set pattern and thermal loading

Results of UDEC final runs indicate that thermal loading is an important parameter affecting most performance measures: magnitudes of maximum principal stress, maximum joint shear displacement, maximum joint closure and separation, and extent of yield zone increase as thermal load increases. An increase in thermal load reduces opening convergence. The effects of important parameters on affected performance measures are given in table 7-2.

**Table 7-2. Effects of parameters studied on selected performance measures**

Parameter Increased	Performance Affected					
	Maximum Principal Stress	Maximum Joint Shear Displacement	Maximum Joint Closure	Maximum Joint Separation	Maximum Roof-to-Floor Convergence	Extent of Yield Zone
Subvertical Joint Inclination	I	N (50 yr) I (100 yr)	N	D	D (50 yr) N (100 yr)	N
Subhorizontal Joint Inclination	N	N	N	I	N	N
Subvertical Joint Spacing	I	N (50 yr) D (100 yr)	N	N	N (50 yr) D (100 yr)	D
Joint Friction Angle	N	N	N	D	D	D
Thermal Load	I	I	I	I	D	I
Intact Rock Friction Angle	N	N	N	N	N	D
Intact Rock Young's Modulus	I	N (50 yr) I (100 yr)	N (50 yr) I (100 yr)	I	D (50 yr) N (100 yr)	I
Intact rock Cohesion	N	N	N	N	N	N (50 yr) D (100 yr)
Thermal Expansion Coefficient	I	N	I	I	D (50 yr) N (100 yr)	I

Note: I = increase; D = decrease; N = no effect

General results show that shear displacement usually occurs along joints near the drift following excavation and increases after heating, particularly along the horizontal-subhorizontal joint set. Although in most cases the extensiveness and magnitude of joint shear displacement are limited, there are cases in which thermally enhanced joint shear displacement becomes so extensive that it could greatly increase shear-induced permeability (Barton et al., 1985) and, therefore, increase the possibility of groundwater flowing into the drift. Figure 7-2 depicts the distribution of joint shear displacements after heating for Case 12 [case numbers and associated input parameters are described in Ahola et al. (1996)].

Yielding occurs in some of the cases after heating, mostly by tensile failure. Although yield zones in most cases are localized to the immediate areas around the drift, they cover the entire pillar in the worst cases. Figure 7-3 shows yielding zones after 100 yr heating for Case 26. Most studies show that yielding of intact rock causes the rock mass to dilate which, in turn, could increase rock permeability (Wawersik and Brace, 1971; Wawersik and Fairhurst, 1970; Bieniawski, 1969; Ofoegbu and Curran, 1992). It is important in emplacement drift design to make sure the extent of yielding is limited to avoid direct hydraulic connections between drifts and overlying strata that could facilitate groundwater inflow from potential perched water zones.

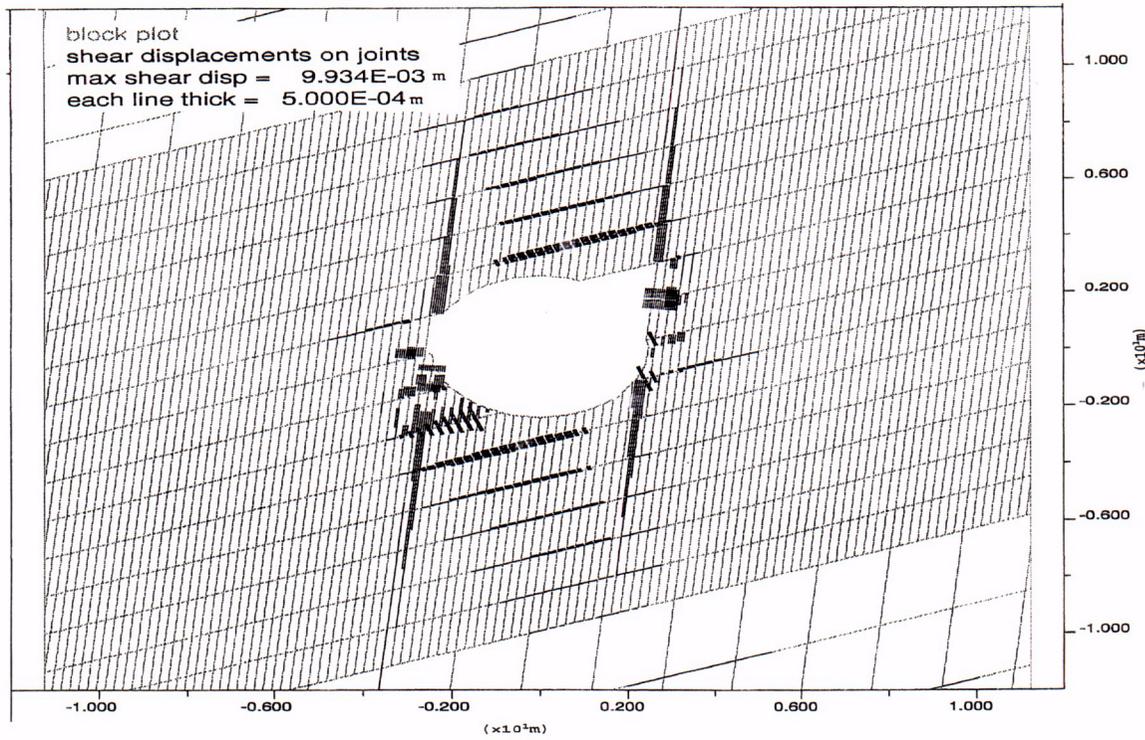


Figure 7-2. Distribution and magnitude of joint shear displacements after 100 yr of heating for Case 12

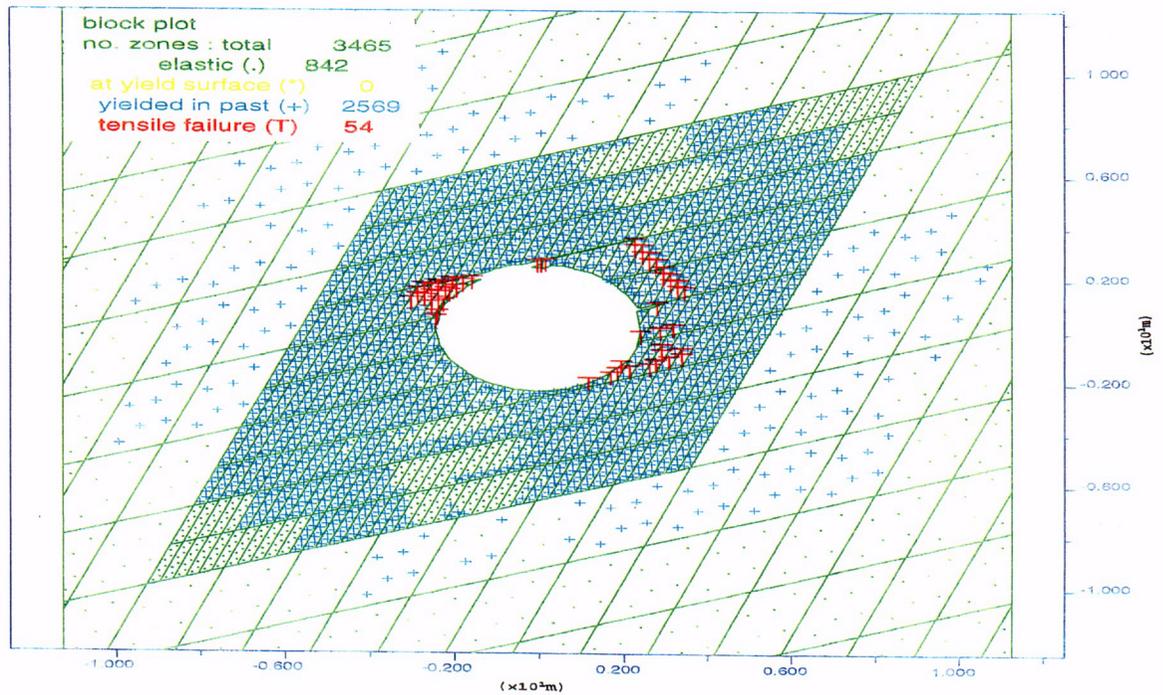


Figure 7-3. Failure distribution after 100 yr of heating for Case 26

In most cases, subvertical joints near the sidewalls of the drift tend to dilate due to stress relaxation immediately after drift excavation. This dilation tends to increase during heating. However, the extent of the zone where joints dilate does not appear to increase significantly during heating. Heating increases closure along subvertical joints above and below the drift. In general, the extent of these zones of joint dilation is less than one drift diameter. Figure 7-4 shows the distribution of joint opening and closure for a typical case.

The maximum compressive stress usually occurs in drift sidewalls following excavation. Its magnitude increases and its location shifts to the immediate roof and floor areas as heating progresses. Although tensile stresses are predicted following drift excavation as well as after heating, heating appears to change the location of the maximum tensile stress from roof and floor areas to the sidewalls of the drift. Circumferential stress generally increases in the roof with heating, while it decreases in the ribs of the drift due to thermal expansion. This phenomenon occurs because thermal expansion creates a stress state that tends to counteract with the mining-induced stresses in the rib of the drift while enhance the mining-induced stresses on the roof and floor areas.

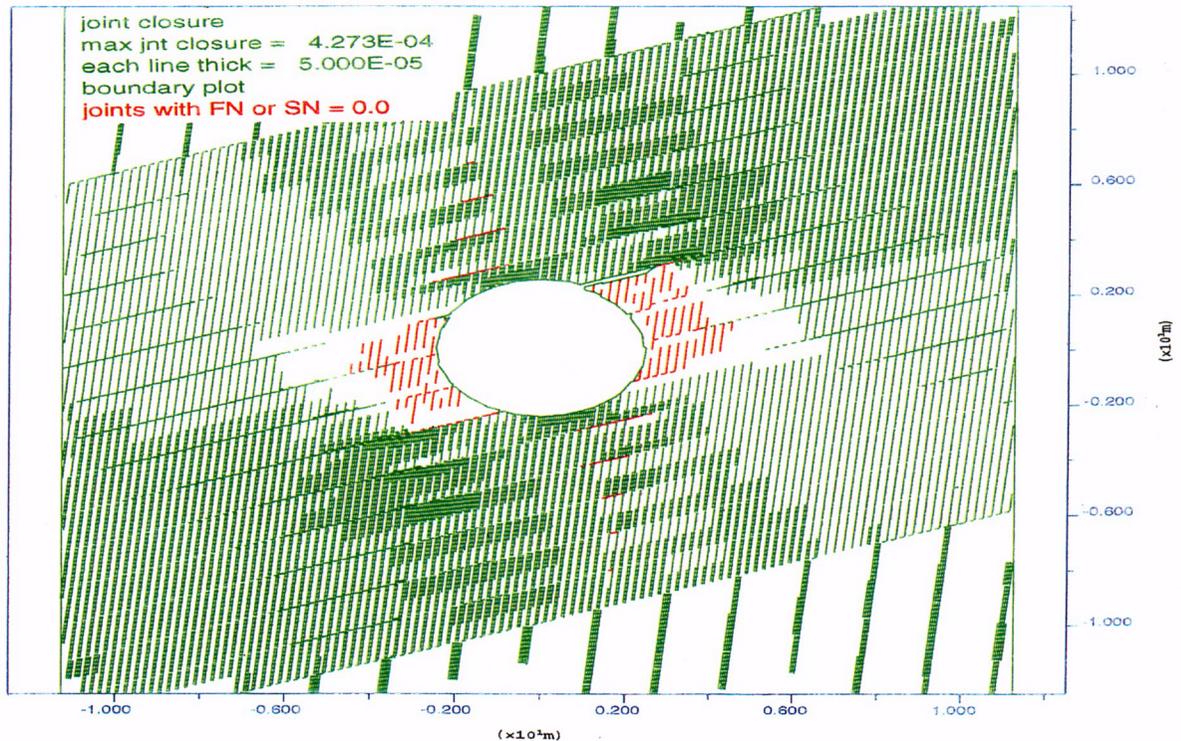
Increasing the coefficient of thermal expansion increases the magnitude of maximum principal stress, maximum joint separation, maximum joint closure, and extent of yield zone, and reduces the short-term convergence. Increasing the intact rock Young's modulus results in higher maximum principal stress, greater maximum joint separation, more extensive yield zone, and increased maximum joint shear displacement and closure after 100 yr of heating while it reduces short-term drift convergence. Higher subvertical joint inclination seems to be associated with higher maximum principal stress when either subhorizontal joint inclination or the coefficient of thermal expansion is at its higher value. Increasing the subhorizontal joint inclination increases maximum joint separation, whereas increasing the subvertical joint spacing reduces joint shear displacement, drift convergence, and extent of yield zone, and increases maximum principal stress. These effects are observed only after 100 yr heating. Joint friction angle has a significant effect on maximum joint separation, convergence, and extent of yield zone. Intact rock friction angle affects only the extent of the yield zone (i.e., a larger intact rock friction angle results in less extensive yielding). Variation of intact rock cohesion does not appear to have an effect on any performance measures other than the extent of the yield zone after 100 yr of heating; that is, an increase in intact rock cohesion reduces the extent of the yield zone.

#### 7.3.4.3 Summary

The most interesting aspects of the results are the increase in joint shear displacement and in the extent of yielding zones around the drift due to heating. As discussed earlier, heating causes significant increases in joint shear displacements over a large area and induced yielding of almost the entire pillar in some extreme cases. Both joint shear displacement and yielding of intact rock could induce dilation that would increase permeability of the rock mass and therefore, affect groundwater flow and radionuclide transport. Phase I TM parametric study shows that thermal load is an important parameter affecting most of the performance measures studied herein. Other parameters also influence drift stability by affecting certain performance measures to various degrees of significance.

#### 7.3.5 Development of Rock Joint Model

Seismic events at YM will take place in an environment of *in situ*, excavation-induced, and thermal stresses. Seismic load will affect both drift stability and hydrological properties of the rock mass in the near-field environment of the proposed HLW repository at YM. Thus, it is necessary to study the effect of seismic load, including the effect of repeated seismic load (Nuclear Waste Technical Review



**Figure 7-4. Distribution of joint opening and closure after 100 yr of heating for typical UDEC run case**

Board, 1992) on proposed repository performance. Experimental results of direct shear tests on joints subjected to cyclic pseudostatic and dynamic loads (Celestino and Goodman, 1979; Gillette et al., 1983; Zubelewicz et al., 1987; Fishman, 1988; Jing et al., 1992; Huang et al., 1993; Wibowo et al., 1993; Hsiung et al., 1994a) have shown that rock joint responses, in terms of both shear strength and dilation, appear to be different in forward and reverse directions of shearing. In reverse shearing, the shear strength is smaller than that in the forward direction. Moreover, dilation realized in forward shearing is almost completely recovered in the reverse direction. Hsiung et al. (1994b) showed that three commonly used rock joint models were unable to simulate joint behavior in reverse shear. Using these models could result in an overestimation of excavation stability, as well as prediction of an unreasonable pattern of fast water flow paths. The objective of developing a new rock joint model, using results of the rock mechanics research project (Hsiung et al., 1994a), is to provide an improved prediction tool to assess seismic effects on the pre- and post-closure performance of the proposed repository and to assist in testing the two DOE hypotheses relevant to the RDTME KTI.

From observation of fractal characteristics of natural rock joint surfaces (Hsiung et al., 1994b), a conceptual model was proposed to represent the joint surfaces in direct shear tests [figure 7-5(a)]. The joint surfaces in this model contain three components: primary, secondary, and tertiary and higher-order asperities. The first component is the basic V-shape of the surface (primary asperity) with an inclination angle  $\phi_1$  that acts as an additional friction angle [figure 7-5(b)]. Friction realized by secondary asperities has an equivalent friction angle  $\phi_2$ , whereas the friction realized by tertiary and higher-order asperities has an equivalent friction angle of  $\phi_3$  [figure 7-5(c)]. Both secondary and tertiary and higher-order

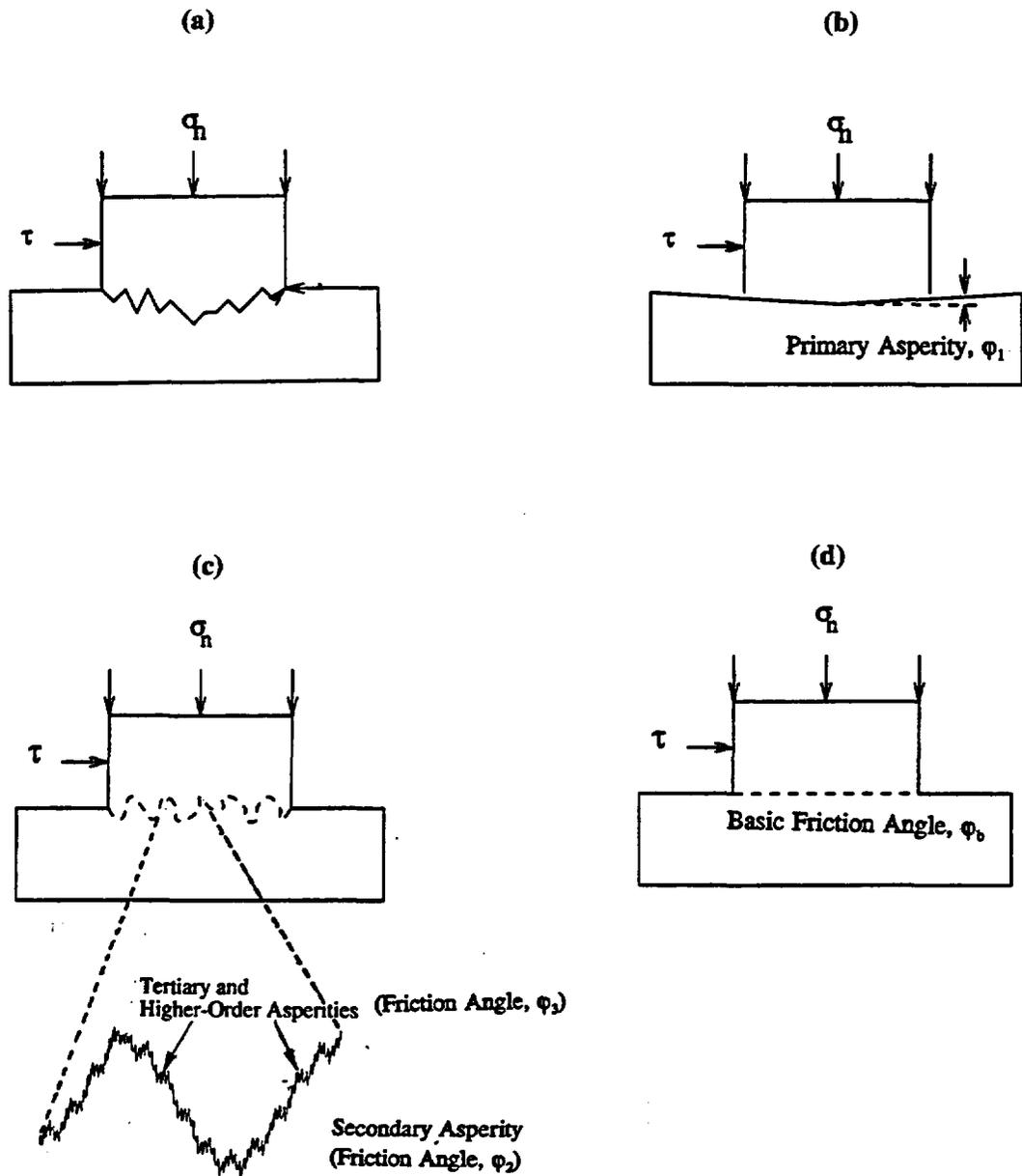


Figure 7-5. Schematic diagrams of rock surface conceptual model

asperities wear off quickly with shear displacement; tertiary and higher-order asperities ( $\phi_3$ ) wear off at a much faster rate than secondary asperities ( $\phi_2$ ). If shear displacement is continued for a long time, the joint surface will tend toward a perfectly smooth and plane surface [figure 7-5(d)] ( $\phi_1$ ,  $\phi_2$ , and  $\phi_3$  approaching zero) having the basic friction angle  $\phi_b$ .

Based on the previous discussion on the rock joint model, shear response of the natural rock joint subjected to cyclic pseudostatic load in the forward direction is

$$\tau = \sigma_n \tan \left[ \text{Sign}(v) \left( \phi_b + \phi_3 e^{-C_3 W^p} + \phi_2 e^{-C_2 W^p} \right) + \phi_1 \tanh(\eta u_s) e^{-C_1 W^p} \right] \quad (7-1)$$

In this equation,  $\tau$  is the shear stress of the joint subjected to a normal stress  $\sigma_n$  and  $u_s$  is the shear displacement.  $C_3$  is the rate of wearing of  $\phi_3$ . Similarly,  $C_2$  and  $C_1$  are the rates of wearing of  $\phi_2$  and  $\phi_1$ .  $W^p$  is the plastic work and the product of normal stress and cumulative shear displacement.  $\text{Sign}(v)$  is the sign of the shear velocity  $v$  (either positive or negative). Shear velocity is a vector quantity and is negative in the reverse direction. Therefore, the resultant shear stress takes the negative sign when the top block is shearing in the reverse direction.  $\eta$  is an empirical constant.  $\tanh(\eta u_s)$  basically controls the smooth transition of the shear stress versus shear displacement curve in the reverse direction. In the reverse direction, the effect of the downslope (angle  $\phi_1$ ) is to help movement of the sheared block, whereas the available friction from surface roughness will oppose the motion.

There is one more aspect of cyclic shearing that warrants discussion. When the top block passes the initial point during reverse shearing from one side of the initial starting point to the other (i.e., from side marked A in figure 7-6 to side marked B), it experiences the fresh surface of the bottom block. Consequently, the frictional resistance offered by these blocks will be higher than when the top block was at the other side of the initial point. Although the rate of wear may remain the same on both sides, the amount of wear needs to be accounted for separately on both sides of the initial point for appropriate modeling. Therefore, one version of the Eq. (7-1) must be provided for each side of the blocks, namely, A and B. Cumulative shear displacement for calculation of plastic work can then be determined separately for each side. Figure 7-7 shows a plot of shear stress versus shear displacement curves for test no. 20 of Hsiung et al. (1994a) and predicted results using the proposed model. The characteristics of the curve are similar to those of the experimental results.

When one rough surface slides past another rough surface, the volume change of the interface or change in aperture is generally described by the normal displacement (dilation) of the interface. In this model, joint dilation at a given shear displacement is proportional to the mobilized friction angle at that shear displacement. The mobilized friction angle is ( $\phi_2 + \phi_3 + \phi_1$ ) in the forward direction and ( $\phi_2 + \phi_3$ ) in the reverse direction. Friction angle for tertiary and higher-order asperities  $\phi_3$  will wear off relatively quickly during the first cycle and make a small contribution to the dilation. Methods for generating the equation constants (including  $\phi_1$ ,  $\phi_2$ ,  $\phi_3$ ,  $C_1$ ,  $C_2$ ,  $C_3$ , and  $\eta$ ) are currently under development.

## 7.4 ASSESSMENT OF PROGRESS TOWARD MEETING OBJECTIVES

Activities conducted during FY96 as reported in section 7.3 were aimed at addressing certain components of two of the three KTI subissues: (i) design of the repository to meet preclosure and

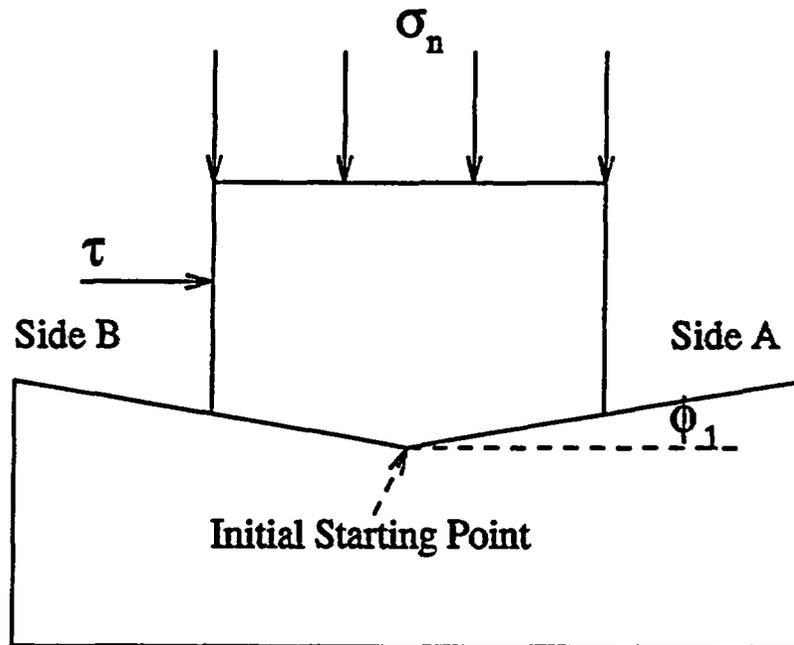


Figure 7-6. Schematic diagram of the rock joint model

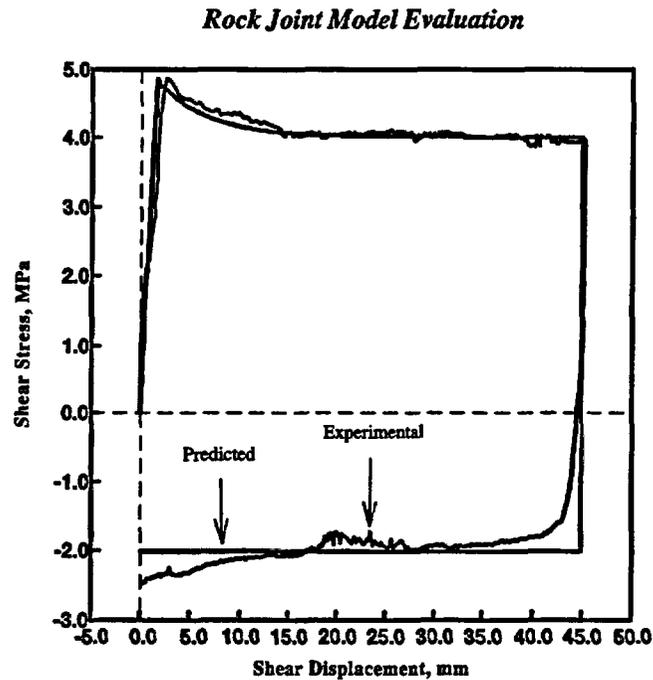


Figure 7-7. Plot of shear stress versus shear displacement curves showing results from test no. 20 (Hsiung et al., 1994a) and predicted results using the proposed rock joint model ( $\phi_1=18.46^\circ$ ,  $\phi_2=2.03^\circ$ ,  $\phi_3=5.53^\circ$ ,  $C_1=0.05$ ,  $C_2=0$ ,  $C_3=0$ ,  $\phi_b=24.7^\circ$ ,  $\sigma_n=3.988$  MPa,  $\eta=3.0$ )

postclosure performance objectives and (ii) evaluation of thermal effects on design of the underground facility. Specifically, activities related to review of seismic TR2, rock joint model development, ESF design package review, and review of the DOE regulatory compliance review report attempted to address concerns related to the DOE design program for subissue (i). The concern related to identification of TM parameters and effects for subissue (ii) is addressed through activities on parametric study of drift stability in jointed rock mass and the DOE *in situ* heater tests.

Review of the DOE seismic TR2, ESF Main Drift design report, and regulatory compliance review report contributed to resolution of NRC concerns related to the DOE repository design program. The NRC and CNWRA recommendations made to modify the DOE proposed seismic design methodology, if accepted by DOE, will resolve the NRC concerns in early FY97. The NRC recommendations made on DOE design of the ESF Main Drift will provide guidelines to the DOE in its future repository design considerations. These will also be factored into the NRC development of review procedures and acceptance criteria for repository design. Review of DOE design control process report made it possible to resolve all related NRC concerns. The only item left is to assess DOE implementation of the NRC-approved design control process.

A TM parametric study and review of DOE ESF heater tests identified thermal load and site specific rock mechanical and thermal parameters that may significantly affect emplacement drift stability and waste retrievability. These will provide input to the basis for resolution of the RDTME subissue on consideration of thermal effects in underground facility design.

The enhanced rock joint model, when completed and incorporated in the TM compliance determination codes UDEC and 3DEC, will be used as a prediction tool to resolve the RDTME KTI subissue on design of the proposed repository to meet preclosure and postclosure performance objectives.

## **7.5 INTEGRATION WITH OTHER KEY TECHNICAL ISSUES**

The Structural Deformation and Seismicity (SDS) KTI provided updated YM seismic ground vibration and fault displacement data to RDTME KTI for the review of seismic TR2. RDTME KTI provided to SDS KTI fault and fracture modeling tools and techniques that have been used for fault slip study, hangingwall deformation investigation, and FAULTING module development. Integration between RDTME and SDS KTIs will continue in areas involving site geologic and geomechanics parameters, seismic and faulting hazard assessments, prediction tools and techniques for these assessments, and underground and surface facilities design against seismic and faulting hazards.

The RDTME KTI provided comments to the audit review of the 1995 DOE Total System Performance Assessment (TSPA-95) (TRW Environmental Safety Systems, Inc., 1995), which was coordinated by the Total System Performance Assessment and Integration (TSPAI) KTI, using the updated TM parametric study data. The effects of thermal and seismic loads on repository postclosure performance will be provided by the RDTME KTI to the TSPAI KTI through the EBSPAC and SEISMO codes, which will be incorporated as models in the TPA code. Updated data on the importance of thermal and seismic loads and seals on repository performance will be provided to the RDTME KTI by the TSPAI KTI based on its TPA sensitivity analysis results.

The RDTME KTI provided to the Evolution of the Near-Field Environment (ENFE) KTI the mechanical and hydrological field investigation data from the Lucky Friday Mine, shaking table rock mass

test data, and TM parametric study data for review of the hypotheses on evolution of the near-field environment.

Integration between the RDTME and Container Life and Source Term (CLST) KTIs is through input to the EBSPAC code (Mohanty et al., 1996). Because the DOE is considering the option of not backfilling the emplacement drifts, TM effects related to drift stability are expected to become important for postclosure system performance. The EBSPAC code has the option to incorporate mechanical and hydrological effects on WP caused by instability of emplacement drifts. The RDTME KTI will provide the CLST KTI with predictions of drift stability and rock fall under thermal and seismic loads. Likewise, the CLST KTI will identify important parameters and data needed from RDTME KTI for the EBSPAC module.

The temperature distribution and fracture opening data predicted by TM parametric study have been provided by the RDTME KTI to the Thermal Effects on Flow (TEF) KTI. These data were used by the TEF KTI for review of the DOE thermal testing program.

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## **8 TOTAL SYSTEM PERFORMANCE ASSESSMENT AND INTEGRATION**

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**Key Technical Issue Co-Leads:** *R.G. Baca (CNWRA) and R.G. Wescott (NRC)*

### **8.1 INTRODUCTION**

The standard currently being developed by the U.S. Environmental Protection Agency (EPA) for the Yucca Mountain (YM) site is expected to require the proposed repository to meet both dose and risk limits. To determine compliance with such a standard, the Nuclear Regulatory Commission (NRC) will conduct a total system performance assessment (TSPA) to evaluate the isolation performance of the engineered and natural barriers. In this evaluation, the TSPA will address, in a probabilistic manner, the propagation of uncertainties associated with inherently complex natural phenomena such as unsaturated flow in fractured-porous media and repository processes such as waste package (WP) corrosion. Where appropriate, the TSPA will use bounding assumptions to compensate for uncertainties in both data and technical knowledge. In addition, TSPA takes into account uncertainties in model parameters and conceptual models as well as the relevant features, events, and processes (FEPs) (for both anticipated and unanticipated conditions) into an analysis that estimates the radiologic risks to a hypothetical member of a critical group. The integration aspect of TSPA ensures that the key technical issues (KTIs) develop technical bases for use in issue resolution and that the transfer of information among program areas will result in assessments of compliance that are transparent, defensible, and sufficiently comprehensive.

A long compliance period (e.g., 10,000 yr) may require consideration of combinations of disruptive events, coupling of processes, and possible changes to the flow and transport in the geologic system. To ensure the proposed repository does not pose an unacceptable risk to public health and safety or the environment, such complex phenomena cannot be considered only within the subsystem process models but must be reflected in the modeling from an overall system perspective. Examples of such complex phenomena include the distribution of water over WPs in the proposed repository and how this distribution can change with time; quantification of thermal, hydrologic, and chemical processes in the near-field of the WP and determination of how these processes may interact with each other; and radionuclide dilution and transport in the groundwater system, including interaction with the biosphere. Analyzing total system performance requires a broad knowledge and modeling expertise from a variety of technical disciplines. The need for strong coordination among KTI teams is recognized as an essential aspect to the success of a TSPA and must be pursued in a deliberate manner.

The three principal subissues associated with the Total System Performance Assessment and Integration (TSPA) KTI consist of

- Do the hypotheses described in the U.S. Department of Energy (DOE) Waste Containment and Isolation Strategy<sup>1</sup> (WCIS) adequately represent and rigorously test the major performance characteristics of the proposed YM repository?
- What is the relative importance of the individual NRC KTIs and is there is a need for change in emphasis?
- Are the major components of the DOE TSPA methodology (e.g., model abstractions, probability and consequences of relevant FEPs, parameter and model uncertainties, and bounding assumptions) sufficiently comprehensive that it will provide a defensible safety case?

In addition to addressing these subissues, the TSPAI KTI was tasked with developing and maintaining an independent technical assessment capability, reviewing the DOE Total System Performance Assessment (TSPA-95) (TRW Environmental Safety System, Inc., 1995)<sup>2</sup>, and supporting documents, promoting technical integration among KTIs, and developing the Consolidated DOCUMENT System (CDOCS) software. The fiscal year (FY) 96 accomplishments in this KTI discussed in greater detail are (i) audit review of the DOE TSPA-95, (ii) expert elicitation, (iii) CDOCS, and (iv) Licensing Support System Pilot Program (LSSPP). Progress on other activities include (i) initiation of a detailed review of TSPA-95, (ii) work on an acceptable scenario analysis methodology, and (iii) development of an independent technical assessment capability.

## 8.2 OBJECTIVES AND SCOPE OF WORK

The major objectives of the TSPAI KTI are two-fold: enhance the NRC capability to conduct independent reviews of the DOE TSPAs [such as the forthcoming TSPA-Viability Assessment (VA)] and use the TSPA capability to evaluate the relative importance of the NRC KTIs. Specific programmatic objectives pursued this fiscal year included providing technical comments to the DOE on TSPA-95, issuing generic guidance on an acceptable procedure for use in formal elicitations of expert judgment, and completing the CDOCS software and transferring it to the NRC for use in a variety of prelicensing activities within the NRC high-level waste (HLW) program.

An audit review of the DOE TSPA-95 report was conducted for the purposes of identifying vulnerabilities of the assessment and recommending approaches for enhancing the defensibility of future DOE TSPAs. The audit review consisted of independent analyses of selected components of the TSPA, direct comparisons of calculational results with those produced by the DOE, and then identification of primary factors causing the differences. In general, the major calculational differences were explained by distinct conceptual models, mathematical modeling approaches, bounding assumptions, and/or interpretations of available data. The independent analyses performed for the audit review provided the basis for developing constructive technical comments transmitted to the DOE in presentations at the

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<sup>1</sup>U.S. Department of Energy. 1996. *Highlights of the U.S. Department of Energy's Updated Waste Containment and Isolation Strategy for the Yucca Mountain Site*. DOE Concurrence Draft. July 1996. Washington, DC: U.S. Department of Energy.

<sup>2</sup>The DOE TSPA-95 document is extensively referenced in this chapter. For ease of reading, the reference to TRW Environmental Safety Systems, Inc., is omitted from all subsequent citations.

DOE/NRC Technical Exchange on the Audit Review of TSPA-95, and transmitted in a technical report (Baca and Brient, 1996). The success of the audit review is reflected in the TSPA-VA Plan (TRW Environmental Safety Systems, Inc., 1996) which makes note of the NRC comments/recommendations and outlines actions to be taken by the DOE in the conduct of the TSPA-VA.

Because of the pervasive nature of expert judgment in the repository program, the NRC recognized the need for guidance on an acceptable expert elicitation procedure. To meet this need, a general elicitation procedure was developed and demonstrated for the case of future climate scenarios for the YM site. This work established the framework for guidance documented in a draft branch technical position (BTP). The BTP was then distributed for public comments, revised in accordance with resolutions and issued as NUREG-1563 (Kotra et al., 1996).

The CDOCS software was developed to provide the Division of Waste Management (DWM) technical staff with an enhanced computer capability for management, retrieval, and visualization of technical and regulatory information (DeWispelare et al., 1993). CDOCS-related work included development of the CDOCS software, preparation of the user's manual, and conduct of a technology transfer seminar. Assistance was also provided to the NRC with the installation and testing of the document management system on the NRC advanced computer system.

## **8.3 SIGNIFICANT TECHNICAL ACCOMPLISHMENTS**

### **8.3.1 Audit Review of the U.S. Department of Energy Total System Performance Assessment-95**

The DOE recently issued the third in a series of TSPAs for the proposed repository at YM. The latest TSPA report referred to as TSPA-95 presents the DOE performance assessment approach, assumptions, data, and principal findings of the evaluation. Overall system performance is quantified in the TSPA-95 report using both cumulative release at 5 km (over 10,000 y) and peak dose (i.e., drinking water dose assuming 2 L/d).

In accordance with the NRC Overall Review Strategy (Johnson, 1993), the NRC conducted an audit review of TSPA-95 (Baca and Brient, 1996). The review consisted of technical comments developed by the NRC and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staffs. These comments formed the basis for presentations and discussions at the DOE/NRC Technical Exchange on the Audit Review of TSPA-95 on May 22-23, 1996. This audit review identified some areas of agreement and a number of areas of technical difference (i.e., methodology issues). Most of these technical differences were clarified during the technical exchange and in some cases resolved.

The audit review consisted of a two-level review process that involved probing component model abstractions of the TSPA-95 and a broad review of TSPA methodology. In the first level, independent analyses were conducted to evaluate such aspects as the appropriateness of technical approach, adequacy of treatment of parameter uncertainties, appropriateness of conservatism through the use of bounding assumptions, sufficiency of site data. Computational results from these independent analyses were used to develop specific technical comments regarding the DOE performance evaluation. The more general comments addressed aspects that the TSPA-95 asserted were not significant but did not specifically address in the TSPA-95 report. For example, the TSPA-95 states that disruption scenarios associated with igneous activity and seismicity are not considered significant to overall performance. To clearly present the NRC

position on this statement, general comments were prepared to indicate that the DOE had not provided sufficient basis (in a TSPA context) to support such a statement.

The audit review focused on five primary review topics:

- Infiltration and Deep Percolation
- Groundwater Dilution
- Temperature and Humidity
- WP Failure Modes
- Subsystem Abstractions

These five review topics were selected because of their relevance to WCIS (U.S. Department of Energy, 1996). The fact that the NRC/CNWRA staffs had performed detailed technical studies on these topics was also a consideration. Each of the focus topics was probed through the conjunctive use of abstracted and detailed process models, as well as through the application of the NRC Iterative Performance Assessment (IPA) Phase 2 (Nuclear Regulatory Commission, 1995) version of the total performance assessment code. These areas are discussed in the following sections.

#### **8.3.1.1 Infiltration and Deep Percolation**

Distribution of percolation flux is identified in TSPA-95 as the primary site characterization issue because of impacts on WP degradation and radionuclide transport rates through the unsaturated zone. The infiltration rate at the soil surface and percolation flux at depth are highly correlated. Both quantities are water fluxes. If no significant lateral diversion of flow can be demonstrated, then the assumption that percolation flux is synonymous with infiltration rate is bounding.

Water fluxes and velocities in the matrix and fractures are not directly calculated in the total system simulations reported in TSPA-95. Rather, an abstracted representation for these quantities is used. Using a single representative vertical column with constant thickness, random matrix properties obtained from Schenker et al. (1995) [essentially identical to the properties used in the TSPA-93 report (Wilson et al., 1994)], and a single set of constant fracture properties for all stratigraphic layers, the velocities and fluxes obtained from simulations using TOUGH2 (Pruess, 1987; 1991) for a small number of material-property realizations are abstracted into probability distribution functions (PDFs) for matrix velocity, fracture velocity, and a flux-partitioning factor distributing flux between matrix and fractures.

To independently assess the impact of the assumptions used for the unsaturated flow abstraction, the method presented in the TSPA-95 was evaluated for several flux rates. The particle travel times were calculated for each pathway in the one-dimensional (1D) column where a pathway consists of a combination of matrix flow for some layers and fracture flow for the remaining layers. The fastest pathway typically consists of fracture flow for each of the layers and the slowest pathway consists of matrix flow. The fastest and shortest pathways have the shortest and longest overall travel times. The largest flux pathway represents the most likely pathway for a particle, since the largest fraction of the flux goes through the pathway. For conservatism, particles were assumed not to move between matrix and fracture within a layer but may transition at layer interfaces.

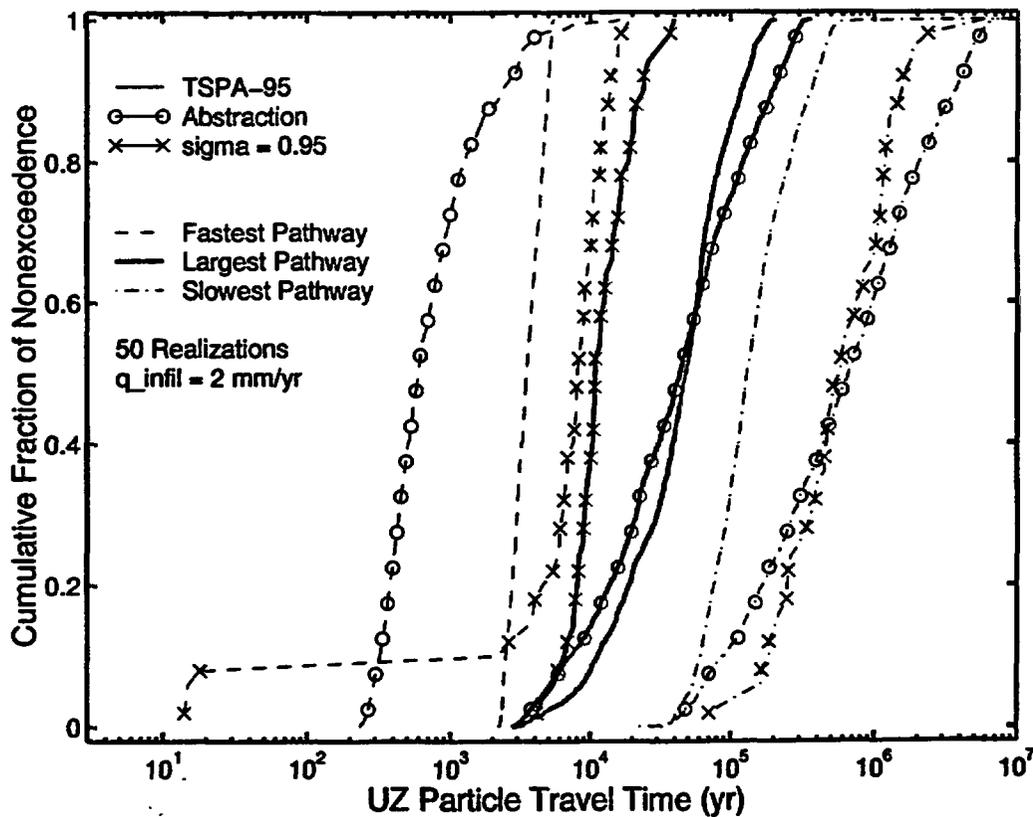


Figure 8-1. Comparison of process-level simulations with abstractions for an infiltration flux of 2 mm/yr

The highest infiltration rate considered in the TSPA-95 report was 2 mm/yr. This value was used to compute the fastest, slowest, and largest flux pathways shown in figure 8-1. The line style for a curve represents the type of pathway and the symbol type denotes whether the curve represents process-level simulations ( $\sigma = 0.95$ ), the abstraction based on the simulations (abstraction), or the TSPA-95 abstraction (TSPA-95). Each curve was constructed using results from 50 process-level realizations. The cumulative fraction of realizations with the particle travel time for a specified pathway not exceeding a given particle travel time is presented for each pathway. The process-level simulations were performed by integrating Darcy's law from the water table to the proposed repository, using the steady-state calculational methodology described by Baca et al. (1994) and adapted to incorporate the equivalent continuum model. As a comparison, the corresponding pathway analysis was performed for the TSPA-95 abstraction.

For the 2 mm/yr case shown in figure 8-1, the statistical character of the particle travel times for the process-level pathways is distinct from the behavior of the corresponding abstraction pathways. In particular, the process-level simulations exhibit a relatively low but non-negligible probability of extremely fast pathways, on the order of decades, while the largest-flux pathways and most of the fastest

pathways are on the order of thousands of years. Incorporating a total of 320 simulations (not shown here due to space limitations) suggests there is a small probability that the largest flux pathways may also be on the order of decades. On the other hand, the abstraction from these process-level simulations indicates a minimum of 200 yr for the fastest pathways but more typically on the order of 1,000 yr. The largest flux pathways generally tend to be several times slower than the corresponding process-level simulations. By comparing the 50 process-level realizations with the TSPA-95 abstraction, it can also be seen that considering 50 rather than 10 realizations has the effect of making the fastest pathways faster and the slowest pathways slower.

Specific recommendations (Baca and Brient, 1996) made at the NRC/DOE Technical Exchange on TSPA-95 as a result of this independent analysis included (i) modifying the equation to calculate pore velocity to account for saturation level, (ii) increasing the number of realizations in their process-level models, and (iii) reviewing the abstractions incorporated in Markovian particle model that result in relatively long particle travel times (i.e., solute residence times) in the unsaturated zone. The recently issued TSPA-VA Plan (TRW Environmental Safety System, Inc., 1996) notes and discusses these recommendations. From the technical activities identified in the TSPA-VA Plan (TRW Environmental Safety System, Inc., 1996), it appears the DOE will be implementing the recommendations.

### 8.3.1.2 Groundwater Dilution

Groundwater dilution at the YM site is a component of the DOE WCIS and may be of key importance to a dose- or risk-based standard. Consequently, the estimation of dilution merits a combination of (i) groundwater modeling, detailed site scale (e.g., 5 km) and regional scale (e.g., 30 km); (ii) evaluation of geochemical parameters indicating the degree of mixing; and (iii) estimation of macro-scale dispersivities based on field tracer test data. Such a combination of investigations would better support the DOE development of a more defensible basis for the TSPA-VA (TRW Environmental Safety System, Inc., 1996). In the DOE TSPA-95, groundwater dilution was quantified by a dilution factor defined as the ratio of steady-state radionuclide concentration in the unsaturated zone to the concentration in the saturated zone. Defined in this manner, the dilution factor accounts for groundwater mixing immediately below the repository and along the saturated zone flow path.

In TSPA-95, two models were used to estimate dilution factors: a stirred-tank mixing model and a line source advection-dispersion model. The stirred tank model implicitly assumes that radionuclides leaving the proposed repository are uniformly distributed throughout the entire repository footprint and, upon reaching the water table, are instantaneously and completely mixed over a 50-m-thick zone (i.e., screen-interval depth). In contrast, the advection-dispersion model makes no assumption of mixing depth but rather assumes that radionuclides enter the saturated zone along a line equal to the width (e.g., 4 km) of the proposed repository and that macro-scale dispersion reduces concentrations along the flow path from the proposed repository to Amargosa Desert.

Based on the stirred tank model, TSPA-95 calculates dilution factors ranging from  $8 \times 10^2$  to  $3.3 \times 10^4$  for a 5 km path length. With the advection-dispersion model, TSPA-95 estimates centerline dilution factors of  $4.5 \times 10^3$  to  $1.9 \times 10^5$  for a 5 km path length and  $3.1 \times 10^4$  to  $1.3 \times 10^6$  for 30 km. Embedded in the calculations with the advection-dispersion model is the assumption that dispersion coefficients are linearly dependent on path length.

Using an advection-dispersion model, independent estimates of dilution factors were calculated and presented in table 8-1. These calculations differ from TSPA-95 calculations only by having more

**Table 8-1. Dilution factors computed using conservative values for transverse dispersivity and unsaturated zone flux**

Unsaturated Zone Flux (m/yr)	Dilution Factor (DF)	
	5 km	30 km
$1.25 \times 10^{-3}$	$9.5 \times 10^2$	$8.0 \times 10^3$
$3.0 \times 10^{-5}$	$4.0 \times 10^4$	$3.4 \times 10^5$

conservative values of transverse dispersivity and saturated zone flux, which can be supported by information in the technical literature (Gelhar et al., 1985; Gelhar, 1993; Whitfield et al., 1985; Wittwer et al., 1995).

These calculated dilution factors are about 1/3 to 1/5 of those estimated in TSPA-95. In addition to these estimates, the maximum dilution factors calculated using assumptions from the NRC IPA Phase 2 (Nuclear Regulatory Commission, 1995) are about two to three orders of magnitude smaller than those calculated in TSPA-95. The much smaller dilution factors arise primarily because the infiltration rates from IPA Phase 2 are much larger than those assumed in TSPA-95 and the estimated saturated zone fluxes are much smaller than those assumed in TSPA-95. Similarly, TSPA-93 (Wilson et al., 1994) presents results for a detailed three-dimensional (3D) transport model indicate dilution factors at 5 km in the range of  $5 \leq DF \leq 20$ . These estimates are again smaller than those in TSPA-95. It is important to acknowledge, however, that dilution factor estimates derived from the TSPA-93 (Wilson et al., 1994) transport calculations are likely to be more conservative than those of TSPA-95 because they neglect the initial mixing and dilution immediately below the repository.

In summary, the conclusion was that the DOE assessment of dilution may be overly optimistic. Moreover, the large dilution factors postulated in TSPA-95 appear to be inconsistent with the heterogeneous hydrochemistry evident from available field data. It was recommended (Baca and Brient, 1996) at the NRC/DOE Technical Exchange on TSPA-95 that the defensibility of dilution factor estimates could be enhanced through the use of improved modeling techniques as well as available field tracer and geochemical data. Alternatively, more conservative bounds for dilution effects could be developed. The recently issued TSPA-VA Plan (TRW Environmental Safety System, Inc., 1996) paraphrases these recommendations. It is evident from technical activities identified in the TSPA-VA Plan (TRW Environmental Safety System, Inc., 1996) that the DOE will be implementing the recommendations.

### 8.3.13 Temperature and Humidity

One conclusion of TSPA-95 is that the thermohydrologic environment of WPs strongly affects the initiation and rate of aqueous corrosion. Because the thermohydrologic environment of the WP affects many near-field processes important to TSPA, independent calculations were initiated to reproduce TSPA-95 results using the same data and dimensions and evaluate the differences introduced by using a 3D instead of a two-dimensional (2D) model.

In TSPA-95, the FEHM thermohydrologic code (Zyvoloski et al., 1995) is used to predict the evolving hydrothermal conditions near WPs. TSPA-95 results appeared to have anomalies in the predictions prior to backfilling, hence independent calculations were performed by the CNWRA to reproduce the results using the ABAQUS (1995) and MULTIFLO (Seth and Lichtner, 1996) codes. METRA, a submodule of MULTIFLO, simulates coupled heat and mass transfer in a porous medium—the same processes included in the DOE FEHM code. ABAQUS simulates transient conduction heat transfer, considered the dominant mode of heat transfer for low and intermediate areal mass loadings (AMLs). ABAQUS uses the finite element method and accurately represents the geometry of the system. MULTIFLO uses rectangular grids.

A portion of the computational mesh near the WP is provided in figure 8-2 for a 2D model similar to that used in TSPA-95 and a 3D model. For clarity, the backfill elements are not shown in the figure but do exist in the mesh. The 2D model averages the heat source along the drift (in the third dimension). This tends to produce lower WP temperatures. The 3D model has a more accurate representation of the geometry and should yield more accurate predictions of WP conditions. Both conceptual models were considered in the CNWRA investigations.

Calculations were performed for the 25 MTU/acre and 83 MTU/acre AMLs. Thermohydrologic parameters were taken from figure 4.2-1 and table 4.2-3 of TSPA-95. Because a few thermal properties were not fully described in TSPA-95 some judgment and interpretation was necessary. Key assumptions were made that the package supports and concrete inverts have a conductivity of 1.0 W/(m-C) and that the effective conductivity of the drift prior to backfilling was 10 W/(m-C).

Relative humidity (RH) was calculated using the same approach as Eq. 4.2-1 on page 4-6 of TSPA-95. RH is a measure of the tendency for liquid films to develop on the WP surface. Within the emplacement drift, the absolute humidity was assumed to be uniform because the relative ease with which vapor flows within the drift. The vapor pressure at the WP surface was then dictated by the vapor pressure at the drift wall.

In figure 8-3, TSPA-95 and the CNWRA results are compared for the 25 MTU/acre case. The temperatures and RH are in good agreement at long times for the 2D models. For the first hundred years, the TSPA-95 results show a higher WP temperature and lower RH. After reviewing TSPA-95, it is believed that this trend is due to underestimating the rate of heat transfer from the WP to the drift wall prior to 100 yr. This could not be confirmed because of sparse documentation of details in TSPA-95. The report states that a radiative transfer model was employed but does not discuss how view factors were calculated or provide emissivity values for the package and drift wall.

The differences arising from using a 2D instead of a 3D model were also compared. It was found that the 3D model calculated WP temperatures that were about 55 °C higher than the 2D results for times after backfill was assumed to be emplaced (140 °C compared to 85 °C) for the 25 MTU/acre case. The RH was also affected so that the 3D model predicted lower values. The overall effect of higher WP temperatures and lower RH on system performance was unclear and depends on the sensitivities of the WP corrosion and source term models. Unless the 2D models are shown to be more conservative (predict earlier WP failure times and higher radionuclide release rates), then the DOE should consider use of 3D models because they can more accurately predict WP conditions.

In summary, the independent calculations reproduced many of the thermohydrologic results found in TSPA-95. Some differences were noted where TSPA-95 has higher WP temperatures before backfilling.

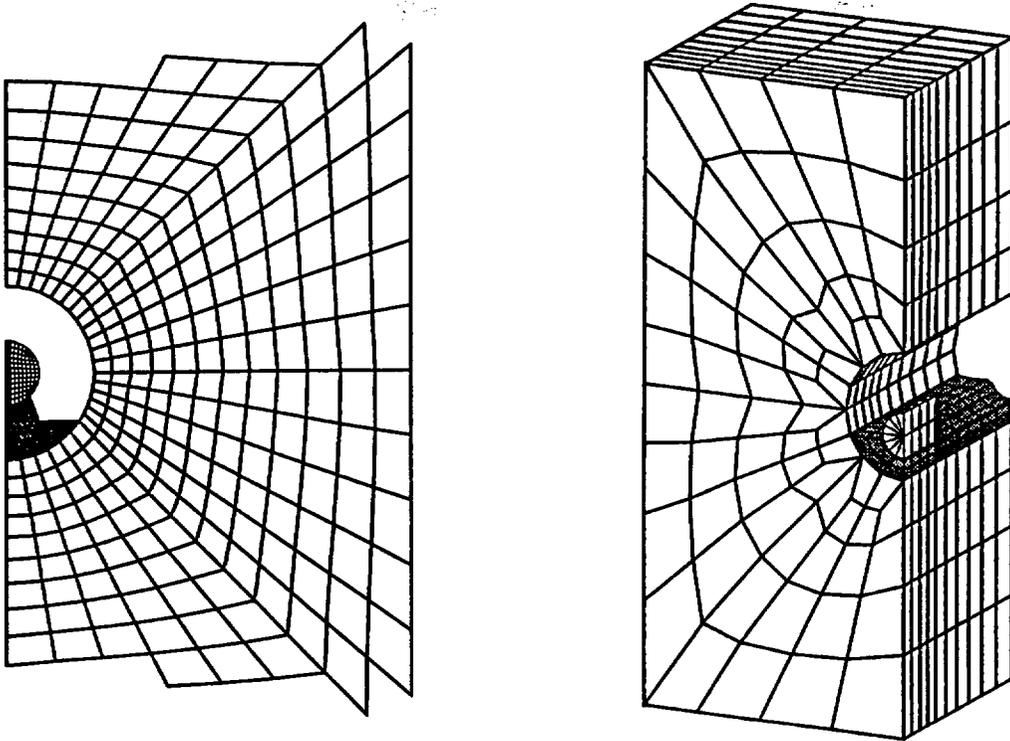


Figure 8-2. Two and three-dimensional computational models near the waste package

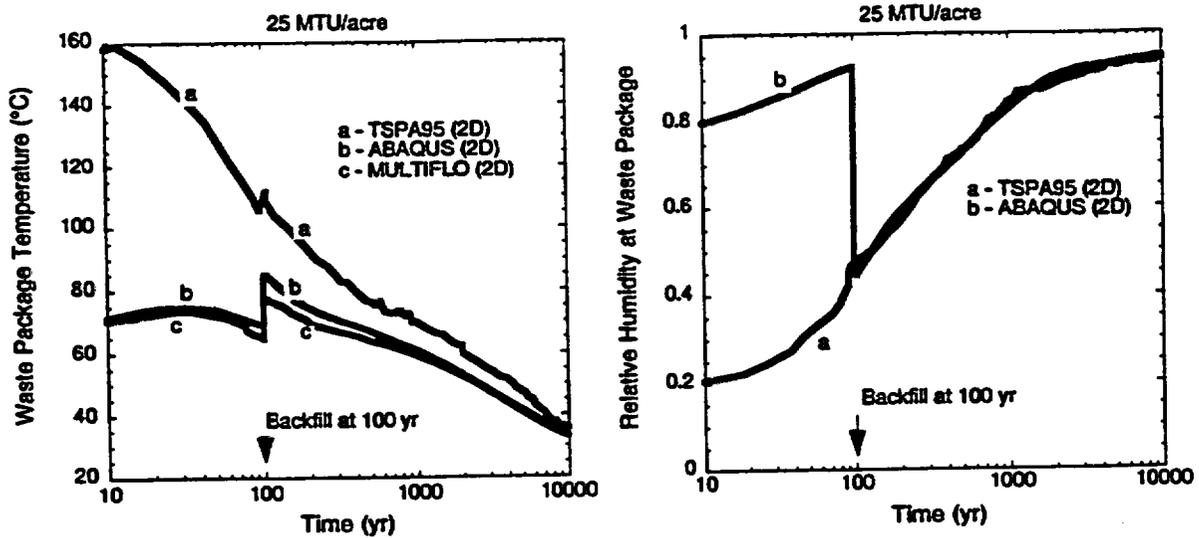


Figure 8-3. Comparison for 25 MTU/acre areal mass loading

As a result of this work, it was recommended (Baca and Brient, 1996) that the DOE review the heat transfer models used in the unbackfilled drift case and consider using a 3D model to more accurately predict WP conditions. The TSPA-VA (TRW Environmental Safety System, Inc., 1996) notes this (and other recommendations) and indicates that the DOE is implementing this recommendation for the 3D analyses. It also indicates that the DOE is considering other NRC recommendations made at the DOE/NRC Technical Exchange on the Audit Review of TSPA-1995 (Baca and Brient, 1996).

#### **8.3.1.4 Waste Package Failure Modes**

The performance characteristics of the current conceptual design of the WP for spent fuel (U.S. Department of Energy, 1994) were evaluated in TSPA-95 using a stochastic WP performance model. The design of the WP used in TSPA-95 is a significant departure from the single-wall container concept evaluated in TSPA-93 (Wilson et al., 1994). The design consists of an outer disposal overpack of a corrosion-allowance material (carbon steel) and an inner container of a corrosion-resistant alloy (Alloy 825). An additional containment barrier of a moderately corrosion-resistant material such as Alloy 400 is included in the low thermal-load repository design (U.S. Department of Energy, 1994). This additional containment barrier was not considered in TSPA-95 because models for predicting the performance of this type of material are not currently available. Also, the multi-purpose canister made of type 316L stainless steel and the pour canister for vitrified defense HLW are not included in TSPA-95 since no credit is assigned by the DOE to these canisters as containment barriers.

Although several corrosion modes, including crevice corrosion, stress corrosion cracking, microbially influenced corrosion, and galvanic corrosion, are briefly mentioned in TSPA-95 as potential failure modes for the WP, the performance calculations in TSPA-95 include only general corrosion and pitting corrosion as relevant models. Calculations in TSPA-95 are considered to be nonconservative because relevant failure modes, such as crevice corrosion, stress corrosion cracking, microbially influenced corrosion, and thermal embrittlement of steel, are not included in the analysis and the chemistry of the environment contacting the WP does not correspond to bounding environments described in the DOE long-term testing program (Lawrence Livermore National Laboratory, 1995). Furthermore, no technical basis was provided for consideration of various atmospheric and river water corrosion test results as representative of corrosion in the expected repository environment.

In summary, a number of potential failure mechanisms associated with container failure were not quantitatively addressed in TSPA-95. As a result of this review, it was recommended (Baca and Brient, 1996) that the DOE consider additional WP degradation modes, possible wet/dry near-field environments, and alternative waste dissolution models. The TSPA-VA (TRW Environmental Safety System, Inc., 1996) acknowledges these and other recommendations. In addition, it indicates the DOE will be improving the WP degradation model to take into account such phenomena as recommended.

#### **8.3.1.5 Subsystem Abstractions**

Currently, the DOE quantifies overall repository performance using a complementary cumulative distribution function (CCDF) plot of total radionuclide releases (at 5 km) to the accessible environment (over  $10^4$  yr) and CCDF of drinking water dose (for 2 L/d). Both the DOE and the NRC use computer codes to assess repository performance. Previous CCDFs calculated by the DOE TSPA codes such as Total System Analyzer (Wilson et al., 1994) and Repository Integration Program (RIP) (Golder Associates, Inc., 1993) differed significantly from those computed by the NRC/CNWRA TPA code, (Sagar and Janetzke, 1993). These differences in computational results are believed to be primarily because of distinct

- Model abstractions for repository subsystems
- Parameter ranges and distributions
- Underlying and/or bounding assumptions

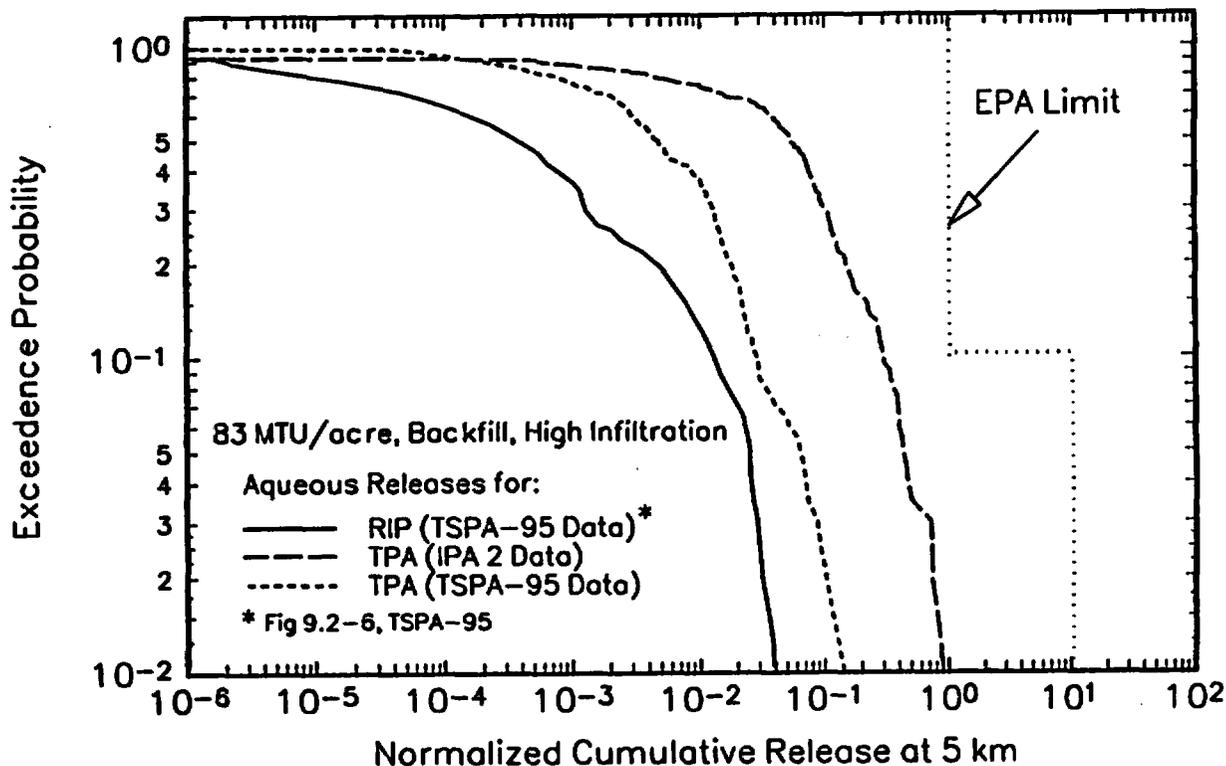
In TSPA-95, a series of CCDFs computed with the RIP code are presented for various combinations of heat load, backfill, infiltration ranges, and alternative thermohydrologic models. None of these CCDF results are explained using causal factors or basic performance indicators [e.g., residence time in the engineered barrier system (EBS), timing of condensate refluxing, particle travel times through the unsaturated and saturated zones]. Thus, determining the correctness and reasonableness of CCDF results requires independent calculation.

The RIP code used in TSPA-95 is a generalized driver that can execute component models that describe (i) WP behavior and radionuclide release from the EBS, (ii) radionuclide transport pathways, (iii) disruptive events, and (iv) biosphere dose/risk. The components describing disruptive events and biosphere dose/risk, however, were not used in TSPA-95. The NRC/CNWRA developed the TPA computer code that was used in the NRC IPA Phase 2 (Nuclear Regulatory Commission, 1995). The approach in the audit review was to use the TPA code with WP lifetime and hydrostratigraphic representations to match those in TSPA-95. Independent CCDFs could then be generated and compared with those in TSPA-95. In this exercise, the WP lifetime was not calculated using the TPA code but a range of lifetimes was assumed based on digitizing figure 5.7-10a of TSPA-95.

In figure 8-4, two independently calculated CCDFs for cumulative release are compared with the corresponding CCDF from TSPA-95. The CCDFs generated by the TPA code used (i) the original IPA Phase 2 data and the digitized TSPA-95 WP lifetime curve together with (ii) the approximate representation of TSPA-95 input data and the digitized WP lifetime curve.

In the first case, the CCDF calculated with TPA code is within one order of magnitude of the EPA limit, whereas the CCDF taken from TSPA-95 (i.e., calculated with RIP) is about two orders of magnitude below the EPA limit. The TPA code calculations produced fewer lower releases and more high releases than indicated by the TSPA-95 result. This suggests that the IPA Phase 2 assumptions and site subsystem abstraction may be more conservative than those used in RIP. For example, in the TPA code calculations it was assumed that once a WP failed in a given zone of the repository, all WPs within that zone also failed—a more conservative assumption than that used in TSPA-95. Also, TSPA-95 computes radionuclide releases through a given number of pits/perforations. In contrast, the TPA code does not limit the releases by the number of perforations with the exception that the releases will not take place until the water in the WP reaches a certain level. The combined effect of these differences is relatively complex so that differences in the CCDF are not easily explained.

In addition to the CCDFs, TSPA-95 also presented results of calculations based on single values of parameters. One such calculation in TSPA-95 was the calculation of drinking water dose from  $^{237}\text{Np}$  as a function of time based on expected values of infiltration and solubility limits.  $^{237}\text{Np}$  was selected for this calculation because it is very long lived and an important contributor to dose. Thus the peak  $^{237}\text{Np}$  dose occurring at long times will be insensitive to assumptions regarding the thermal period, waste container, and release rates for spent fuel. Two calculations were performed—one for the high infiltration rate (1.25 mm/yr), and one for the low infiltration rate (.03 mm/yr). For the staff calculation, the infiltration rate remained constant (in the TSPA-95 calculation, the infiltration rate increased). Results of



**Figure 8-4. Comparison of complementary cumulative distribution functions for cumulative release**

the calculation were approximately two orders of magnitude greater than doses presented in TSPA-95. The apparent extra dilution is believed to come from the model abstractions for interunit connectivity (Markovian particle approach) used in the DOE RIP code.

The model for radionuclide transport used in DOE TSPA-95 was compared to the model used in the NRC IPA Phase 2. In both models, particles moved along 1D flow paths representing either the fractures or the matrix in the Markovian particle approach (i.e., a particle starting in a given pathway—fracture or matrix—moves a distance  $\Delta x$  before transitioning to the other pathway). The time  $\Delta t$  for a particle to move  $\Delta x$  is sampled from an exponential distribution. Upon leaving a layer and entering the next, the process repeats itself until the particle translates all layers. The Phase 2 approach is similar, but particles move entirely through the layer in either the fracture or matrix flow paths, and only transition between layers.

The two models were compared for a four-layered unsaturated flow system using parameters typical of TSPA-95. Results for an instantaneous release of 5,000 particles showed obvious differences. The particle arrival times are much more spread out using the Markovian particle approach. The NRC

model would lead to a higher peak concentration at an earlier time. Conclusions from this analysis are that the Markovian particle approach may be taking unwarranted credit for diffusion between the fracture and matrix flow paths.

As a result of this work, it is recommended (Baca and Brient, 1996) that the DOE provide sufficient explanations of subsystem abstractions using basic physical factors and assess the potential optimism or conservatism of the abstracted models. Many abstractions appear prudent and defensible, but intermediate calculations and sensitivity studies would enhance reviewer understanding and confidence in the abstractions. One questionable abstraction is radionuclide transport along fractures. The Markovian particle approach used in TSPA-95 appears to neglect potential fast paths and, hence, it was recommended that alternative abstractions be pursued. The TSPA-VA (TRW Environmental Safety System, Inc., 1996) notes this recommendation and indicates that the DOE will be examining alternative modeling approaches.

### **8.3.2 Expert Elicitation**

During this fiscal year, the staff issued a BTP on the formal use of expert elicitation in the HLW program. In the review of license applications, traditionally the NRC has accepted expert judgment in the evaluation and interpretation of the factual bases. Thus, it is expected that the NRC will give appropriate consideration to the judgments of the DOE experts regarding the geologic repository. In the BTP, designated NUREG-1563 (Kotra et al., 1996), the NRC staff proposed set forth technical positions that (i) provide general guidelines on those circumstances that may warrant the use of a formal process for obtaining the judgments of more than one expert (i.e., expert elicitation) and (ii) describe acceptable procedures for conducting expert elicitation when formally elicited judgments are used to support a demonstration of compliance with the NRC geologic disposal regulation.

In February 1996, the availability of a draft BTP for public comment was announced in the *Federal Register* (Nuclear Regulatory Commission, 1996). In its comments on the draft BTP, the DOE indicated it was in substantial agreement with the NRC staff technical positions (Brocoum, 1996). Moreover, the State of Nevada commented that the draft BTP was favorably responsive to earlier concerns regarding the DOE programmatic guidelines in this area (Loux, 1995). Thus, with issuance and acceptance of this guidance, the NRC staff was inclined to recommend a path to resolution of site characterization analysis comment no. 3 (Nuclear Regulatory Commission, 1989). Moreover, the staff also plans to review and possibly close open items related to expert elicitation.

The NRC and the DOE achieved a high level of agreement on an appropriate process for formal elicitation of expert judgment. For example, the DOE recently indicated to the Nuclear Waste Technical Review Board (NWTRB) that they plan to follow the NRC nine-step process (outlined in the BTP) in elicitation for the TSPA-VA (TRW Environmental Safety System, Inc., 1996). The recently issued DOE TSPA-VA (TRW Environmental Safety System, Inc., 1996) indicates that expert judgments will be used in a number of areas to supplement other sources of scientific and technical information.

### **8.3.3 Consolidated Document Management System**

The CDOCS software was developed to provide the DWM technical staff with an enhanced computer capability for management, retrieval, and visualization of technical and regulatory information (DeWispelare et al., 1993). CDOCS Version 1.0 was documented and delivered to the NRC this fiscal

year. The NRC has a requirement for increased capability in making independent technical analysis to conduct prelicensing and licensing review activities.

CDOCS is intended to complement the technical computing capabilities of the NRC and the CNWRA technical staffs currently being provided by the Advanced Computer Review System. CDOCS provides the staffs with the capability to create, modify, and maintain documents containing both text and images in a full-text search and retrieval environment. This capability facilitates the capture of a broad spectrum of technical and regulatory materials making these available to the staffs to support work in the KTIs to resolve associated subissues, prepare for technical exchanges, review progress by the DOE, document concerns as open items, and track these open items.

As illustrated in figure 8-5, CDOCS uses a suite of commercial off-the-shelf (COTS) software combined by custom interface codes in a modern client-server network implementation supporting computers used by the NRC and the CNWRA staffs. The modular design of CDOCS allows for managed evolution of software products as their capabilities change over time. In figure 8-5, the database is continually updated by a custodian, to be then used by technical staff.

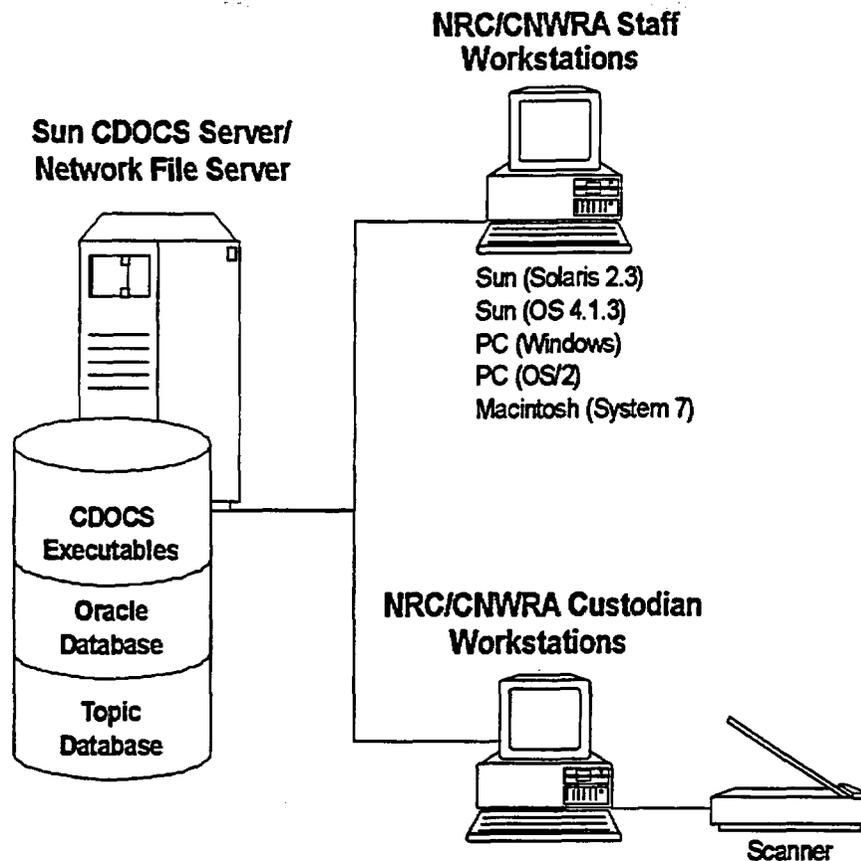
Currently, holdings in CDOCS include technical documents, technical document bibliographic headers, regulations, NUREGs, technical positions, regulatory records (compliance determination strategy and compliance determination method), and open items. CDOCS is implemented and available to staffs at the NRC and the CNWRA. Documents entered at either the NRC or the CNWRA are passed to servers at both locations for processing and inclusion into the local database. A synchronization process will be used to ensure that the NRC and the CNWRA databases are fully consistent.

### **8.3.4 Licensing Support System Pilot Program**

The NRC License Support System (LSS) computer server test bed (LSSTB) was developed under a pilot program to evaluate the feasibility of a LSS concept using COTS technology. The LSSTB, accessible through the public Internet (outside the NRC network security firewall), will (i) provide a basic document search and retrieval capability from among a sample of HLW documents, (ii) allow downloading documents selected by the user, and (iii) obtain feedback from users by allowing on-line comments.

The CNWRA established a public Internet computer server site that can be accessed by commonly available World Wide Web (WWW) browsers (e.g., Netscape) as illustrated in figure 8-6. Authorization was obtained from the NRC before the server was placed on the Internet for public availability (URL: <http://www.nrc.lsstb.gov>). This server has an NRC LSSTB Home Page that was produced after design consultation with the NRC. The WWW server Home Page provides the user interface for searching the loaded-document repository. The WWW server application also provides for logging user comments and conducting four types of user searches (i.e., title, author, date, and document text). The server hardware uses a SUN workstation. The search and retrieval software used by the server is a COTS product that was quickly acquired.

The LSSTB was loaded with a sampling of documents from the HLW program including correspondence and SECY papers from the NRC Commission Data Tracking System, select CNWRA technical reports, and regulations. The goal of the LSSTB in FY97 is to provide downloading both text of documents and associated linked images, as well as provide a mechanism for users to submit/load pertinent documents. The full LSS will eventually document material of the DOE, the NRC, and others

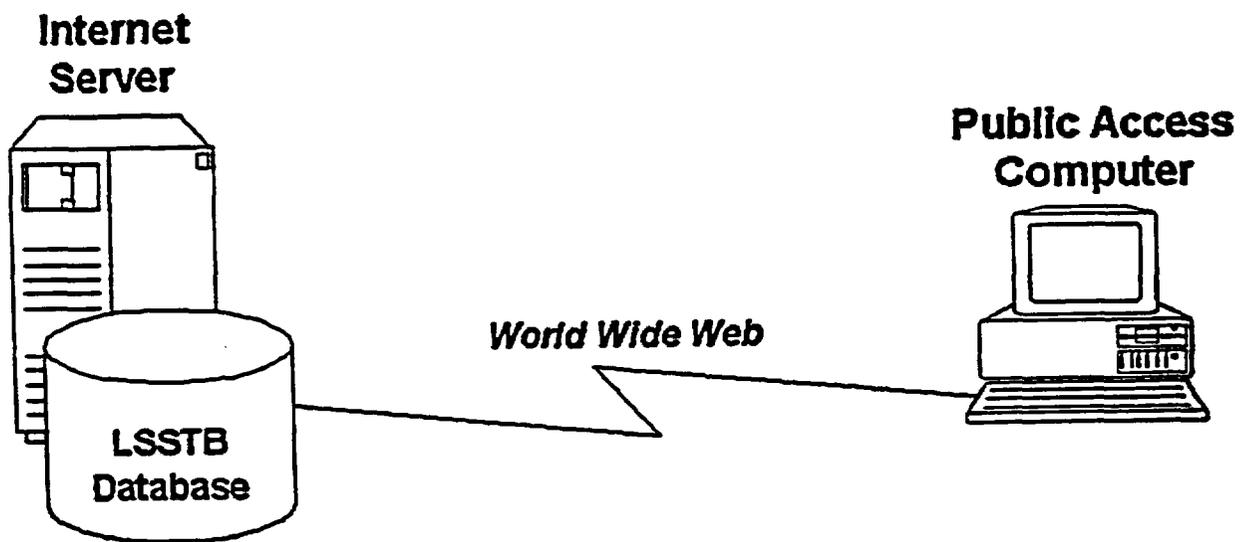


**Figure 8-5. CDOCS architecture**

to the HLW licensing proceeding that may be relevant to the license application review process. It is intended to facilitate the license review by supporting (i) electronic access to discoverable documents before the DOE license application is filed, (ii) early technical review of materials by all potential parties, and (iii) electronic transmission of all filings during the hearing.

#### **8.4 ASSESSMENT OF PROGRESS TOWARD MEETING OBJECTIVES**

The technical work conducted in the TSPA-95 audit review was completed in April 1996. Although all KTI teams participated, focus areas were chosen in four KTIs: Total System Performance Assessment and Integration, Unsaturated and Saturated Flow Under Isothermal Conditions, Thermal Effects on Flow, and Container Life and Source Term. Other KTI teams also provided technical comments that will be used in the detailed review of TSPA-95. Analyses performed for the audit review were discussed with the DOE in a technical exchange held on May 22–23, 1996. A letter summarizing the results of the audit review was sent to the DOE in July 1996 and a more detailed report of the analyses was transmitted to the DOE in September 1996. In addition, data collection and analyses on select topics were initiated as planned for the detailed review.



**Figure 8-6. Licensing Support System Test Bed**

A draft BTP on the Formal Use of Expert Elicitation in the High-Level Waste Program was issued for public comment in February 1996. Public comments were incorporated into a final version of the BTP that will be issued as NUREG-1563. The DOE provided favorable comments on the BTP and is expected to use this guidance in formal elicitation planned in FY97. The NRC staff believes that agreement has been achieved on an acceptable methodology for the formal use of expert elicitation. This acceptance is reflected in the recent DOE presentations to the NWTRB which states that the DOE will follow the elicitation procedure outlined in the NRC BTP. Additional work will be needed to develop guidance on acceptable techniques for aggregation of expert judgments.

Progress in scenario analysis methodology consisted of resolving three site characterization plan (SCP) comments: 101 (partial performance measures), 103 (Ross sequence numbers), and 115 (independence of scenario classes). Other comments about scenario analysis methodology were left open

and reasons explained: 95 (scenario development and screening) and 105 (justification for elimination of scenarios). Actions are based on a review of the DOE Mined Geologic Disposal License Application Annotated Outline distributed in March 1995. Results of this review were documented and sent to the DOE on March 28, 1996. This review helped provide some basic guidance to the DOE on an acceptable scenario analysis methodology. Specific disruptive scenarios needing to be considered in TSPAs, however, remain as a KTI subissue. Although the TSPA-95 contends that the volcanism and seismic disruption scenarios have been previously analyzed and found not to be of sufficient consequence, the DOE plan for the TSPA-VA (TRW Environmental Safety System, Inc., 1996) indicates these scenarios will be addressed.

Progress in developing an independent TSPA technical assessment capability was primarily concerned with modifying the IPA Phase 2 TPA code so it could be used in detailed reviews of the TSPA-95 and TSPA-VA (TRW Environmental Safety System, Inc., 1996). The TPA code is being updated to evaluate the latest repository designs and site characterization data. Assistance is also being provided to other KTI teams to develop updated modules to be added to the TPA code. Presently, the TPA code can run on a SUN workstation as well as on a Cray supercomputer. To make the code more user friendly, the TPA code is being modified to facilitate its general use in the evaluations of the remaining NRC KTIs and the corresponding DOE WCIS attributes.

## **8.5 INTEGRATION WITH OTHER KEY TECHNICAL ISSUES**

**Activities Related to Development of the EPA YM Standard KTI:** The major input to the this KTI from TSPAI KTI was a scoping study for a human intrusion scenario. This and other scoping studies are expected to be included in a NUREG report. The information contained in the NUREG is planned to provide the basis for revising the NRC technical criteria for consistency with the EPA YM Standard. Information from the EPA Standard KTI includes tentative definitions of the reference biosphere used to guide near future TSPA calculations and likely criteria to be considered for dose and performance assessment (PA).

**Unsaturated and Saturated Flow under Isothermal Conditions KTI:** This KTI provided analyses for two focus topics to the audit review of TSPA-95 infiltration and dilution. Integration will continue with this KTI through the detailed review and the independent TSPA technical assessment capability effort. Using available geochemical data, the TSPAI KTI is working with this KTI to develop updated percolation flux distributions for the base case and pluvial climate case, groundwater dilution, and mixing parameters.

**Container Life and Source Term (CLST) KTI:** This KTI developed the Engineered Barrier System Performance Assessment Code (EBSPAC) (Mohanty et al., 1996) that will be used in the detailed review of TSPA-95 and as an integrated module within the TPA code. The CLST KTI also provided the results of technical evaluations as part of the audit review of TSPA-95. Because of FY97 budget reductions, no further development of EBSPAC code will be performed; maintenance and application of the code will be conducted under the TSPAI KTI. Discontinuance of EBSPAC code development is expected to limit the ability to independently review aspects of the DOE WP performance in the forthcoming TSPA-VA (TRW Environmental Safety System, Inc., 1996) report.

**Evolution of the Near-Field Environment KTI:** This KTI provided models and data to EBSPAC to be used within the TPA code. Insight gained from exercising the TPA code will be transmitted to the KTI regarding the relative importance of parameters and phenomena associated with the near-field

environment. This KTI will also prepare input to radionuclide transport models that will be incorporated in the TPA code.

**Repository Design and Thermal-Mechanical Effects KTI:** This KTI primarily focused on postclosure thermal-mechanical effects but also considered preclosure aspects such as drift stability and retrievability of the waste. As a result of FY97 budget reductions, the preliminary study of drift stability under thermal and seismic loads will be completed under the TSPA KTI and, no further work on preclosure PA will be conducted. This will impact TPA code development in regards to repository system changes that occur during the 100–150 yr operational phase.

**Igneous Activity KTI:** This KTI prepared probability estimates for various types of igneous occurrences and is developing the modeling theory for eruption style and radionuclide transport. This model will be used to determine the contribution to risk from igneous activity through the airborne pathway. If this contribution is significant, the model will become part of the VOLCANO module in the TPA code.

**Structural Deformation and Seismicity KTI:** This KTI prepared an updated hydrostratigraphy for use in the detailed review of TSPA-95 and as input to the TPA code. The KTI developed the FAULTING module for evaluating the impact of fault displacement on WP lifetime. If fault displacement is found to contribute significantly to risk, the module will be added to the TPA code.

**Thermal Effects on Flow KTI:** This KTI furnished input to the audit review of TSPA-95 and will give additional information for the detailed review, as well as for the TPA code. Specifically, the KTI provided time-dependent WP temperature and RH for typical repository conditions under different AMLs.

**Radionuclide Transport KTI:** This KTI contributed to the audit review by using geochemical data to support estimates of mixing in the saturated zone. The KTI developed a geographic information system specific to hydrologic flow and transport. This was then combined with existing geographic information system coverages of geology and structure to support the detailed review. Because of budget reductions in FY97, no further work will be performed on determination of radionuclide transport properties (e.g., sorption and solubility) and dependence on such factors as pore fluid chemistry, mineralogy, and flow regime. Termination of this work will limit the NRC capability to review the DOE data and the appropriateness of certain input assumptions that may be used in the TSPA-VA (TRW Environmental Safety System, Inc., 1996).

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# 9 ACTIVITIES RELATED TO DEVELOPMENT OF THE U.S. ENVIRONMENTAL PROTECTION AGENCY YUCCA MOUNTAIN STANDARD<sup>1</sup>

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## 9.1 INTRODUCTION

Through the Energy Policy Act of 1992 (EnPA — Public Law 102-486), Congress directed the U.S. Environmental Protection Agency (EPA) to promulgate new environmental standards applicable to a potential geologic repository for high-level radioactive waste (HLW) at Yucca Mountain (YM). The EnPA stipulates that new EPA Standards be based on and consistent with the recent findings and recommendations of the National Academy of Sciences (NAS) (National Research Council, 1995). Once final standards are promulgated, the EnPA directs the NRC to modify its requirements in 10 CFR Part 60 to conform to the new EPA Standards. Under the EnPA, the Nuclear Regulatory Commission (NRC) has one year to make the necessary modifications.<sup>2</sup>

To support technical bases for revised disposal standards for YM, section 801(a)(2) of the EnPA directed NAS to provide EPA with recommendations on the following issues

- Whether health-based standards based on doses to individual members of the public from releases to the accessible environment . . . will provide a reasonable standard for protection of the health and safety of the general public.
- Whether it is reasonable to assume that a system of postclosure oversight of the proposed repository can be developed, based on active institutional controls, that will prevent an unreasonable risk of breaching the repository engineered or geologic barriers or increasing the exposure of individual members of the public to radiation beyond allowable limits.

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<sup>1</sup>Revision to EPA HLW standard is currently under consideration. The NRC will need to consider revision to its geologic disposal regulation after a new EPA Standard for YM is promulgated. The information presented in the following chapter is not intended to convey a preference or position of the NRC or the CNWRA staffs regarding how either of these two regulations might be revised.

<sup>2</sup>In addition to recent NAS recommendations, Congress is contemplating other legislative proposals that would affect regulation of HLW at YM. See summary pp 46-48 in Nuclear Waste Technical Review Board (1995).

- Whether it is possible to make scientifically supportable predictions of the probability that the repository engineered or geologic barriers will be breached as a result of human intrusion over a period of 10,000 yr.

In August 1995, NAS issued its findings and recommendations on a revised environmental standard for HLW disposal. The NRC staff is coordinating with EPA to ensure development of reasonable and implementable HLW standards, considering the recommendations of NAS. Once EPA issues its final standards, the NRC must conform its regulations accordingly.

Important differences exist among NAS findings and recommendations, prior EPA Standards for HLW, and existing geologic disposal regulations in 10 CFR Part 60. Through the Activities Related to Development of the EPA Yucca Mountain Standard Key Technical Issue (KTI), the NRC staff is conducting requisite technical analyses to review and comment on EPA revised environmental standards, especially in those areas not addressed by previous HLW regulations. Some of the key subissues for evaluating a revised EPA Standard are (i) definition of the compliance period and the associated approach used in compliance calculation; (ii) specification of the exposure scenarios; (iii) treatment of disruptive events; and (iv) evaluation of the effects of human intrusion. Using its Iterative Performance Assessment (IPA) capability, the NRC staff and its technical assistance contractor—the Center for Nuclear Waste Regulatory Analyses (CNWRA)—undertook a series of focused technical analyses in FY96 to assess these subissues. Results of these analyses were documented by the respective staffs and are summarized in this report.

The primary objectives for this KTI are to (i) support the NRC in their interactions with the EPA regarding the development of an EPA Standard for the YM site and (ii) subsequent to promulgation of the EPA standard to assist in developing the technical bases for future revisions to NRC regulations required to conform with the new EPA Standard. As noted previously, a number of subissues have been defined that must be addressed to resolve the primary objective by providing specific staff assessment capabilities. These subissues are discussed in the following paragraphs.

- **Defining a Compliance Period and Method:** The current compliance period in the remanded HLW standards is 10,000 yr. NAS recommendations noted that long-term stability of the geologic setting at YM is on the order of one million years and recommended that compliance be evaluated for the time of peak risk. Selection of the appropriate compliance period must consider the recommendations of NAS as well as regulatory precedent and available assessment techniques. The specific assessment criterion (e.g., mean or median of dose to a specified group or individual) must also be specified.
- **Selecting a Critical Group(s):** Adoption of the NAS recommended critical group approach requires consideration of reference biosphere(s) and exposure pathways. There are numerous options for critical group parameter specifications, each presenting particular technical and regulatory uncertainties.
- **Evaluating Results of Potential Human Intrusion:** NAS determined there was no scientific basis for predicting the occurrence of human intrusion subsequent to repository closure and recommended that a stylized calculation be made to provide an indication of the resiliency of repository performance to such intrusions. The current regulations include requirements for considering human intrusion within the context of unanticipated processes and events which apply only to the containment limits for sites other than YM, Nevada. NAS

recommendations would require a consequence analysis for human intrusion to measure the resilience of the repository as measured by individual risk. The NRC must be able to evaluate the adequacy of any such stylized scenario calculation.

- **Considering Disruptive Events:** While NAS noted that the geologic setting in the YM area should be stable for approximately one million years, certain processes could occur in the region which might affect repository performance. These processes may include seismicity, volcanism, and climate change. Criteria for screening these processes and incorporating their effects into assessments of proposed repository performance must be evaluated.

To varying degrees, all of these issues were addressed in FY96. The following sections of this report detail the extent of these activities and their results.

## 9.2 OBJECTIVES AND SCOPE OF WORK

The previously applicable EPA environmental standards and the current NRC implementing regulations are somewhat different from the proposals for a health-based standard (e.g., limiting individual dose or risk) suggested by the EnPA. 40 CFR Part 191 establishes containment requirements that limit the releases of radioactive material to the accessible environment, weighted by a factor approximately proportional to radiotoxicity, and integrated over a period of time (e.g., a span of 10,000 yr is the current regulatory requirement) after permanent closure of the geologic repository. 10 CFR Part 60 incorporates 40 CFR Part 191 as the overall performance requirement for a geologic repository. The requirements in 10 CFR 60.112 establish an overall system performance objective that supports EPA containment requirements, whereas certain other sections (10 CFR 60.113) set forth subsystem performance objectives.<sup>3</sup>

The forthcoming revisions to both the EPA Standards and the NRC conforming regulations notwithstanding, it is expected that the NRC regulations will continue to require compliance with applicable EPA environmental standards as the overall system performance objective for the proposed repository, and that demonstration of compliance with this objective will necessitate a quantitative performance assessment (PA) to estimate postclosure performance of the repository system.

Among the NAS findings and recommendations is a key recommendation that the revised standard limit individual risk to a member of the public and abandon the existing quantitative release limit with its implied population protection basis. Specifically, NAS recommended that the level of protection provided by the new environmental standard be comparable to that level of risk considered acceptable to society at large, given that society currently tolerates certain *involuntary* risks (e.g., in the range of  $10^{-5}$  to  $10^{-6}$  fatalities per year). To demonstrate that the proposed geologic repository can be designed to provide comparable protection to society, NAS therefore recommended that assessments of individual risks be conducted for certain target populations in the YM vicinity, using the approach specified in 1985 by

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<sup>3</sup>The use of subsystem performance objectives is consistent with the Commission multiple barrier, defense-in-depth concept. At their time of inclusion in 10 CFR Part 60, these criteria were viewed as important contributors to the NRC ability to find, with reasonable assurance, that the EPA Standards would be met.

the International Commission on Radiological Protection (ICRP) (e.g., "critical groups").<sup>4</sup> As EPA considers this particular recommendation, the NRC staff is evaluating how a PA methodology, used to demonstrate compliance with its implementing regulation, might be revised to accommodate such a standard. Anticipating that some type of dose-based standard will be adopted, the NRC has begun to evaluate methodologies for implementing such a standard to provide some insights into the subissues cited previously. For these reasons, the efforts of NRC staff in FY96 focused on the objectives presented in the following paragraphs.

#### **Defining a Compliance Period and Method**

The objective for work on this subissue in FY96, was to provide some initial analyses of techniques for evaluating an appropriate compliance period. There is regulatory precedent related to this issue and selecting a compliance period that represents a departure from that precedent would require a supporting rationale. Accordingly, a comparative analysis of the hazards presented by a HLW repository and an equivalent uranium ore body was conducted. This comparative analysis provides insights on radiological hazard as a function of time and therefore supports decisions concerning an appropriate compliance period. A peak dose calculation was also completed, providing additional information on appropriate compliance determination periods and methods to be used in reviewing a proposed revised EPA Standard for YM.

#### **Selecting a Critical Group(s)**

In FY96, efforts by the NRC focused on determining whether sufficient information exists to support identifying a critical group (or groups) for the Yucca Mountain region (YMR). Specific items addressed included (i) evaluation of the applicability of the critical group concept to the YMR, (ii) discussions with EPA staff to determine whether early drafts of the revised environmental standard would be compatible with the critical group concept, (iii) analysis of wells and water usage in the YMR to provide information related to lifestyles and exposure pathways, (iv) evaluation of approaches to defining exposure scenarios and reference biospheres, (v) reviews of previously compiled data on exposure pathways at YM, and (vi) considerations of the appropriate level of specificity to be used for including critical group parameters in a revised EPA Standard for YM.

#### **Evaluating Results of Potential Human Intrusion**

The FY96 effort on this subissue was limited to examining whether using a stylized human intrusion scenario for the purpose of evaluating the resiliency of a repository to such intrusion was implementable through a revised EPA Standard for YM. Scoping calculations and evaluations were conducted for this purpose.

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<sup>4</sup>The term dose generically refers to the quantity of radiation energy absorbed by body organs or tissue. The NRC defines dose for its regulatory purposes in 10 CFR Part 20. In its recommendations, the NAS adapts the ICRP terminology to its proposed risk-based framework.

## Considering Disruptive Events

In FY96, techniques for assessing the effects of volcanic disruption on the proposed repository were evaluated through refined modeling of the dispersion of radionuclides as a result of such disruption. The calculations included doses to persons who might reside at various distances from a proposed YM repository. These calculations could also assist in identifying the critical group. This assessment of volcanic disruption provides an example of methods that can be used to evaluate the incorporation of other disruptive events in a revised EPA Standard for YM.

These four particular topics were selected for study because they (i) provided some preliminary insights into NAS recommendations; (ii) focused on the major implementation issues that the Commission would need to address as it reviews and comments on a revised EPA Standard, and (iii) could be completed within the time constraints.

### 9.3 SIGNIFICANT TECHNICAL ACCOMPLISHMENTS

This section describes the technical accomplishments for the EPA Standard KTI during FY96. The significant technical accomplishments described herein are (i) scoping calculations that were performed to support the NRC review and comment on technical issues associated with a dose-based standard, (ii) documentation of investigations related to critical group(s) and reference biosphere, and (iii) documentation of background information to support the assessment of a stylized human intrusion calculation that may be required by a revised EPA Standard for YM.

#### 9.3.1 Scoping Calculations for Interactions with the Environmental Protection Agency

The following sections provide short summaries of the analyses that are being published as NUREG-1538.<sup>5</sup>

##### 9.3.1.1 Relative Hazards of High-Level Waste Over Long Time Periods

The time period of regulatory concern for geologic disposal of HLW is an issue that has been discussed and debated for well over 20 yr. The NAS recently recommended (National Research Council 1995)

. . . [the] calculation of the maximum risks of radiation releases whenever they occur as long as the geologic characteristics of the repository environment do not change significantly. The time scale for long-term geologic processes at YM is on the order of approximately one million years.

NAS also stated that probably the most significant difference between their findings and recommendations and the existing HLW standard is the time period of regulatory interest (TPI) (National Research Council, 1995). Based on recent total system performance assessment (TSPA) studies, the time of maximum risk

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<sup>5</sup>Nuclear Regulatory Commission. 1996. *Preliminary Performance Assessment Analyses Relevant to Dose-Based Performance Measures*. In preparation. NUREG-1538. Washington, DC: Nuclear Regulatory Commission.

may well be hundreds of thousands of years into the future (e.g., TRW Environmental Safety Systems, Inc., 1995). This NRC/CNWRA study examines one basis for limiting the time period of concern—the natural decrease in gross radioactivity and radiological hazard from a geologic repository hazard with time that results from radioactive decay.

A number of studies have examined the technical bases for limiting the TPI (Environmental Protection Agency, 1985; 1982a,b). Natural decay of the waste, in conjunction with other considerations, was used to support the limited time period for regulatory concern in the since-remanded standard 40 CFR Part 191. The 1985 version of the EPA Standard contained both a 1,000 yr time period for individual protection requirements and a 10,000 yr time period for the cumulative release requirement. A court remanded this regulation requesting (among other things) a more thorough explanation of the reasons underlying the choice of a 1,000 yr regulatory period. In 1993, EPA extended the time period for individual protection to 10,000 yr on the basis that it would encourage the selection of a good disposal site and robust barriers, but not because it was deemed necessary to ensure adequate protection for the environment or the public (Environmental Protection Agency, 1993a; 1993b).

A scoping study compared the variation in total radioactivity and radiological hazard for a geologic repository containing 70,000 MTU of spent nuclear fuel (SNF<sup>6</sup>) and a hypothetical equivalent uranium ore body, over a one hundred million year time period. The hypothetical ore body is defined to have the same amount of uranium and occupy the same volume as the proposed geologic repository at YM. The primary difference between the potential geologic repository and the hypothetical ore body is that repository waste has a significant man-made radioactive hazard (through neutron irradiation and fissioning) compared to the hazard from the ore body that is from naturally occurring nuclides.

In calculating the relative radiological hazard, the staff assumed the primary hazard would be from drinking contaminated groundwater, where the contamination was predicted using modeling assumptions and data specific to YM. The model consisted of steadily percolating groundwater flowing through the repository and into the saturated zone. Some of the percolating groundwater contacted some of the waste packages (WP). The water that contacted the waste became contaminated with radionuclides. For the analyses, 43 different radionuclides were considered from ten to one hundred million years after irradiation (Lozano et al., 1994). The drinking water pathway dose conversion factors ( $DCF_{dw}$ ) were based on previously published results (Environmental Protection Agency, 1988; Department of Energy, 1988) and an assumed drinking rate of two L/d. The solubilities of the radionuclides were modeled with probability distributions based largely on earlier TSPA work (Wilson et al., 1994; Nuclear Regulatory Commission, 1995). The release of radionuclides was modeled as either solubility limited or rate limited. The limiting radionuclide release rate was based on subsystem requirements in 10 CFR 60.113 (Nuclear Regulatory Commission, 1995). The relative radiological hazard was defined as a ratio of doses

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<sup>6</sup>The principal waste forms to be disposed at YM will be SNF and vitrified waste. Other waste forms that may possibly be disposed include low-level, greater than class C, or transuranic wastes. Only SNF was considered for this analysis.

$$\frac{D_{dw,rep}}{D_{dw,ob}} = \frac{\sum_i DCF_i \min(sol_{i,rep} \cdot F_g \cdot A_i, R_{i,rep} \cdot F_w \cdot I_{i,rep} / Q)}{\sum_i DCF_i \min(sol_{i,ob} \cdot F_g \cdot A_i, R_{i,ob} \cdot F_w \cdot I_{i,ob} / Q)} \quad (9-1)$$

where

- $D_{dw,rep}$  = dose from drinking groundwater contaminated by the repository (rem/yr)  
 $D_{dw,ob}$  = dose from drinking groundwater contaminated by the ore body (rem/yr)  
 $DCF_i$  = dose conversion factor from drinking groundwater contaminated by the  $i^{th}$  radionuclide [(rem/yr)/(Ci/L)]  
 $sol_{i,rep}$  = solubility of the  $i^{th}$  radionuclide in 70,000 MTU of waste (mol/L)  
 $sol_{i,ob}$  = solubility of the  $i^{th}$  radionuclide in hypothetical ore body (mol/L)  
 $F_g$  = fraction of seeping groundwater that becomes contaminated (2 percent)  
 $F_w$  = fraction of waste inventory that is contacted by groundwater (1 percent)  
 $A_i$  = activity of the  $i^{th}$  radionuclide (Ci/mol)  
 $R_{i,rep}$  = maximum release rate for the  $i^{th}$  radionuclide in 70,000 MTU of waste (1/yr)  
 $R_{i,ob}$  = maximum release rate for the  $i^{th}$  radionuclide in hypothetical ore body (1/yr)  
 $I_{i,rep}$  = total inventory of  $i^{th}$  radionuclide in 70,000 MTU of waste (Ci)  
 $I_{i,ob}$  = total inventory of  $i^{th}$  radionuclide in hypothetical ore body (Ci)  
 $Q$  = volumetric flow rate of groundwater through the repository/ore body (L/yr)

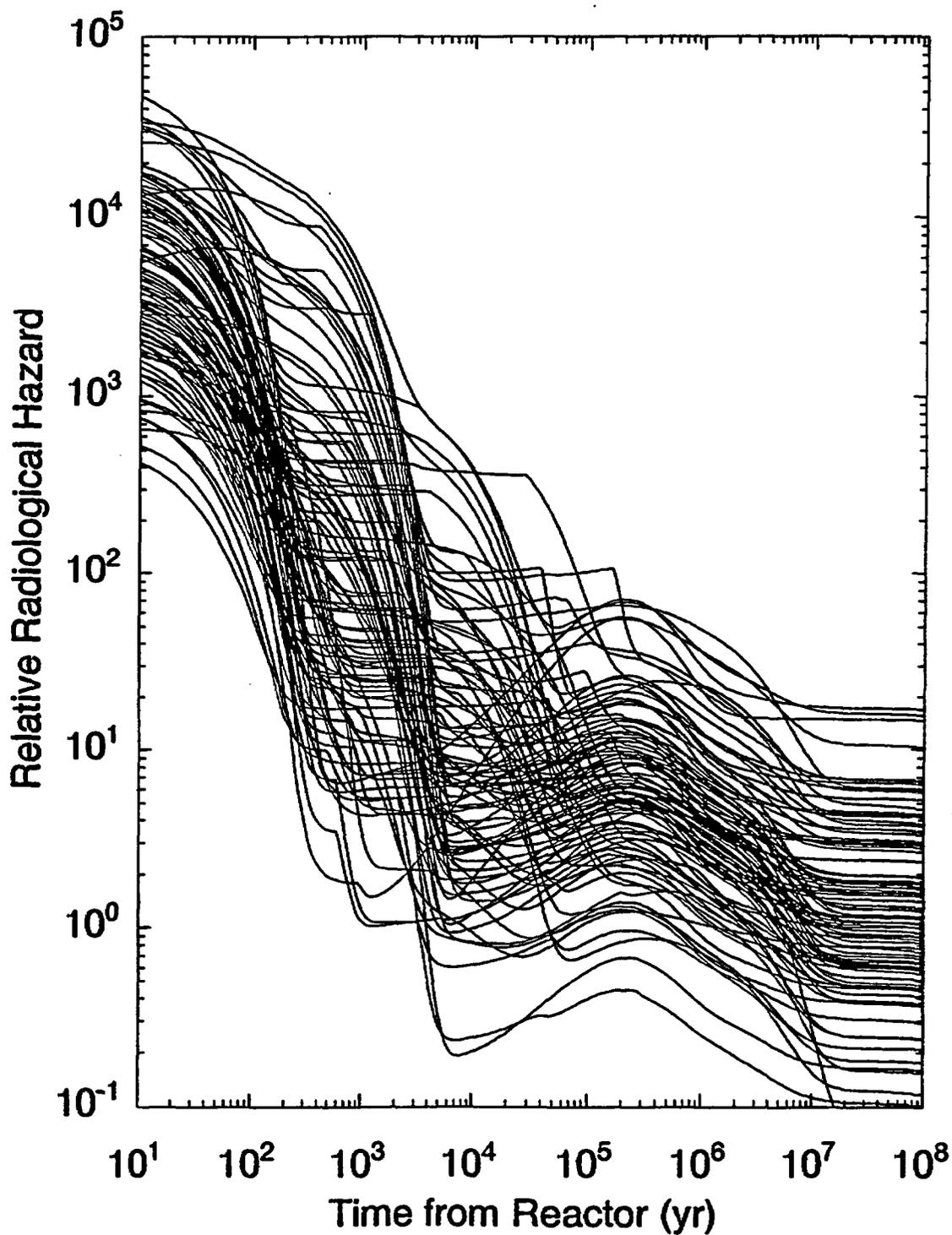
The minimum operator is used in Eq. (9-1) to select either solubility or rate limited release.

Figure 9-1 shows the range of relative radiological hazard due to uncertainties in radionuclide solubilities and release rates. For both the spent fuel repository and the hypothetical ore body, 100 distinct estimates were generated by sampling the radionuclide solubilities and release rates [the common logarithm of the release rate was assumed to be  $-5$  with a standard error of 0.5 based on previous staff work (Nuclear Regulatory Commission, 1995)].

The relative radiological hazard of the spent fuel repository is initially about four orders of magnitude greater than that of the hypothetical ore body. The radiological hazard diminishes rapidly over the first few hundred to few thousand years. The relative hazard diminishes by 90 percent at 100 yr, 99 percent at about 1,000 yr, and 99.9 percent at 10,000 yr. By 10,000 yr, the relative radiological hazard will be within an order of magnitude of the hypothetical ore body. The apparent increase in hazard at 100,000 to 500,000 yr is due to the ingrowth of radionuclides such as  $^{230}\text{Th}$ ,  $^{229}\text{Th}$ ,  $^{226}\text{Ra}$ , and  $^{210}\text{Pb}$ . A TPI for a proposed repository of about 10,000 yr would therefore focus attention on the time period when the waste has a significant man-made hazard component that is readily discernable from a hypothetical ore body, even after considering uncertainties associated with solubilities and release rates. The findings of this study are consistent with those of earlier studies (Environmental Protection Agency, 1982a, 1985).

### 9.3.1.2 Preliminary Calculations of Expected Dose from Extrusive Volcanic Events at Yucca Mountain

The purpose of this analysis was to demonstrate a calculational technique and provide a preliminary estimate of radiation doses for an extrusive volcanic scenario at YM. Calculations are based in part on a probabilistic volcanic ash (tephra) distribution model developed by Suzuki (1983) and



**Figure 9-1. Comparison of spent nuclear fuel repository and hypothetical uranium ore body hazards accounting for uncertainties in radionuclide solubilities and release rates**

extended by Jarzempa (1995). In addition, a new model for distributing only SNF within the ash particles has been developed to more realistically (than previous methods) model radionuclide distributions on the earth surface after a volcanic event. Dose modeling of radiation exposures from the contaminated ash blanket has also been performed. The dose pathways considered in these analyses were (i) ingestion from contaminated animal products and crops, (ii) inhalation from resuspension, and (iii) external radiation. Dose Conversion Factors (DCFs) as a function of these most important pathways, and as a total of all the pathways, were derived for contaminated soil for a hypothetical critical group resident at selected dose points on the earth surface [i.e., 20, 25, and 30 km directly south from the proposed repository (down gradient)] immediately after the volcanic event occurs. The extrusive volcanism analysis was performed for two different TPIs: 10,000 yr (current HLW regulations) and one million years (NAS proposed time frame).

The progression of events in the exposure scenario is as follows:

- Magma enters the repository and becomes contaminated with SNF particles.
- Contaminated magma forms into contaminated ash. The level of contamination of these particles is a function of the particle size (described in NUREG-1538).
- Eruption parameters are sampled according to the procedure given in Jarzempa (1995).
- The eruption column and contaminant plume form and produce volcanic ash fallout at distances and directions as determined in Jarzempa (1995).
- Doses are received by a member of the hypothetical critical group at specified dose points.

It is assumed the critical group member is exposed immediately after the particle plume deposits the contaminated ash blanket. The critical group in these investigations is composed of a single Amargosa Desert-type farmer/rancher at points 20, 25, and 30 km directly south of the proposed repository. For these preliminary analyses no other critical groups were investigated. NUREG-1538 contains a description of the lifestyle of this critical group. In addition, the following four assumptions were used:

- Volcanic ash dispersal model and parameter ranges described in Jarzempa (1995) are valid for modeling volcanic ash dispersals at YM.
- Doses are calculated for an Amargosa Desert farmer/rancher as described in LaPlante et al. (1995) with all of the associated assumptions and limitations.
- Selected dose points describe reasonable possible locations of the critical group.
- Assumptions used in modeling the SNF transport and subsequent dose calculations detailed in NUREG-1538 are valid.

Expected doses and standard deviations were calculated for the three dose points and the two TPIs. These results show a generally decreasing dose with distance from the location of the volcanic event (table 9-1). Increasing the TPI from 10,000 yr to one million years generally appears to increase the expected value of the peak effective dose equivalent by a factor of 2 to 4, although the magnitude of this change is somewhat uncertain because of the large standard deviation of the estimates. These results affirm

that by increasing the TPI, the importance of low-probability, high-consequence events such as volcanism is significantly enhanced when compared with scenarios that are certain to occur, such as an undisturbed repository leaching small amounts of radionuclides to the water table with subsequent drinking water pathway doses.

### 9.3.1.3 Dilution Analyses

Groundwater dilution is expected to be an issue of key importance in assessing the YM site because it directly determines the degree of dose reduction. For example, if mixing a contaminant stream with groundwater flow in the tuff aquifer produces a dilution factor of 100, then the dose (and associated radiologic risk) would be reduced by this same factor. Dilution of radionuclides released into the groundwater will be a result of mixing along the flow path between the source point(s) and the location where the contaminated groundwater is withdrawn. Mixing of a dissolved contaminant is, in general, the result of variations in both the magnitude of the fluid velocity and its direction (i.e., hydrodynamic dispersion). These variations are principally caused by small- and large-scale heterogeneities in the geologic media (Fetter, 1993). Large-scale features such as faults may in some instances induce flow variations and thereby enhance natural mixing, while in other cases they may produce highly channelized flow with limited mixing.

Only generic analyses of mixing and dilution have been performed by the DOE to date for the YM site (TRW Environmental Safety Systems Inc., 1995). These analyses suggest that natural or passive groundwater mixing will produce dilution factors (DF) on the order of  $10^3$  to  $10^5$  at 5 km from the edge of the proposed repository and  $10^4$  to  $10^6$  at 30 km. NRC and CNWRA staff believe these estimates are optimistic because (i) the technical bases were neither conservative nor bounding, (ii) such large DFs imply a homogeneous hydrochemistry—inconsistent with available data, and (iii) the DFs were much higher than those suggested by previous transport calculations in the DOE TSPA-93 (Wilson et al., 1994). The DOE estimates inferred from TSPA-93 calculations suggest DFs ranging from 5 to 20 at 5 km. In comparing the two independent dilution factor estimates, however, it is important to recognize that the TSPA-95 DFs take into account mixing below the repository whereas the DFs inferred from the TSPA-93 (Wilson et al., 1994) calculations neglect dilution immediately below the repository.

The scoping analysis was performed to study groundwater dilution characteristics associated with the proposed repository at YM. The objectives of the analysis were two-fold:

- Gain insight to the site specific factors that may affect groundwater mixing and attendant dilution of dissolved radionuclides at the YM site, and
- Determine if there are any methodology issues that may impact implementation of a dose- or risk-based standard as proposed by the NAS report.

Meeting these objectives provides a basis for staff review and comment on a revised EPA Standard for YM. As used in this analysis, the dilution factor was defined as the ratio of the peak groundwater concentration below the repository to the concentration at any other point in the saturated zone. This definition assumes that the initial mixing below the repository is small, which introduces conservatism.

Although available field data for the YM site were used, the scoping analysis did not consider parameter uncertainties associated with the spatial variability of hydraulic properties. In addition, the

**Table 9-1. Expected values and standard deviations as a function of position and the time period of interest**

Dose Point Number	Time Period of Interest (yr)	Dose Point Location		Expected Peak Annual Effective Dose Equivalent in the TPI (rem/yr)	Standard Deviation (rem/yr)
		x (km)	y (km)		
1	10,000	0	-20	$2.7 \times 10^{-6}$	$2.2 \times 10^{-3}$
2	10,000	0	-25	$7.5 \times 10^{-7}$	$7.6 \times 10^{-4}$
3	10,000	0	-30	$2.5 \times 10^{-7}$	$3.4 \times 10^{-4}$
1	1,000,000	0	-20	$7.7 \times 10^{-6}$	$6.1 \times 10^{-4}$
2	1,000,000	0	-25	$1.8 \times 10^{-6}$	$1.4 \times 10^{-4}$
3	1,000,000	0	-30	$4.4 \times 10^{-7}$	$4.1 \times 10^{-5}$

hydrogeologic system was treated as an equivalent porous continuum and no attempt was made to account for flow and transport through discrete fractures or include matrix diffusion effects. Mixing induced by water well pumping was also not considered.

To assess groundwater dilution and its dependence on the heterogeneous characteristics of the YM setting, a series of two-dimensional (2D) computer simulations of groundwater flow and radionuclide transport were performed. Computer models were applied to calculate four quantities: hydraulic head distributions, flow paths, particle travel times, and radionuclide plume distributions. Dilution of <sup>99</sup>Tc was modeled because it is a radionuclide of importance to dose and reflects the dilution behavior of radionuclides with relatively large inventories, long half-lives, and nonsorbing characteristics. Numerical calculations and graphical display of these four quantities were used to gain insight to the nature of the hydrogeologic processes that may control the degree of dilution at the YM site.

Two computer codes were used in performing the scoping analysis: (i) MAGNUM-2D, a saturated flow model (England, et al., 1985) and (ii) CHAINT, a multicomponent radionuclide transport model (Kline and Baca, 1985). Hydraulic head distributions simulated with the MAGNUM-2D code were used to calculate flow paths (i.e., streamlines) from various locations and associated particle travel times along the streamlines. Radionuclide concentrations computed with the CHAINT code were contoured to depict plume spreading and dilution patterns.

A model of lateral groundwater flow from the proposed repository site to the Amargosa Desert region was developed to assess the flow patterns through the relatively long and heterogeneous flow path. Groundwater flow paths and particle travel times for a particular parametric case are shown in figure 9-2a; circled numbers refer to the distinct hydrogeologic subregions of the flow domain. From this visualization it is evident that, depending on location of the release, mobile radionuclides could travel along paths with

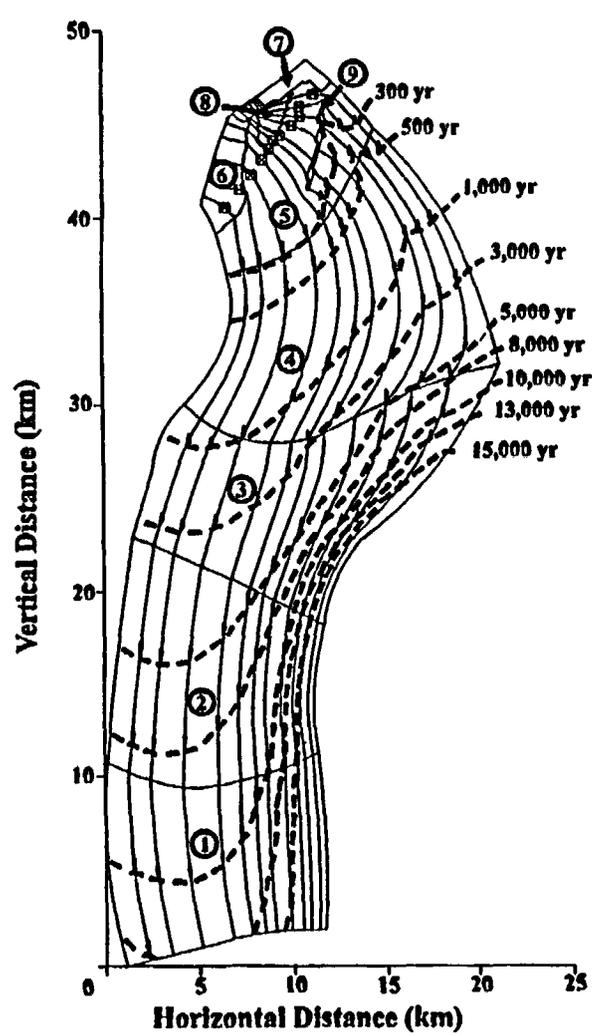
very large particle travel times (i.e., on the order of  $\approx 10,000$  yr) or along more direct paths with smaller travel times (i.e.,  $\approx 5,000$  yr). It can also be noted from figure 9-2a that structural features such as the Bow Ridge fault can play a role in determining flow directions. The range of Darcy fluxes, which are relevant to mixing, were calculated for each of the nine subregions. The magnitude of the flux in the tuff aquifer beneath the proposed repository foot print ranged from about 0.5 to 1.9 m/yr while immediately down gradient of the repository the flux was estimated to range from 0.01 to 3.7 m/yr. In the alluvium, where the Amargosa Valley region is located, the magnitudes of the Darcy fluxes ranged from about 0.4 to 0.7 m/yr.

Hypothetical releases of  $^{99}\text{Tc}$  from discrete locations in the proposed repository site were also modeled to estimate possible spread and dilution of radionuclides. DFs were computed and contoured for various time frames. Depictions of the  $^{99}\text{Tc}$  plumes at 10,000 yr (after the contaminant reaches the groundwater) are shown in figure 9-2b. From this radionuclide transport simulation, it appears that degree of dilution in the vicinity of the proposed repository would be relatively small. Even at long times, after the plume has reached the Amargosa Desert region, the DFs appear to be relatively low. Although these estimates may be relatively conservative, particularly at larger distances from the proposed repository, actual DFs would not be expected to be orders of magnitude larger.

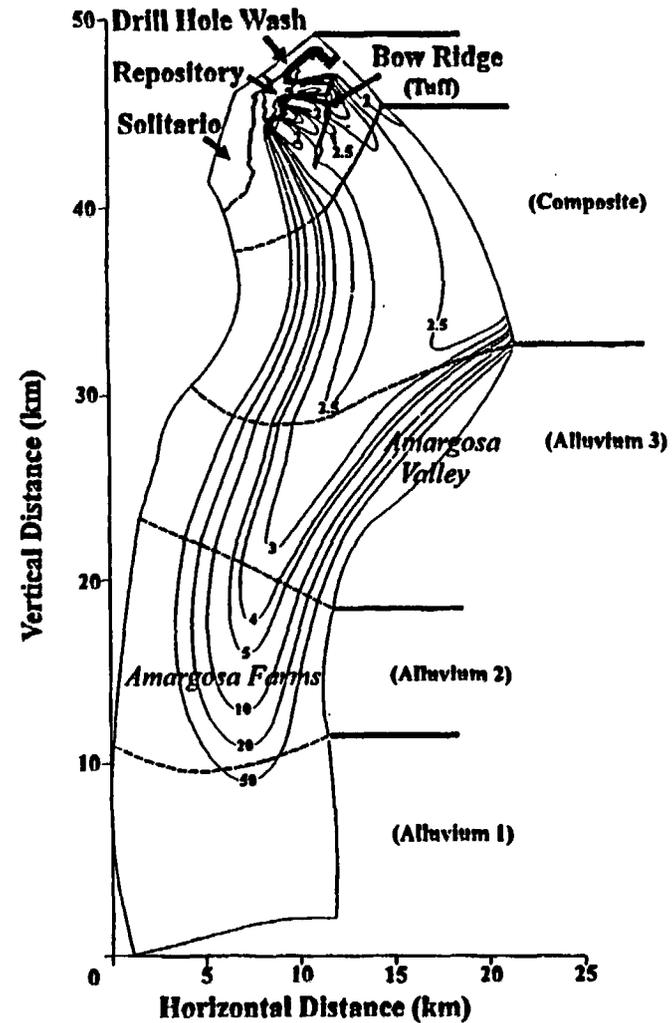
Flow and transport along a cross section through the site was also modeled. The purpose of this part of the scoping analysis was to examine smaller scale mixing processes that occur immediately beneath the site. In this case, plume dilution is controlled by channelized flow through the complex geometry of the dipping hydrostratigraphic units, large permeability contrasts of adjacent units, and discontinuities associated with fault zones. The flow paths were calculated for the cross section defined by boreholes USW H-5 and USW H-4, shown in figure 9-3a. This figure depicts the streamlines originating from points along the Ghost Dance fault. The arrow heads placed along each streamline mark a 100 yr interval of particle travel time. From this visualization it is evident that flow paths are predominantly along hydrostratigraphic units except near fault zones where there are large discontinuities in the hydrostratigraphy. Transport calculations are for  $^{99}\text{Tc}$ , assumed to be introduced at the Ghost Dance fault. The radionuclide distribution at 1,000 yr, shown in figure 9-3b, illustrates that (i) the plume remains near the surface of the water table, (ii) the DFs at the water surface are relatively small, and (iii) large fault zones can induce significant vertical mixing.

The overall finding of this preliminary scoping analysis was that dilution at the YM site is not likely to produce large reductions in groundwater concentrations of radionuclides (or the associated radiation doses). In the immediate vicinity of the proposed repository, DFs on the order of 2 to 5 are expected based on model calculations. Relatively low DFs are likely if the plume is confined to fracture zones that are pervasive in the tuff aquifer (Geldon, 1993). Alternatively, if the plume spreads vertically as a result of flow through vertical fractures or faults, then the DFs will tend toward the higher end of the range. Passive mixing along the long flow path (from the proposed repository site to the Amargosa Desert region) are conservatively estimated to produce DFs on the order of 5 to 50. Other factors, such as interbasin transfers and water well pumping, may contribute to enhanced dilution, but a much stronger technical basis and relevant field data are needed to support DFs of the magnitudes presented in the DOE (TRW Environmental Safety Systems, Inc., 1995).

While this scoping analysis did not directly identify any methodology issues related to implementing a dose- or risk-based standard, an important consequence of such a standard is that it will require the DOE to place greater emphasis on characterization of the local and regional groundwater system. Additional tracer tests such as those conducted in the C-well complex (Geldon, 1995) may be

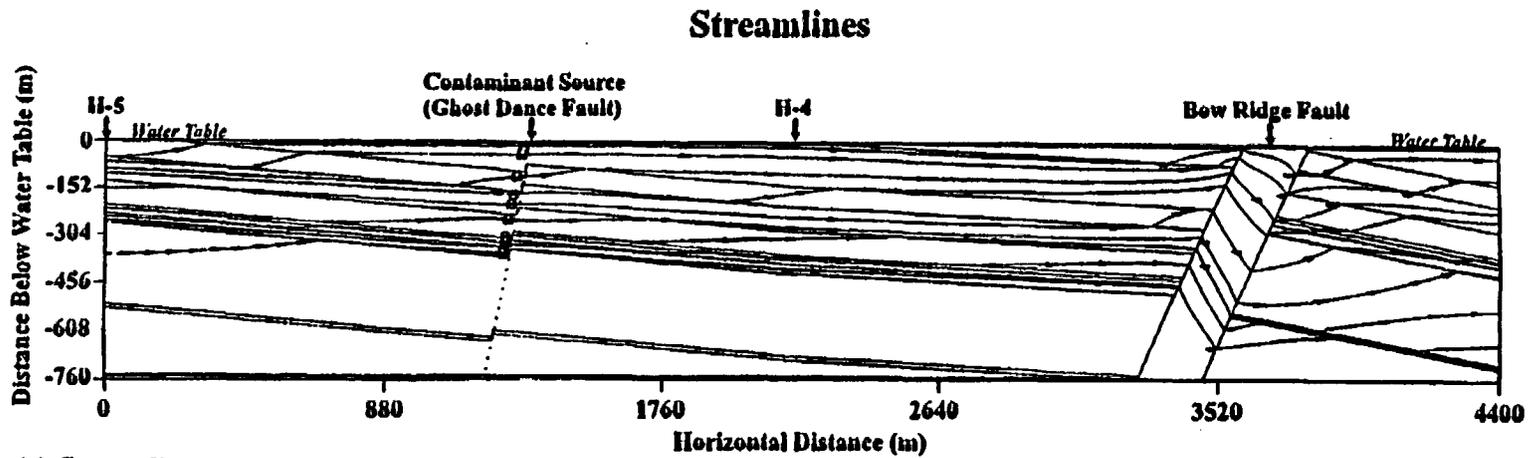


(a) Streamlines and travel times

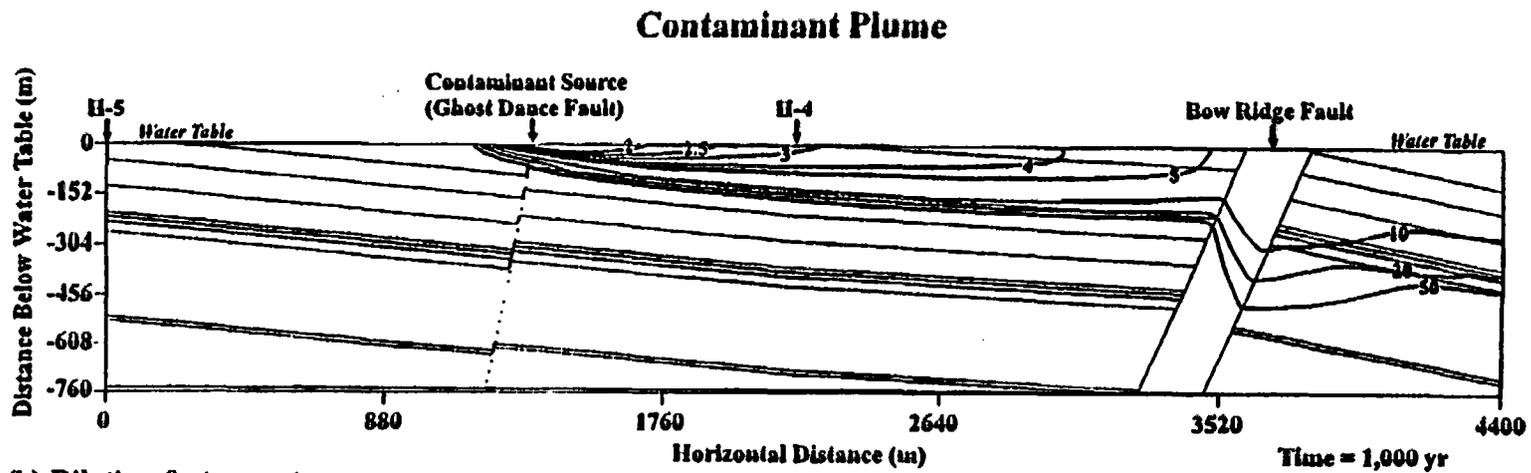


(b) Dilution factor contours

Figure 9-2. Streamlines (solid lines), particle travel times (dashed lines), and plume for lateral flow model (solid lines with arrows)



(a) Streamlines



(b) Dilution factor contours

Figure 9-3. Streamlines (solid lines with arrows) and contaminant plume for vertical cross section model

needed to acquire data on transport parameters (e.g., mass dispersivities and effective porosities) but representative of larger length scales. The hydraulic properties of the various faults will also be important.

#### **9.3.1.4 Human Intrusion**

Human intrusion has been analyzed as a disruptive scenario in prior TSPAs [e.g., Codell, et al. (1992), Barnard, et al. (1995), Wilson, et al. (1984), and Nuclear Regulatory Commission, (1995)] performed to examine compliance with the requirements of 10 CFR Part 60. Each of these analyses required basic assumptions regarding human behavior and future technology. As stated in section 9.1 of this report, the NAS (National Research Council, 1995) determined that there was no scientific basis for predicting the occurrence of human intrusion. Consequently, the NRC staff performed scoping analyses to consider the requirements for a stylized calculation (consequences only) of human intrusion.

The scoping analysis for human intrusion consisted of calculating drinking water dose resulting from a single WP damaged by exploratory drilling from the ground surface. Neither direct exhumation nor other sources of human intrusion were considered in the analysis. The source term and transport of radionuclides were modeled using the methodology of section 9.3.1.5 as developed in the NRC IPA program (Nuclear Regulatory Commission, 1995). Dissolution of spent fuel and leaching of radionuclides from within a single WP were determined taking individual radionuclide solubilities into account, and radionuclide concentrations at a 5 km distant well were calculated, assuming a representative transport pathway. The first set of calculations assumed the WP to be damaged at times of 0, 500, 1,000, 10,000, and 100,000 yr after closure. For each of these times of failure, surface runoff was assumed to enter the borehole from a catchment of either 10 m<sup>2</sup>, 1 m<sup>2</sup>, or the inside area of the 150 mm diameter casing. Geochemical retardation was ignored so that the condition of either a fast fracture pathway or a nearby borehole path to the saturated zone could be approximated. Another purpose of this initial calculation was to determine the relative importance of time of failure and water inflow to consequence (drinking water dose). It was readily apparent that surface water inflow had a strong effect on dose and that time of failure had a relatively minor effect. It was also determined that water inflow affected the relative contributions of various radionuclides to dose.

The next set of analyses included geochemical retardation during transport. This was considered a more credible scenario than a direct short circuit to the saturated zone next to a damaged WP, given that the drilling event occurs. The inclusion of geochemical retardation reduced the calculated drinking water dose at the receiving well to about 1 millirem or less, depending on water inflow to the WP.

Considering such factors as (i) the depth to groundwater from the top of YM, (ii) the scarcity of water users and arable land on the mountain, and (iii) the absence of known resources below the proposed repository, it is reasonable to argue that disruption of the repository by exploratory drilling or drilling for water resources is relatively unlikely. Because of the expected low likelihood and low consequence, the NRC staff concludes that human intrusion from surface based drilling need not be directly incorporated into a TSPA.

#### **9.3.1.5 Annual Individual Dose Estimates**

Prior TSPAs for YM analyzed system performance primarily with respect to the integrated release requirement of the remanded EPA Standard. As discussed previously, NAS recommendations called for a performance objective based on an annual individual dose using a critical group approach. Preliminary dose calculations were conducted to gain insight on implementation issues associated with a

dose-based standard and the relative importance of site-specific assumptions and parameters at YM. These insights will be used to support the NRC analysis of a proposed EPA Standard for YM.

Evaluation of annual individual dose requires specification of an exposure scenario that defines the geosphere and biosphere pathways that can transport radionuclides released from a repository to a human receptor in the biosphere. Simulation of radionuclide release and transport in the geosphere was based on models already developed in the NRC IPA program (Nuclear Regulatory Commission, 1995). Some modifications were necessary to allow investigation of sensitivities of the dose calculation, improve calculational efficiencies, and allow the calculation to go beyond a 10,000 yr performance period to the time of peak dose. Two exposure pathways were developed for release of radionuclides to groundwater. One exposure pathway, consistent with the distance used for integrated release calculations performed in previous IPA efforts (Nuclear Regulatory Commission, 1995), assumes a critical group exists at a distance of 5 km. Radioactive exposure results from drinking water from a well that intercepts the potential release plume. The other exposure pathway, consistent with current populations in Amargosa Valley region, assumes a critical group is located approximately 30 km down gradient from YM. Radioactive exposure results from drinking contaminated water and consumption of locally grown crops irrigated using contaminated water.

The NRC staff performed probabilistic analyses to quantify the variation in dose estimates due to uncertainties in the geosphere models (i.e., source term release, hydrologic flow, and radionuclide transport) for the two critical group locations. Important attributes and assumptions of the analyses are as follows.

- Simplifications of the flow and transport models include a steady-state flow system; no thermal effects; fracture retardation assumed to be a fraction of the matrix retardation (a range of 0-10 percent was used for the uncertainty analyses); assumed WP container lifetime of 1,000 yr; disruptive scenarios not considered; and a source term based on leach rate, solubility, and amount of water contacting the waste.
- A continuous transport path is assumed to exist from the saturated zone below YM to the receptor locations at 5 and 30 km.
- All releases from the proposed repository eventually pass the receptor locations and are uniformly mixed in the annual volume of water pumped by the critical group (1 million gallons per day for the 5 km location and 8 million gallons per day for the 30 km location). Water usage was based on broad assumptions regarding minimum pumping rates required to intercept the entire contaminant plume (applied to the 5 km location) and water usage consistent with a farming critical group (applied to the 30 km location).
- The critical group at 5 km uses untreated groundwater for drinking water and household chores only.
- The critical group at 30 km uses untreated groundwater for home and irrigation. The average member of this critical group is assumed to supply half of the food needs and all the water and milk consumption from the farm/ranch.

The maximum annual individual dose [Total Effective Dose Equivalent, (TEDE)] for the pathways considered in the uncertainty analysis is presented in figures 9-4 and 9-5 for the 5 km location

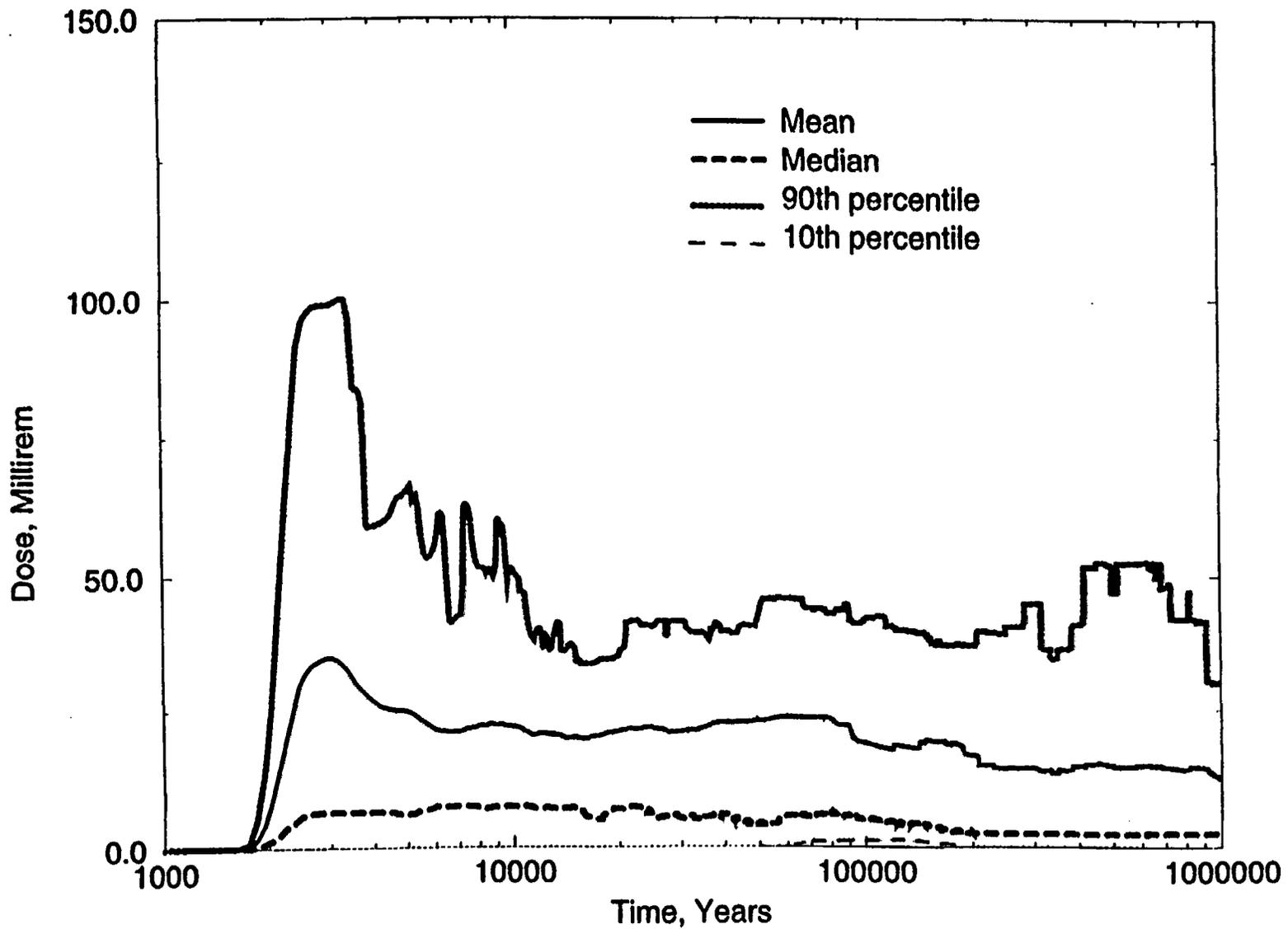


Figure 9-4. Uncertainty analysis of dose for one hundred vectors at a point 5 km down gradient from the proposed repository

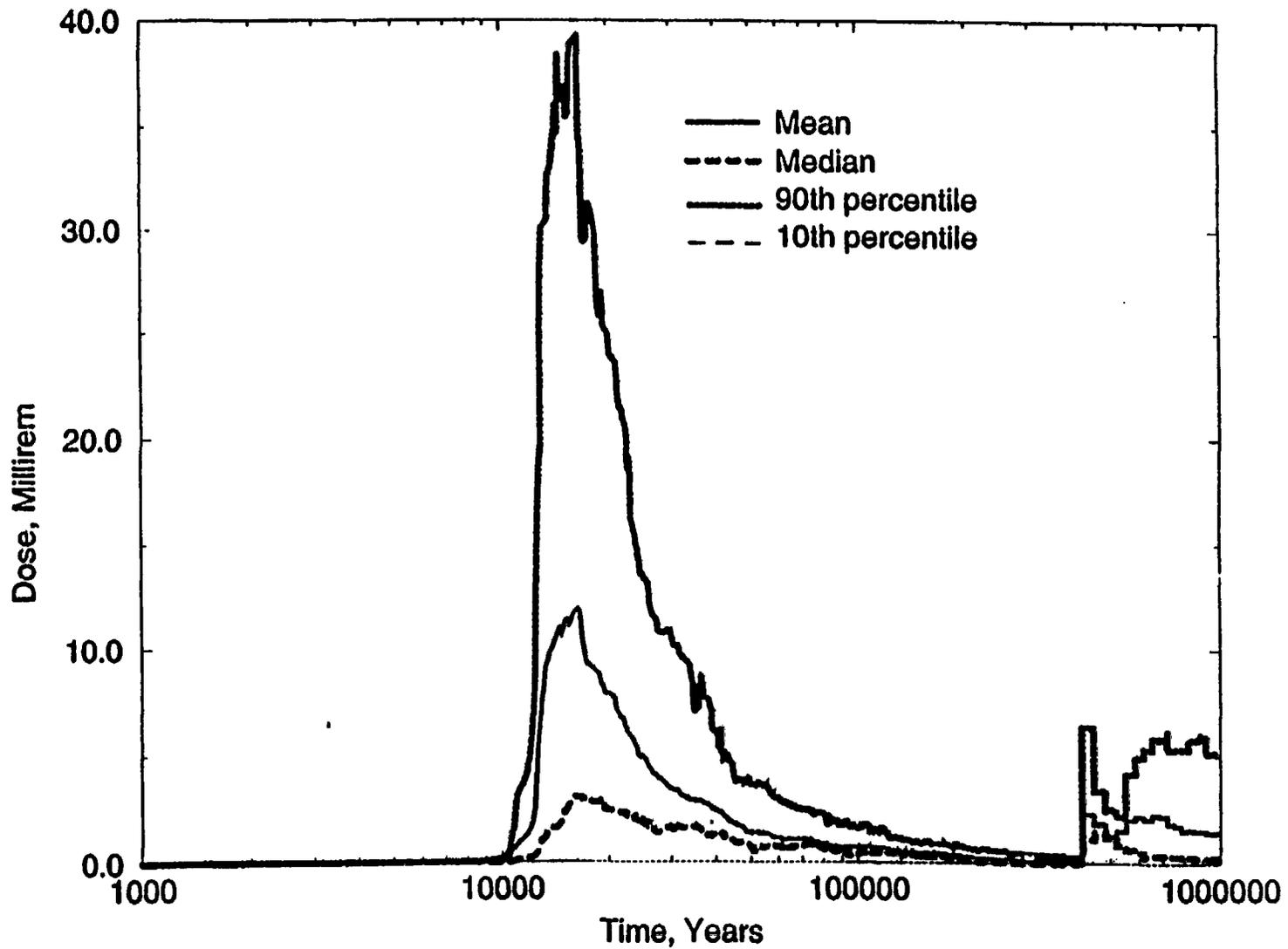


Figure 9-5. Uncertainty analysis of dose for one hundred vectors (all dose pathways) in the Amargosa Desert region 30 km down gradient from the proposed repository

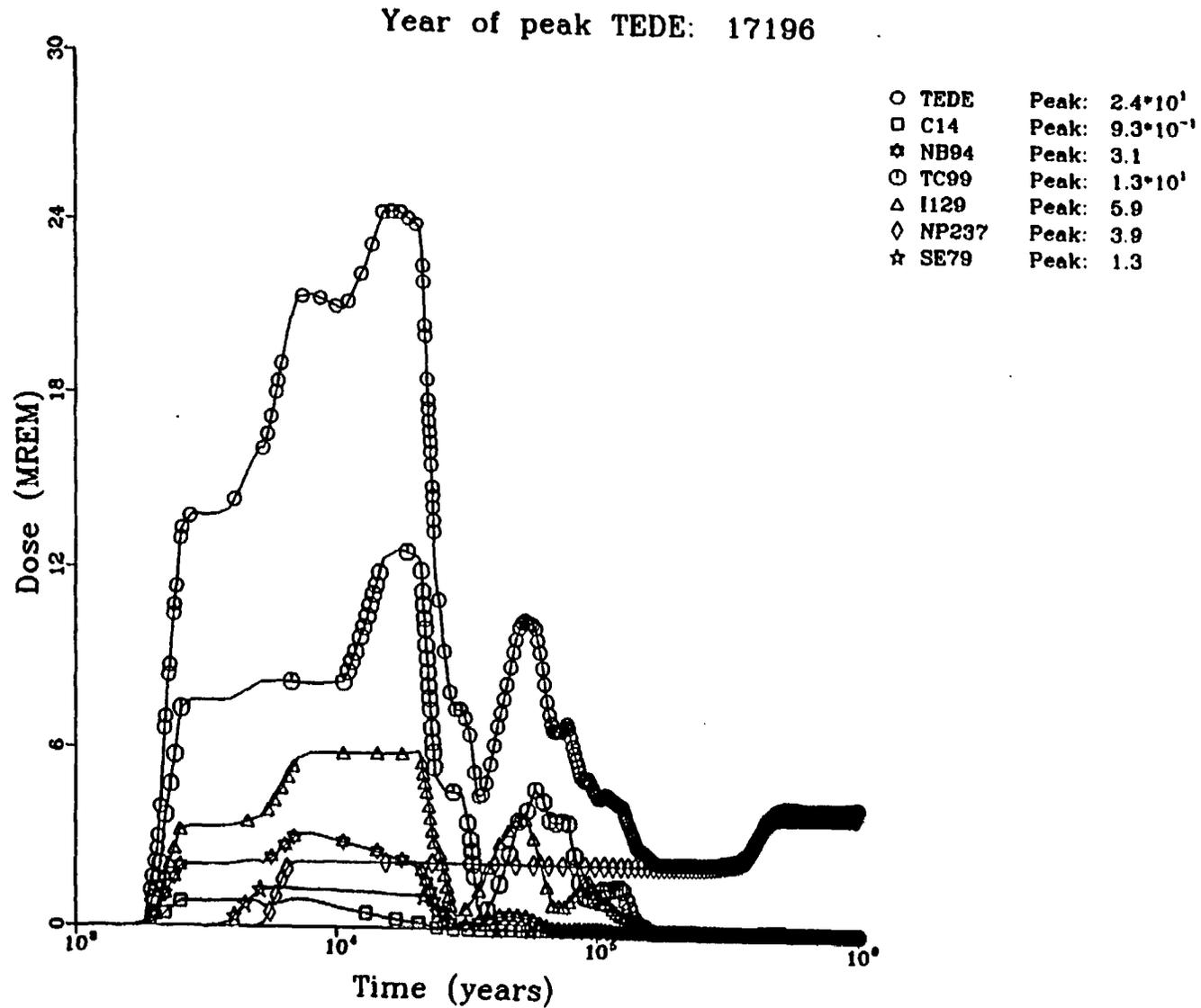


Figure 9-6. Annual individual dose from all radionuclides total effective dose equivalent and for selected radionuclides for the drinking water pathway at a distance of 5 km (mean parameter values were used including fracture retardation)

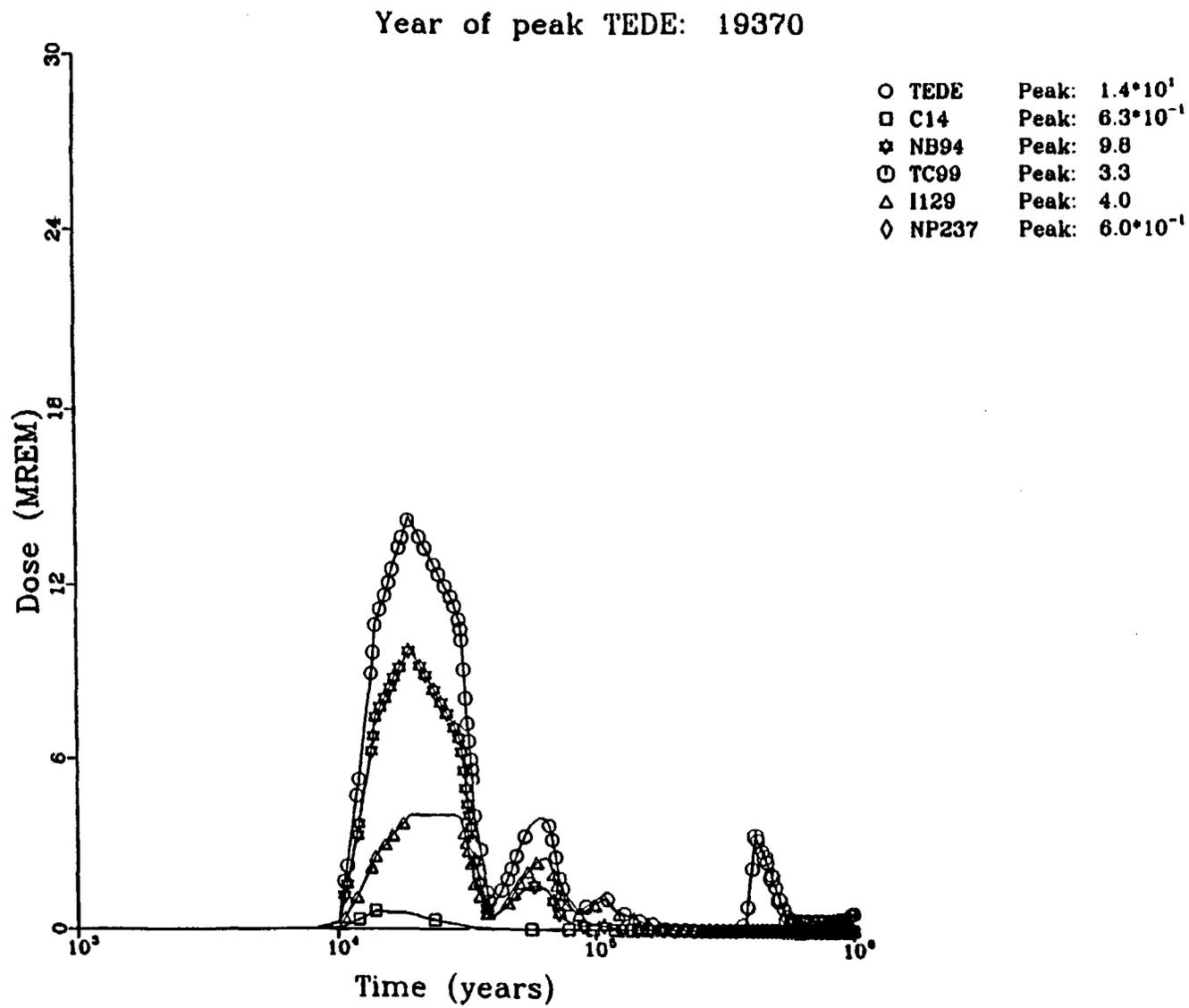


Figure 9-7. Annual individual dose from all radionuclides total effective dose equivalent and for selected radionuclides for the drinking water pathway at a distance of 30 km (mean parameter values were used including fracture retardation)

and the 30 km location, respectively. These figures represent the calculated annual individual dose at each point in time. Doses for 100 sampled vectors were calculated versus time, and the results were grouped into 100 yr bins. The values in each bin were then ranked, and the 10th, 50th, and 90th values in the rank (100 being the largest) were plotted to provide the curves denoted as 10th percentile, median, and 90th percentile, respectively. The curve marked mean is the arithmetic average of all the values in each bin. Note that over a large range of times for both curves, the 10th percentile value was essentially zero, and is coincident with the time axis. The maximum annual individual dose estimates for both locations occur shortly after the initial arrival time of radionuclides at the two locations. This result is believed to be due to high percolation values (deep percolation in the 2 to 5 mm/yr range) which result in large releases of a small set of long-lived, mobile radionuclides which arrive at the well location at generally overlapping times. After the initial peak, the dose versus time curve is complicated by both short duration spikes (e.g., spikes that appear between 3,000 and 8,000 yr in figure 9-4) and secondary peaks which are significantly less than the initial peak (e.g., secondary peaks at 50,000 and 700,000 yr in figure 9-4 and 700,000 yr. in figure 9-5). The short duration spikes are believed to be due to variation in arrival times of individual radionuclides due to varying flow velocities and retardation. The secondary peaks are due to the distinct arrival times from specific sub-areas of the repository (the repository was divided into seven sub-areas) or from the same sub-area but along differing flow paths (i.e., an initial peak could be due to releases which are transported in the fracture flow path with a later peak occurring from releases which are transported in the slower matrix flow path).

A set of mean value simulations that used mean values from the parameter ranges used in the uncertainty analysis was performed to determine the radionuclides most important to dose. While the mean simulation results are considered appropriate for identifying particular radionuclides, the probabilistic results (presented in figures 9-4 and 9-5) are more representative of total system behavior. The figures are in reasonable qualitative agreement, but there are differences between the probabilistic results and the deterministic results. Generally, attempts to draw inferences based on comparison of the probabilistic and deterministic results were not meaningful.

Figures 9-6 and 9-7 present the doses for specific radionuclides for two locations as well as the total dose for all radionuclides from the pathways considered, which is denoted in the legend as TEDE (for Total Effective Dose Equivalent). The parameter values for these simulations used mean values of the parameter ranges from the uncertainty analysis. A cursory examination of figures 9-6 and 9-7 reveals that: (i) the magnitudes for the peak dose for the two locations are quite similar (14 mrem versus 24 mrem), and (ii) the times of occurrence of the peaks are similar (both around 20,000 yr) although estimated releases initially arrive at the 5 km location at a much earlier time than for the 30 km location (2,000 yr versus 10,000 yr). This apparent similarity in results is due to several significant differences in key assumptions (see previous bullets) that have counterbalancing effects on the results. For example, the dose at the 5 km location should be larger than the dose at the 30 km location due to differences in the assumed dilution volumes [1 million gallons per day (MGD) versus 8 MGD] which reduce concentrations at the further location. If drinking water dose was the only ingestion pathway, then the dose at the 30 km location might have been an order of magnitude or more lower than the dose at the 5 km location. However, the increased dilution volume at the farther location is due to the greater water needs of an agricultural community which requires consideration of additional ingestion pathways from animal products and crops that are not included in the ingestion pathway for the 5 km location. Thus, doses at the 30 km location are increased due to inclusion of additional pathways, counterbalancing the decreased dose due to lower concentrations. The similarity in the two times for occurrence of the peak is a result of the different contributions from specific radionuclides responsible for time of the peak. At the 5 km location, the peak dose is significantly influenced by arrival of  $^{99}\text{Tc}$  and  $^{129}\text{I}$  from more than one sub-area as evidenced by the multiple peaks for  $^{99}\text{Tc}$  (note: in the IPA flow and transport model, the repository is

represented by 7 sub-areas). At the 30 km location, the peak dose is influenced more by arrival of <sup>94</sup>Np. However, at both locations, it is long-lived, mobile radionuclides that are the key contributors to dose.

Three general conclusions may be drawn from the present analysis: (i) preliminary indications are that a relatively small number of long-lived, mobile radionuclides will be important to performance; (ii) there do not appear to be any technical difficulties that might preclude estimating an annual individual dose; and (iii) assumptions concerning critical group location and lifestyle could be important in determining an appropriate approach for establishing radionuclide concentrations at receptor locations.

### **9.3.2 Reference Biosphere/Critical Group**

NAS recommended that the concepts of reference biosphere and critical group (RB/CG) be adopted for the revised EPA Standard for YM. These concepts were not included in prior EPA Standards (e.g., 40 CFR Part 191), and a number of new implementation issues must be considered by the NRC to prepare for review and comment on a new EPA Standard for YM. In addition, a joint NRC/CNWRA working group within the EPA KTI was formed to consider acceptable options that EPA might select for adopting the RB/CG concepts. This working group focused on understanding and summarizing relevant NAS recommendations and identifying important implementation issues regarding RB/CG at YM. The absence of a completed standard during FY96 required staff to limit consideration of issues to general concepts. When a standard is completed, the NRC implementing role will be clarified and details of the implementation approach will be addressed.

Initial efforts relating to RB/CG were directed at understanding relevant NAS recommendations. This effort was important for developing a common understanding of the recommendations, and to support discussions between the NRC and EPA on options for revised standards. The approach provided in appendix C of the NAS report (i.e., the probabilistic critical group) was found to be unnecessarily complex and confusing. Consistent with NAS recommendations, the KTI team concluded that an alternative approach, which also satisfies the NAS recommendations, would be preferable. Special attention was placed on examining how NAS recommendations helped to define and limit speculative assumptions about lifestyle characteristics and potential locations of the critical group(s).

NAS recommendations were considered by the KTI team to provide the staff with the flexibility needed to select alternative methods for implementation. The team agreed that RB/CG characteristics should be based on reasonable assumptions supported (to the extent possible) by site specific information. The team also agreed with NAS that the critical group concept is only a framework for performance assessment and is not intended to predict future human behaviors. Nonetheless, available information on present human populations provides a reasonable basis for defining critical group characteristics. It may be necessary for EPA or NRC to provide additional definition of critical group characteristics through rulemaking or issuance of supporting guidance; however, NAS recommendations relating to use of the critical group approach were found to be implementable.

Scoping calculations focused on providing EPA early input on current techniques, capabilities, and implementation issues to consider prior to drafting a dose-based standard. For the exposure assessment portion of the calculations in NUREG-1538, a site-specific farming/ranching exposure scenario representative of potential exposure conditions currently existing in the Amargosa Desert area was developed. Exposure scenario parameter information was adopted from previous staff efforts including NUREG-1464 (Nuclear Regulatory Commission, 1995) and LaPlante et al. (1995). Local information on

current farming practices, water use, climate, and soil characteristics was obtained and used. Additional information sources were investigated for population demographics and well water use.<sup>7</sup> Results of the scoping calculations were presented to EPA, and site specific data was provided to allow their staff to conduct exposure assessments and tests. Preliminary results of exposure scenario parameter sensitivity analyses were also provided to EPA for consideration. Discussion of issues within the KTI team helped formulate a general approach which was presented at a BIOMOVs conference and at the 84th Advisory Committee on Nuclear Waste meeting on Exposure Scenarios for YM (June 25, 1996). An examination was conducted to evaluate the EPA claim that a reasonably maximally exposed individual (RMEI) is essentially equivalent to the average member of the critical group recommended by NAS. While EPA did not demonstrate this quantitatively, upon consideration the NRC staff recognized that RMEI appeared to be an adequate concept to consider for the standard. The NRC currently awaits publication of the draft standard before more detailed review and comment can take place.

### **9.3.3 Background Information and Recommendations for a Stylized Human Intrusion Calculation at Yucca Mountain**

The NAS report concluded: “. . . it is not possible to make scientifically supportable predictions of the probability that a repository's engineered or geologic barriers will be breached as a result of human intrusion over a period of 10,000 years.” Based on this conclusion, the NAS recommended that the new standard(s) for YM not require that human intrusion be included directly in PAs of the proposed repository, but might instead require: “. . . [examination of] the site- and design-related aspects of repository performance under an assumed intrusion scenario to inform a qualitative judgement. In this approach, the objective would be to perform a consequences-only analysis without attempting to determine an associated probability for the analyzed scenario.” NAS considered one exploratory borehole of a specified diameter drilled from the surface through the WP canister to the underlying aquifer. NAS suggested that: “. . . the simplest scenario that provides a measure of the ability of the repository to isolate waste and thereby protect the public health is the most appropriate scenario to use for this purpose.”

The purpose of this work was to provide background information and recommendations for identification of characteristics of a representative (e.g., most likely) borehole at YM and identification of the important processes associated with boreholes that penetrate the proposed repository horizon. By studying related documents about exploratory drilling techniques typically used in mineral exploration and water well construction, and considering NAS recommendations for this scenario, the NRC staff developed concepts that will be used to review and comment on a proposed EPA Standard for YM. Building upon the findings of the scoping calculations for the human intrusion scenario described briefly in section 9.3.1.4, a rudimentary study of the size of the catchment area as a function of borehole position was also conducted. Other potentially important considerations associated with drilling that could affect repository performance were identified including borehole size, drilling fluid additives, the use of casing, and borehole sealing techniques.

## **9.4 ASSESSMENT OF PROGRESS TOWARD MEETING OBJECTIVES**

This section evaluates the activities conducted in FY96 with respect to meeting the objectives discussed in section 2.0. The primary issue and each subissue will be discussed.

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<sup>7</sup>Eisenberg, N.A. 1996. Staff Visit to Amargosa Valley: Trip Report. Memorandum to M. Federline, Acting Director, Division of Waste Management. May 14, 1996. Washington DC: Nuclear Regulatory Commission.

Significant progress was made in identifying and conducting the activities necessary to support review and comment on an EPA Standard for YM. Throughout the year, the NRC staff interacted frequently with EPA staff to provide the NRC perspectives on implementation issues regarding the NAS recommendations for a dose-based standard.

### **Defining a Compliance Period and Method**

A number of proposals have been made to define the compliance period and method. These include (i) using the current 10,000 yr compliance period, (ii) evaluating compliance at the time of peak dose, and (iii) using deterministic calculations for shorter time periods with probabilistic methods for longer periods. Calculations of relative hazards and peak dose completed this year, combined with results of the previous NRC TSPAs, provided confidence that the NRC can evaluate any of the compliance periods or methods identified previously that might be proposed by the EPA Standard for YM.

### **Selecting a Critical Group(s)**

Evaluations completed during FY96 show that there is information on conditions and lifestyles in the YM area which supports the identification of critical group characteristics that can be included in a revised EPA Standard. Exposure scenarios and pathways and reference biospheres can be adequately constrained. Issues remain concerning the level of detail for critical group parameters to be specified in the regulatory framework.

### **Evaluating Results of Potential Human Intrusion**

Scoping calculations performed by the NRC staff in FY96 indicate that specifying a stylized human intrusion scenario and calculation is technically feasible. Details of the scenario and associated calculations require further definition in the regulatory framework.

### **Considering Disruptive Events**

Scoping calculations completed for volcanic hazards in FY96 combined with increasing sophistication of the NRC TSPAs provide confidence that potential repository disruptive events can be examined in a technically defensible way. These calculations not only support PAs but also contribute directly to selection of a critical group.

## **9.5 INTEGRATION WITH OTHER KEY TECHNICAL ISSUES**

Throughout FY96, the EPA Standard KTI coordinated its activities with other KTIs to ensure consistency of technical bases and assumptions and to provide results and information to other KTIs. The principal technical integration activities accomplished in FY96 were

- Information was provided to the TSPA I KTI consisting of tentative definitions of the reference biosphere and a critical group. Site specific characteristics (e.g., land use and water well practices) relevant to pathway modeling and dose calculations were compiled that will be used in future TSPAs for YM. In addition, scoping calculations for the human intrusion scenario were coordinated with those conducted in TSPA I KTI.

- Technical knowledge base and data regarding the hydrogeology of the site assembled as part of the USFIC (and previous CNWRA research projects) were used to conduct scoping calculations of the dilution characteristics of the proposed YM site.
- The RT KTI provided information regarding geochemical data for the regional groundwater system at YM that was useful in qualitative checks of the scoping calculations of dilution factors.
- The technical information necessary for modeling the volcanism scenario for YM was provided by the IA KTI. In close collaboration with the IA KTI team, this information was used to model hypothetical eruptions and to simulate the associated entrainment and airborne releases of radionuclides.

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## 10 UNSATURATED AND SATURATED FLOW UNDER ISOTHERMAL CONDITIONS

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### 10.1 INTRODUCTION

Yucca Mountain (YM), Nevada has been proposed as a site for a geologic repository for high-level radioactive waste (HLW) in part because of the favorable hydrogeologic conditions provided by its 700 m thick unsaturated zone. YM is located in the southernmost portion of the Great Basin Desert where the sparse precipitation—a reflection of the Sierra Nevada rain shadow—is greatly exceeded by annual potential evapotranspiration and infiltration rates in the lower elevation valleys and mountain ranges are generally small. Because mean infiltration and deep percolation rates within YM are assumed to be small, it is postulated that waste canisters are unlikely to be contacted by significant amounts of water under ambient thermal conditions and are thus less likely to corrode and expose the waste form. Low flux rates also reduce the likelihood that waste form that is exposed to water will be dissolved and transported rapidly to the water table. When YM was originally proposed, the saturated zone was assumed to play little or no role in demonstrating repository performance inasmuch as applicable regulations were based on a maximum cumulative radionuclide release to the accessible environment and saturated zone transport times to the accessible environment were estimated to be small (less than 170 yr, U.S. Department of Energy, 1988). With the publication of the National Academy of Sciences (NAS) recommendation that the YM standard be risk- or dose-based rather than release-based, the study of mechanisms that may retard the transport of radionuclides in the saturated zone and thus reduce peak doses has received increased emphasis.

The U.S. Department of Energy (DOE) Waste Containment and Isolation Strategy (WCIS)<sup>1</sup> for YM defines seepage and saturated zone dilution as two of the three key attributes of the natural barrier system; radionuclide transport is the third key attribute. The WCIS (Department of Energy, 1996) states that “[p]erformance assessments have shown that seepage into the emplacement drifts is the most important determinant of the ability of the site to contain and isolate waste.” Moreover, the DOE has developed a set of five specific hypotheses, which must be addressed in order to support the DOE assertion that seepage into the drifts will be low: (i) flux that percolates through the repository horizon is substantially less than net infiltration, (ii) rapid fracture flow occurs only within a limited volume of the repository block at any specific time, (iii) capillary effects will reduce seepage into the emplacement drifts to be a small percentage of deep percolation, (iv) effects of heat generated from the waste on the hydrogeologic regime can be bounded, and (v) the effect of climate change on seepage can be bounded. The DOE strategy for saturated zone dilution is to demonstrate that the flow of water that may contact the waste packages and transport dissolved waste to the water table is much smaller than the flow below

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<sup>1</sup>U.S. Department of Energy. 1996. *Highlights of the U.S. Department of Energy's Updated Waste Containment and Isolation Strategy for the Yucca Mountain Site*. DOE Concurrence Draft. July 1996. Washington, DC: U.S. Department of Energy.

the water table. Moreover, the DOE strategy recognizes that further dilution may occur when water from a radionuclide plume is mixed with uncontaminated water in a producing water well. To address issues related to dilution strategy, the DOE proposed the following two hypotheses: (i) flow through the saturated zone beneath YM is much greater than the flow that may come in contact with waste packages and (ii) water that percolates through the repository horizon mixes with flow in the underlying welded tuff aquifer.

Specific technical subissues determined to be important to the resolution of this KTI have been identified. These technical subissues were framed as questions: (i) what is the key information needed to describe the hydrogeologic framework of YM, (ii) what is the amount and extent of present day shallow infiltration at YM, (iii) what are the hydraulic conditions in the unsaturated zone above the repository, (iv) what are the ambient flow conditions through the repository horizon to the water table, (v) what are the ambient flow conditions in the saturated zone, and (vi) which conceptual models provide conservative assessments of groundwater flow? By addressing each of these subissues in detail, it is hoped that technical bases can be developed that will assist in the timely review of the Site Suitability Report as well as the License Application. Moreover, by addressing these subissues the NRC hopes to resolve technical issues such as shallow infiltration and future climate prior to the issuance of the Site Suitability Report. Moreover, resolution of subissues (ii), (iii), and (iv) will directly address the reasonableness of the WCIS low seepage hypotheses, while resolution of (v) will address the reasonableness of the WCIS saturated zone dilution hypotheses.

## **10.2 OBJECTIVES AND SCOPE OF WORK**

The primary objective of the Key Technical Issue (KTI) on Unsaturated and Saturated Flow under Isothermal Conditions (USFIC) is to assess all aspects of the ambient hydrogeologic regime of YM that have the potential to compromise the performance of the proposed repository. The secondary objective of this KTI is to develop technical procedures and to conduct technical investigations for assessing the adequacy of the DOE strategy for characterizing key site- and regional-scale hydrogeologic processes and features that may adversely affect the performance of the repository. These processes and features include (i) those likely to decrease radionuclide transport time from the repository to the accessible environment, (ii) those that affect corrosion of waste packages and dissolution of waste form, and (iii) those affecting saturated zone dilution of radionuclides. During FY96 it was determined that effort would primarily be focused on those processes and features that affect shallow infiltration and deep percolation.

For each subissue described previously, a number of specific technical criteria have been defined that describe in more detail the scope of each subissue. Because efforts during FY96 were focused primarily on shallow infiltration and deep percolation, only the specific technical criteria for subissues (ii) and (iii) will be defined. Specific technical criteria, which must be addressed to resolve subissue (ii) include determination of the average annual infiltration rate, the spatial distribution of infiltration, the maximum instantaneous infiltration rate, and the expected increase in infiltration during a pluvial period. Specific technical criteria for subissue (iii) include determining the potential for existing perched water bodies to flood portions of the repository, the likelihood that additional perched water bodies will form under a pluvial climate, whether perched water bodies are indicators of fast flow paths that extend to the surface, whether the Paintbrush nonwelded tuff (PTn) is laterally contiguous within a fault block and thus acts as a barrier to vertical flow, estimates of fast flow rates where the PTn is breached by faults or fracture zones, and whether radioactive tracers found at depth (e.g.  $^{36}\text{Cl}$ ) are indicators of fast pathways.

## **10.3 SIGNIFICANT TECHNICAL ACCOMPLISHMENTS**

During FY96 significant progress was made in refining estimates of shallow infiltration and deep percolation, and improving understanding of mechanisms that lead to the development of perched water bodies and what the presence of perched water bodies at YM indicates about present and past hydrogeologic and climatic conditions. Three papers were prepared on these subjects and submitted to scientific journals for publication. In addition, significant progress has been made on development of a technical review procedure for assessing whether the DOE has adequately addressed the likelihood that existing or future perched water bodies may saturate the underground facility. Other efforts focused on resolving differences with the DOE on estimates of shallow infiltration and determining appropriate methods for bounding the effects of climatic changes on future hydrogeologic conditions.

### **10.3.1 Progress Toward Resolving Technical Issues at Yucca Mountain**

Assessments of the performance of the proposed repository are unanimous in finding that moisture conditions in the drifts and moisture flux rates in the unsaturated zone below the repository critically impact performance of the repository (Nuclear Regulatory Commission, 1992, 1995b; Sandia National Laboratories, 1992; Wilson et al., 1994; TRW Environmental Safety System, Inc., 1995). Significant progress was made on determining appropriate methods for bounding the effects of climatic changes on future hydrogeologic conditions and resolving differences with the DOE on estimates of shallow infiltration. Both issues are concerned with linking current and possible future climatic conditions to current and possible future hydrologic conditions occurring at and below the proposed repository level.

#### **10.3.1.1 Climate Change, Future Precipitation, and Water Table Rise**

Current regulations of the U.S. Nuclear Regulatory Commission (NRC) require that any performance assessment supporting the license application for a HLW repository must consider potential changes in hydrologic conditions caused by reasonably foreseeable climatic conditions (Nuclear Regulatory Commission, 1995a). The requirement is important because climate will almost certainly change significantly during the many tens of thousands of years that disposed nuclear wastes will remain hazardous. More importantly, climate controls the range of precipitation, which in turn controls the rates of infiltration, deep percolation, and groundwater flux through a geologic repository located in an unsaturated environment. Changes in groundwater recharge will induce other changes such as fluctuations in elevation of the water table. Water table rise would reduce the thickness of the unsaturated zone barrier. Therefore, future changes in climate could significantly influence waste isolation in a repository at YM.

The importance of groundwater flux as the key parameter for waste isolation in an unsaturated zone is well known, and has been further emphasized by the DOE's most recent report (TRW Environmental Safety System, Inc., 1995) on total system performance assessment (TSPA). On page ES-30 of that report it is stated that "... in the overall TSPA analyses, an over-arching theme comes back again and again as being the driving factor impacting the predicted results. Simply stated, it is the amount of water present in the natural and engineered systems and the magnitude of aqueous flux through these systems that controls the overall predicted performance... Therefore, information on... [this issue]... remains the key need to enhance the representativeness of future iterations of TSPA." The DOE WCIS

(U.S. Department of Energy, 1996, p 5)<sup>2</sup> likewise states that “[p]erformance assessments have shown that seepage into the emplacement drifts is the most important determinant of the ability of the site to contain and isolate waste.” The importance of infiltration as a hydrologic parameter was recognized by the NRC staff in Iterative Performance Assessment Phase 2. The NRC (1995b, p 10-4) states that “[a]lthough the flux of liquid water through the repository depends on the parameters infiltration, hydraulic conductivity, and porosity, performance correlates most strongly to infiltration.”

The present environment of the HLW program is one of legislative and regulatory changes. The U.S. Environmental Protection Agency (EPA) is promulgating a new HLW standard. EPA current standard, 40 CFR Part 191, specifies a repository compliance period of 10,000 yr. A new standard may stipulate a similar period or a much longer time period on the order of hundreds of thousands of years. Under an extended compliance period climate change would be expected to play an even greater role in performance assessments. Even if the compliance period remains at 10,000 yr, the DOE may be required to provide longer-term estimates of peak doses dependent on likely climate scenarios to help support the NRC regulatory decisions.

As part of a pilot project in issue resolution, the NRC staff is preparing an issue resolution report that addresses three subissues under the KTI of Isothermal Hydrology. These subissues are future climate change and the related topics of future precipitation and water table rise. There appears to be a clear path to reach a scientific consensus on methods for evaluating past climates and estimating future climatic changes. It is suggested in the report that paleoclimatic and paleohydrologic data provide an excellent foundation to estimate the range of future climate states at YM. The NRC staff report emphasizes paleoclimatic methods to develop a reference scenario for future climate rather than placing reliance on extensive use of climate modeling. This approach is not expected to be significantly affected by any changes to EPA or the NRC HLW regulations that may result from the National Research Council (1995) recent review or by changes in the licensing of HLW repositories being considered in the Congress.

The NRC staff reviewed all available information, not just that provided by the DOE in previous submittals. Based on this prelicensing review, the issue resolution report suggests that sufficient paleoclimatic information exists in various forms to make the following observations:

- Methods based on paleoclimatic data can be used to adequately estimate the range of past climates in the YM region. In particular, the temperature proxy data from Devil’s Hole provide one of the longest and best paleoclimatic records covering a continuous 500,000-yr period (Winograd et al., 1992).
- Variability of future climate over hundreds of thousands of years could be presumed to follow general patterns of the last 500,000 yr as inferred from paleoclimatic data. Glacial/interglacial cycles have typically lasted about 100,000 yr and interglacials have lasted about 20,000 yr (Winograd et al., 1992).
- Recent studies have shown that the water table in the YM region may at times have risen as much as 115 m during the Wisconsin glacial stage. The data also suggest that the water table

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<sup>2</sup>U.S. Department of Energy. 1996. *Highlights of the U.S. Department of Energy’s Updated Waste Containment and Isolation Strategy for the Yucca Mountain Site*. DOE Concurrence Draft. July 1996. Washington, DC: U.S. Department of Energy.

may never have been higher than that in the last 10+ million years, providing confidence that waste packages in a proposed repository at YM would never be inundated by the regional water table.

- Based on recent studies, mean annual precipitation at YM during past pluvial climates may have been two to three times greater than today. This range of precipitation can be used to estimate what might be expected during future pluvial climates and can help establish an upper bound to derive estimated ranges of future infiltration and deep percolation.

The NRC staff approach to issue resolution considers all available information, not just the information provided by the DOE in previous submittals. For this pilot topic the NRC staff is not responding to a specific topical report from the DOE, but instead performed an independent, precicensing review of the broad scientific literature related to future climate. In general, there is sufficient information available today to reach resolution on the range of future climate variability and methods to determine upper thresholds for future precipitation and water table rise. When complete, the NRC staff issue resolution status report will be transmitted to the DOE, oversight committees, the State of Nevada, and other interested parties for review and comment.

#### 10.3.1.2 Infiltration

To estimate deep percolation fluxes using numerical simulation, an estimate of net infiltration (percolation flux escaping the zone of evapotranspiration) is required over the surface of the subregional area. The DOE strategy evolved from potential infiltration maps based solely on matrix properties (Flint and Flint, 1994) as additional data [e.g., neutron-probe borehole measurements (Flint and Flint, 1995)] became available and as numerical simulators appropriate to the site have been developed.<sup>3</sup> The planned DOE strategy for estimating net infiltration over the performance period links climatic forcings to net infiltration using numerical simulators.<sup>1</sup> Current DOE efforts are tied to calibrating the numerical simulators to the neutron-probe data and estimating the spatial distribution of net infiltration.<sup>1</sup>

Independent attempts to use numerical simulators to predict the behavior and distribution of net infiltration are being conducted at the Center for Nuclear Waste Regulatory Analyses (CNWRA) (section 10.3.3). Based on experience gained from comparing modeling exercises to field measurements, it can be concluded that

- Numerical simulations can provide plausible estimates of the relative spatial and temporal distributions of net infiltration,
- Numerical simulations can provide reasonable estimates of hydraulic controls on infiltration,
- Numerical simulations can provide insights into how infiltration might change over time due to climatic changes, and

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<sup>3</sup>Flint, A.L. 1996. Open-meeting presentation to the Nuclear Waste Technical Review Board on July 9–10, 1996 in Denver, CO.

- Numerical simulations only bound estimates of net infiltration to within ranges of perhaps 10 to 20 percent of precipitation.

Spatial distribution patterns for net infiltration predicted by the CNWRA are quite similar in character to patterns reported by Flint<sup>1</sup> (e.g., infiltration increases with increasing elevation and decreasing surface cover). The modeling approaches are similar, insofar as 1D simulations are used on a pixel-by-pixel basis, but the processes involved with shallow infiltration are handled using somewhat different assumptions (e.g., bare-soil evaporation by the CNWRA versus evapotranspiration by the DOE). In addition, the estimated area-average net infiltration values are within a factor of 2 to 4, comparable in magnitude to the variation that the CNWRA model predicts over reasonable ranges of parameter values. Inasmuch as numerical modeling can only bound shallow infiltration estimates, it is appropriate to further constrain infiltration estimates using other sources of data. Various lines of evidence, including (i) aged fracture fillings, (ii) comparing  $^{36}\text{Cl}$  measurements in the Exploratory Studies Facility (ESF) with transport simulations, and (iii) inverse modeling based on borehole measurements of moisture contents, tension, and temperature are cited<sup>4</sup> as suggesting that infiltration lies in the range of slightly under 1 mm/yr to perhaps greater than 10 mm/yr. As comparison, using the base-case CNWRA map, the average net infiltration is approximately 10 mm/yr, estimated over the length of the north ramp of the ESF through the turn to the main drift. As multiple lines of evidence are pointing to a range of values broadly within an order of magnitude for net infiltration, it can be concluded that considerable progress has been made on resolving the issue of estimating shallow infiltration.

### **10.3.2 Perched Water Bodies at the Yucca Mountain Site and Inferences for Recharge Rates**

Specific technical subissues addressed in this section are the hydraulic conditions in the unsaturated zone above the repository, and the ambient flow conditions through the repository horizon to the water table. Resolution of both technical subissues involve evaluating the potential for formation of perched water bodies at YM. Perched water is defined as an unconfined saturated zone separated from an underlying saturated zone (water table) by an unsaturated zone and is deemed significant with respect to infiltration and groundwater flux (U.S. Geological Survey, 1981). Relative to the proposed repository, perched water bodies could occur above, within, and below the repository horizon. Of these three zones, perched water within the repository itself would be of most concern because it is believed that waste canisters will last longer in unsaturated rock than under saturated conditions. The formation of perched water bodies around waste canisters would likely increase the rate of waste canister failure resulting in greater releases of radionuclides. The potential for formation of perched water bodies is identified in federal regulations, for example, 10 CFR 60.122(c)(23), as a potentially adverse condition for the storage of HLW in a geologic repository. Perched water is common in arid environments. For example, perched water flows from seeps into the U12n tunnel through the zeolitized Indian Trail Tuff at Rainier Mesa, 50 km northwest of YM (Thordarson, 1965; Russell et al., 1987; Wang et al., 1993). Perched water bodies tend to be transient features that are formed where there is a contrast in hydrologic properties (Freeze and Cherry, 1979). Contrasts may result from differences between stratigraphic units. Contrasts may also occur by juxtaposition of low conductivity strata with more conductive strata along a structural feature such as a fault or other persistent discontinuity. YM is crisscrossed by numerous faults, thus substantially increasing the probability of locally saturated conditions occurring.

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<sup>4</sup>Bodvarsson, G.S. Open-meeting presentation to the Advisory Committee on Nuclear Waste on September 26, 1996 in Las Vegas, NV.

Perched water bodies would be more likely to form or expand under future, wetter, climatic conditions that cause increased infiltration. It is possible that perched water bodies in the YM area are relict features formed by higher infiltration rates during former pluvial climates. If perched water bodies formed above the repository, this local saturation could induce localized fracture flow along vertical pathways downward into the repository. Past (and contemporary) occurrence of fracture flow that bypassed part of the unsaturated zone where matrix flow would normally predominate, thus transporting released contaminants at greater flow rates, has been recently inferred from  $^{36}\text{Cl}$  measurements at the ESF within the repository host rock at YM (Fabryka-Martin et al., 1996). Elevated levels of  $^{36}\text{Cl}$ , interpreted as being bomb-pulse in origin, was identified at a few distinct, highly fractured zones generally in the vicinity of faults, indicating that a small amount of water at these locations is less than 50 yr old and that it was, most probably, transported through extremely localized pathways.

### 10.3.2.1 Perched Water Body Occurrences at Yucca Mountain

A number of perched zones were found at several boreholes (USW UZ-1, UZ-14, NRG-7a, SD-7, and SD-9) at YM (Burger and Scofield, 1994; Yang et al., 1996). A vacuum-reverse-air-circulation drilling method was used for these boreholes to prevent contamination from drilling fluids and all perched water samples were collected using plastic or stainless steel bailers. As of June 1996, all perched water found occurs in the upper Calico Hills unit with the exception of UZ-14 and USW SD-9, where the perched water body is found on the basal vitrophyre in the Topopah Spring unit. Boreholes UZ-1 and UZ-14, which are on the same drilling pad, encountered a perched zone at a depth of 190 m above the water table. The zone was extensive enough to be pump tested at a rate of  $0.204 \text{ m}^3/\text{hr}$  for 67 hrs, and a total of  $22.71 \text{ m}^3$  produced. It has been estimated, however, that this perched water zone is much more extensive than originally thought, with an approximate volume of  $114,000 \text{ m}^3$  (Yang et al., 1996). In USW SD-9, perched water appeared to be just above the basal vitrophyre of the Topopah Spring unit, 120 m above the water table. Boreholes that encountered perched water within the Calico Hills Tuffs include USW SD-7 and USW NRG 7/7a. The perched zone encountered by SD-7 was extensive enough to be pump tested at a rate of  $0.75 \text{ m}^3/\text{hr}$  for 30 hrs and a total of  $45.42 \text{ m}^3$  produced. This perched water zone is a relatively small body and its total volume estimated at approximately  $300$  to  $500 \text{ m}^3$ . It is quite possible that other perched zones may be discovered at YM during further site characterization.

Within 6 to 8 m sampling intervals in the five boreholes, large  $^{14}\text{C}$  variations are detected ranging from 27.2 to 66.9 percent modern carbon (PMC) with an average of about 37 PMC, indicating a multitude of water sources that contribute to these perched water reservoirs. The apparent (uncorrected)  $^{14}\text{C}$  ages of perched water range from 3,500 to 10,800 yr. If age corrections are made to account for caliche dissolution, perched water residence times of less than 7,000 yr are estimated. The uncertainty in  $^{14}\text{C}$  measurements is  $\pm 0.7$  PMC (Yang et al., 1996).

### 10.3.2.2 Perched Water Body Modeling

This work addresses a specific mechanism that is known to promote development of perched water, the entrapment of water due to faults or fault zones. Faults can affect groundwater by enhancing flow rates, inhibiting flow, or acting in a neutral manner. In this work faults are considered to be neutral due to the lack of data supporting other hypotheses and thus only the effects of the relative positions of the layers of different and perhaps sharply contrasted hydrologic properties would affect the flow. Thus, the first question that needs to be answered is whether a perched water body can form and be sustained under the contrast conditions present at YM.

The effect of differing hydrologic properties of the stratigraphic layers may cause water that is percolating down to be channeled downdip when it encounters a relatively impermeable layer. Faults in YM are common and this faulting has produced offset of the stratigraphic units. If the offset of the fault is such that a relatively permeable unit within the downthrown fault-block is juxtaposed against a relatively impermeable unit downdip of the fault, then the channeled water will be inhibited from continuing downdip and eventually will become trapped at this location. The source of this water may be a combination of both infiltration of precipitation and relict water that accumulated during a cooler, wetter climatic period in the past. Spaulding (1985) conducted research with plant microfossils and dated remains found in packrat middens in the vicinity of the Nevada Test Site (NTS). Based on this work, Spaulding (1985) reported that the climatic conditions at the NTS about 45,000 yr before present (YBP) were similar to the present day conditions in northern Nevada. Even though it is fair to speculate that most of this recharge occurred in the areas of higher elevation north of YM, it is hypothesized that water was also able to find its way down in the area of the proposed repository, at higher rates than present. Moreover, evidence exists suggesting that the water table was approximately 115 m higher in the YM region than it is today (Quade et al., 1995).

Czarnecki (1985), following a numerical modeling approach, investigated the effects a wetter future climate would have on the water table and concluded that a 100 percent increase in precipitation could cause the water table at YM to rise by as much as 130 m. Such a rise in the water table would not be adequate to inundate the repository, but saturation levels above the higher water table would see an increase from present day values.

Some interesting questions pertaining to the YM system are (i) whether the flow system at YM could yield relict perched water bodies starting from a much wetter initial condition in the distant past, (ii) whether these perched water bodies could be sustained at present day levels (i.e., estimated reservoir volumes) under present day recharge conditions, and (iii) whether such sustained perched water bodies agree with  $^{14}\text{C}$  residence times inferred from measurements at YM boreholes.

The first step toward enhancing modeling efforts is to construct a three-dimensional (3D) Geologic Framework Model (GFM) that embodies the current understanding of YM. Efforts at the CNWRA have developed a computerized GFM that includes lithostratigraphy, hydrostratigraphy, and geologic structure (Stirewalt et al., 1994; Stirewalt and Henderson, 1995) of the YM region. Lithostratigraphy and geologic structure are based on surface geologic maps of the site (Scott and Bonk, 1984). Subsurface geology is constrained by both borehole control and through the construction of balanced cross sections. Hydrologic properties include porosity, saturated hydraulic conductivity, and water content. For the hydrostratigraphic model, mean values for hydrologic properties are assigned as constant values for each of seven different lithostratigraphic units. Original data are from the DOE site characterization activities (e.g., Craig and Reed, 1991; Flint and Flint, 1990; Loscot and Hammermeister, 1992; Whitfield et al., 1993).

The area considered for current work is the vicinity of the intersection of the Ghost Dance and Sundance faults in the repository area of the YM site. The modeled area is 1,100 m wide by 650 m deep and is extracted electronically from the CNWRA GFM. The plane of view is the Sundance fault facing northward. The area of interest is above the water table and primarily updip of the Ghost Dance fault. The right border of this model represents an artificial no-flow boundary that causes water to accumulate, whereas in reality the water would continue flowing downdip past this boundary. Given the abundance of normal faults in the YM area, this condition may be a representative depiction since it corresponds to a periodic boundary condition (a fault every so many length units). Any perching to the right of the fault

is eliminated from subsequent calculations. The beds included in this analysis are (from top to bottom): (i) Tiva Canyon welded (TCw); (ii) PTn; (iii) Topopah Spring welded 1,2,3 (TSw); (iv) Calico Hills nonwelded (CHn); and (v) Prow Pass welded (PPw).

Initially, a uniform suction head value of 10 m (approximately equal to the bubbling pressure for most YM units) was assigned to the entire modeled region, which was then allowed to drain under gravity with no flux added in the system. Solution of the flow equation in a transient mode produced pressure head, which were transformed to saturation values. The volume of moisture within zones that exceeded an *a priori* selected percent saturation value (typically 99.95 percent) was then calculated, thus providing perched water volume as a function of time,  $V(t)$ . In this work, all flow simulations have been conducted with the BIGFLOW numerical code (Ababou and Bagtzoglou, 1993) that solves the local mass conservation equation in a slightly compressible and variably saturated porous medium without source/sink terms. The BIGFLOW code is based on a low order, seven point centered finite difference scheme in space and a fully implicit one step (Euler backwards) finite difference scheme in time. The spatial mesh used in this work is rectangular with a  $\Delta x=20$  m and  $\Delta z=10$  m and an automatic time stepping algorithm is invoked. The left and right boundaries are no-flow, the top boundary is constant flux, and the bottom boundary is a water table condition.

Once the  $V(t)$  relationship has been obtained for the base-case state of the flow system (i.e., no flux added) the point of maximum perched water volume was used as an initial condition for a simulation with a uniformly distributed, prescribed flux added at the top of the domain. Depending on the value of this flux, any of the following situations is possible for the perched water volume: (i) it could eventually go to zero (system drained), (ii) it could eventually increase without bound (system flooded), and (iii) it could be sustained at a steady-state level. Figure 10-1 depicts two cases in schematic form: complete drainage and attainment of a steady-state volume consistent with the observed present day volume. Once such a match between predicted and observed volumes is attained, through repeated flow simulations with different input fluxes, the obtained flux is considered optimal and recorded. As indicated in figure 10-1, there exists two hydrological constraints that need to be satisfied. These are (i)  $dV/dt(t=T_{tot})=0$ , and (ii)  $V(t=T_{tot})=V_{pres}$ , where  $V_{pres}$  is the observed (present day) volume of the perched water reservoir. Finally, there exists the additional constraint that the steady-state condition has been attained within a time period less than 18,000 to 20,000 yr, the current climate period. Thus,  $T_{tot} \leq 20,000$  yr is the third hydrological constraint that must be satisfied.

A means of refining computer models of flow at YM is to use available water and mineral chemistry to identify where perched water might have occurred in the geologic past. Hydrochemical facies and environmental tracers such as stable isotopes have long been used to distinguish water bodies and identify potential flow paths (National Academy of Sciences, 1992). Radiometric age dates can be determined for both mineral deposits and groundwater and used to estimate rates of fluid flow and timing of changes in paleohydrological conditions. Chemical data are being gathered at YM as part of the DOE site characterization efforts. These include groundwater chemistry of the unsaturated zone (Yang et al., 1988, 1996; Yang, 1992) and chemical and isotopic analyses of minerals deposited from past and present groundwater (e.g., Bish and Chipera, 1989; Whelan and Stuckless, 1992). Trends in these data have been used to interpret paleohydrology, fluctuations in the static water table (National Academy of Sciences, 1992), and climatic variations (Tyler et al., 1995).

An obvious second step in the work, presented herein, is to investigate whether  $^{14}\text{C}$  data from the YM site could corroborate or refute hydrologically conditioned simulation results. Consider the mass balance of  $^{14}\text{C}$  within a well-mixed reservoir (Pearson and Truesdell, 1978) expressed in PMC

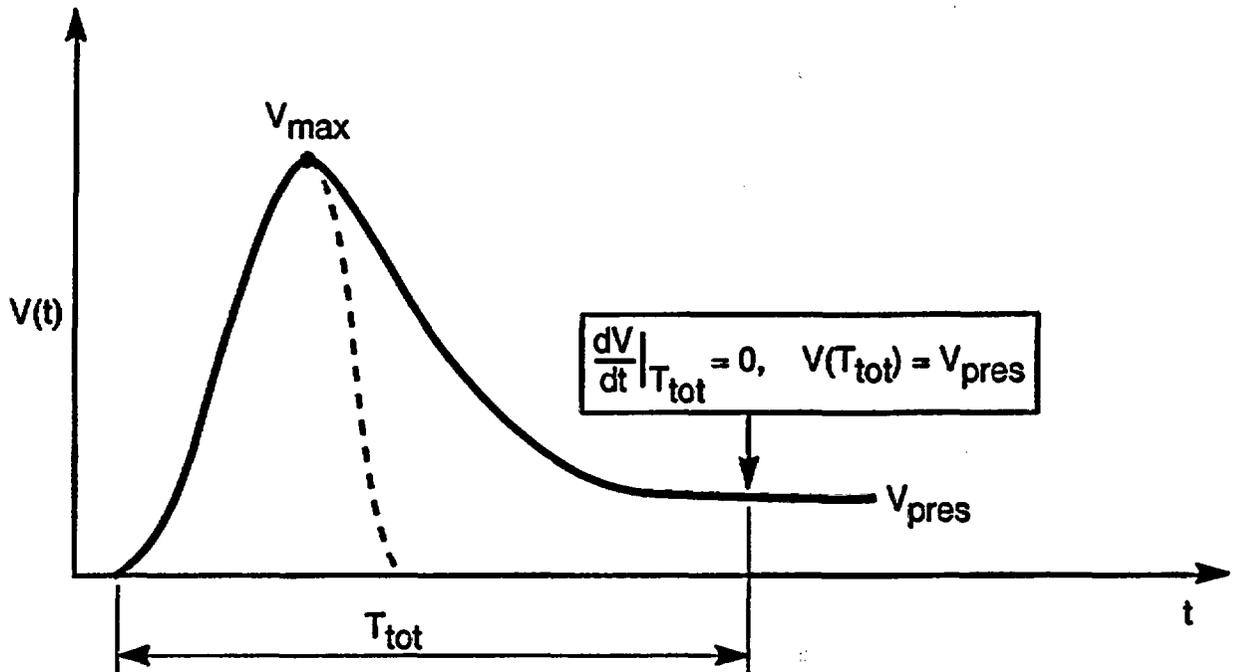


Figure 10-1. Schematic of perched water volume as a function of time for complete drainage and steady-state attainment simulations

$$\frac{d(CV)}{dt} = A q_i C_i - A q C - \lambda CV \quad (10-1)$$

where  $C_i$  and  $C$  are the PMC of young (present day) and mixed-age water;  $\lambda=1.2097 \times 10^{-4} \text{ yr}^{-1}$  is the radioactive decay constant for  $^{14}\text{C}$ ;  $A$  and  $V$  are the horizontal cross sectional area and volume of the perched water body, respectively; and  $q_i$  and  $q$  are the inflow and outflow rates, respectively. The well-mixed model assumes that all sources of water input to the reservoir are completely mixed with the water already in the reservoir. Solution of this equation is obtained by setting

$A_1 = V_o$ ;  $B_1 = A(q_i - q) = \frac{\Delta V}{\Delta t}$ ;  $A_2 = A q_i + \lambda V_o = \frac{\Delta V}{\Delta t} + A q + \lambda V_o$ , and  $B_2 = \lambda \frac{\Delta V}{\Delta t}$  resulting in:

$$\frac{dC}{dt} = -\frac{A_2 + B_2 t}{A_1 + B_1 t} C + \frac{A C_i q_i}{A_1 + B_1 t} \quad (10-2)$$

This is an ordinary differential equation that, unfortunately, has no closed form solution. In the process of arriving at this equation for  $^{14}\text{C}$ , the following assumptions were made: (i) influx ( $q_i$ ) is not changing with time; (ii) optimal flux estimates represent the areal average of a matrix-fracture continuum; (iii) no daughter product contribution ( $C_{\text{tot}} = {}^{12}\text{C} + {}^{13}\text{C} + {}^{14}\text{C}$ ); (iv) transport system is lumped, exhibiting no spatial characteristics; and (v) no  $^{14}\text{C}$  is partitioned in liquid and gas phases. Integration of (Eq. 10-2) was performed numerically using a fourth and fifth order Runge-Kutta-Fehlberg algorithm with a self-adapting

time step. The geochemical constraint that must be satisfied is that after a period of time equal to  $T_{tot}$ , the  $^{14}\text{C}$  in the perched water body cannot be substantially different than a target value  $\text{PMC}_{\text{pres}}$  observed at YM boreholes.

To determine the likelihood of the repository site developing localized perched water zones, the potential for trapping and the areal extent of that perched water zone must be exhaustively evaluated. To do this, the hydraulic conductivity must be determined for all the rock units involved at all possible saturation levels. The hydrologic effects of the difference in hydraulic conductivities of various units must also be evaluated to determine the trapping potential of all the rock units at all saturation levels. Ideally, to make the best final probability estimate for the perching potential, an infinite number of combinations of hydraulic conductivity to saturation level and different saturation levels of different beds should be considered. For each of these combinations the areal extent of the region likely to become perched should be calculated. This task, however, would involve a vast number of calculations. The data used in this study were adopted from the 1993 Total System Performance Assessment (TSPA-93) for YM (Wilson et al., 1994). TSPA-93 uses 10 hydrogeologic units. Because the current CNWRA model of the YM site uses slightly different stratum classifications, some modifications were necessary. Some units are directly equivalent and others were combined by a weighted average based on their relative thicknesses. From the TSPA-93 data (mean, minimum, maximum, and coefficient of variation), a random sampling of possible values from a beta distribution curve were produced using the Latin Hypercube Sampling (LHS) approach (Iman and Shortencarier, 1984) to obtain sufficiently accurate results without using all possible combinations. However, results from only one realization are presented here for the sake of brevity.

### 10.3.2.3 Results and Discussion

The first realization used the mean values from the TSPA-93. As the system began to drain, with no flux added and an initial uniform head value of  $-10$  m, water began to drain from some areas and to accumulate in others. The PTn unit, having a high matrix permeability, allowed water to flow freely down through it. When it encountered the low matrix permeability TSw unit its downward flow was inhibited. This caused the water to be channelled down dip in the PTn until it reached the Ghost Dance fault. The footwall of the fault has been uplifted such that the PTn in the hanging wall is juxtaposed against the relatively impermeable TSw unit in the footwall of the fault. This produces a trap where water that is channelled down dip through the PTn encounters the relatively impermeable TSw at the fault and begins to accumulate, producing a perched water body. As it continues to accumulate, it percolates slowly down through the TSw unit, thus extending the perched water body well in the TSw unit. The perched body continues to grow as long as there is enough water above it to supply water faster than can be dissipated. It reaches a maximum perched volume of  $15,949 \text{ m}^3$  at 455 yr after which the perched water begins to dissipate until it is completely drained by about 1,600 yr.

Starting from the point in time with maximum perched water volume, a flux was added at the surface to approximate a mean infiltration rate. This was allowed to continue until the system reached an equilibrium condition, specifically until the perched water body disappeared or remained at a constant volume. Different flux rates were added until one was found that produced and sustained a perched water body of roughly the same volume of water as actual perched water bodies found in the area (e.g., SD-7), approximately  $400$  to  $500 \text{ m}^3$ . In this case, a constant flux of  $6.2 \text{ mm/yr}$  applied uniformly to the top of the system produced a sustained perched water volume of  $528 \text{ m}^3$  right below the PTn/TSw interface. Figure 10-2 depicts the temporal evolution of the perched water volume for the draining simulation and the simulations with a recharge of  $6.2$  and  $8.0 \text{ mm/yr}$ . Note how the  $8.0 \text{ mm/yr}$  simulation diverges and floods the system, whereas the  $6.2 \text{ mm/yr}$  simulation reaches asymptotically the desired volume. This is

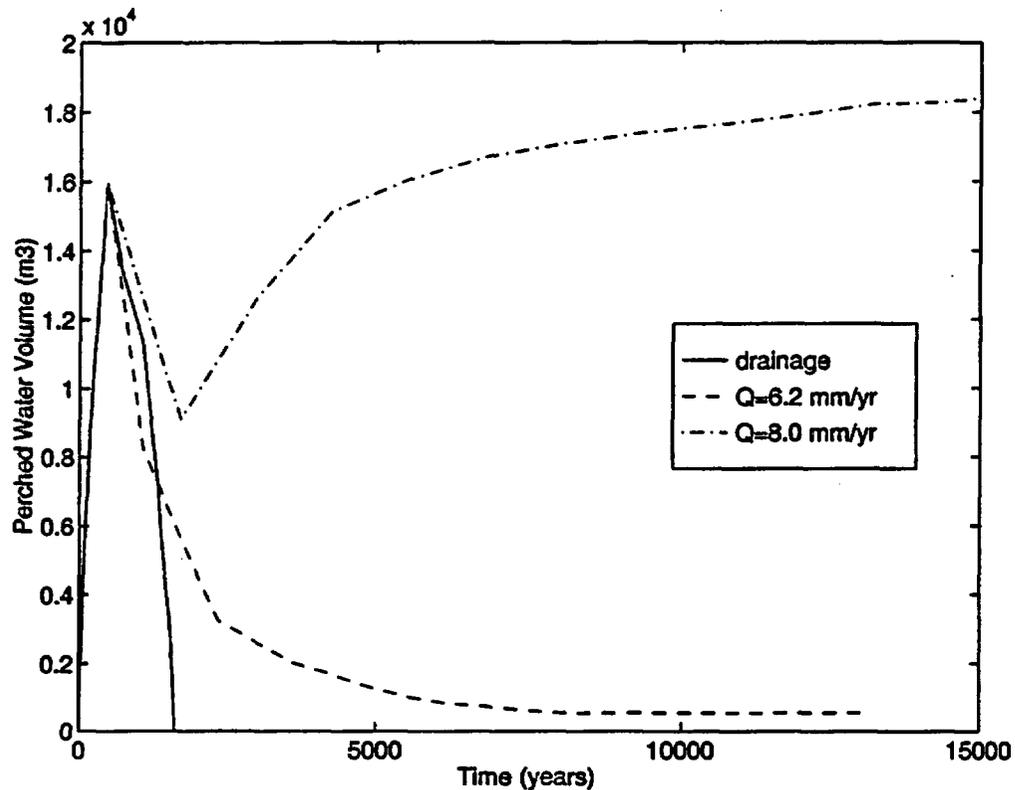


Figure 10-2. Temporal evolution of perched water volume for draining and for  $q=6.2$  and  $8.0$  mm/yr simulations. Mean TSPA-93 hydrologic properties are used.

an indication that the perched water body exhibits a meta-stable behavior near the optimal value of  $6.2$  mm/yr. Any recharge higher than this optimal value exceeds its storage capacity and eventually floods the system. It is worth mentioning that even though this particular realization predicted perched water forming at a depth quite different from that observed at YM, other realizations predicted perched water forming at the base of the TSw unit.

Equation (10-2) was solved numerically with input the  $V(t)$  behavior as inferred from the detailed flow simulations. Since the actual areal extent  $A$  of the perched water body is unknown, a set of simulations have been conducted by varying this parameter. Figure 10-3 depicts the  $^{14}\text{C}$  depletion as a function of time for each material property realization and also for a set of three values for the areal extent parameter. Shown in figure 10-3 also is the reference simulation that corresponds to pure radioactive decay and the target value of  $\text{PMC}_{\text{pres}}=0.28$ . Several observations can be made from this figure. First, the  $q=6.2$  mm/yr simulation, using mean TSPA-93 values, could reach the target  $\text{PMC}_{\text{pres}}$  after a residence time between  $10,000$  and  $20,000$  yr for realistic areal extent values. This timeframe is consistent with the time required for the volume to reach a  $dV/dt=0$  and also with the change of the climate around  $18,000$  to  $20,000$  YBP. Therefore, this realization could be classified as plausible on the basis of the hydrological and geochemical constraints described earlier.

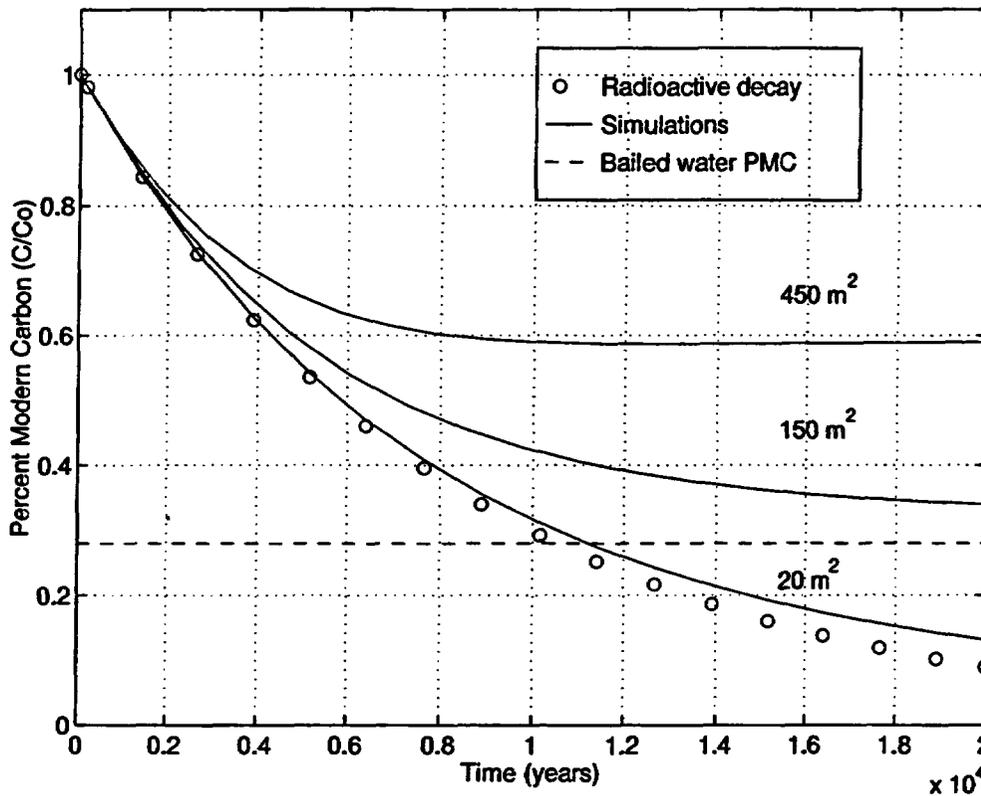


Figure 10-3. Depletion of perched water <sup>14</sup>C as a function of time for  $q=6.2$  mm/yr and three areal extent values. Mean TSPA-93 hydrologic properties are used.

#### 10.3.2.4 Conclusions

It must be stressed that the method presented in this section does not account for the hydraulic properties of fractures, which should be considered when modeling YM. Therefore, conclusions are only valid for the simplified system used to test the approach and may not be valid for YM. There are three major conclusions of this study: (i) a sustainable perched water body can be attained in the simplified system with an average deep recharge rate of 6.2 mm/yr; (ii) an approach that assists in the determination of plausible recharge rates, based on hydrological and geochemical constraints, was proposed and applied to an idealized YM site; and (iii) it appears that for the realization that satisfies both hydrological and geochemical constraints, a present day perched water body that consists of a combination of some minimal relict (past pluvial) water and young water from infiltration is an appropriate hypothesis.

### 10.3.3 Estimates of Infiltration at Yucca Mountain

The study presented in this section is part of an ongoing effort to examine the spatial distribution of shallow infiltration at YM using numerical simulations. A motivation for the study is to provide insight into the spatial distribution of boundary conditions appropriate for simulations of deep subsurface moisture redistribution and examine how these might be affected by hydraulic properties and climatic variation. The first efforts toward the study occurred under the Iterative Performance Assessment Project and a large part

of the work occurred under the Subregional Hydrogeologic Flow and Transport Processes Research Project.

The study abstracts detailed one-dimensional (1D) simulations into a response surface for average annual infiltration (AAI) as a function of hydraulic properties, average annual meteorologic inputs, and depth of surficial cover. Each input parameter to the response surface function is estimated for each pixel of a Digital Elevation Model (DEM) of the study area. Assuming that the response surface is appropriate over the scale of a DEM pixel, the set of input parameters at each pixel is used to predict AAI for the pixel. Using the average of AAI over the study area as a measure, the relative importance of each input parameter is assessed by examining the sensitivity of the measure to the input.

The basic methodology for the study was presented in the CNWRA semi-annual research reports (e.g., Stothoff et al., 1995; Stothoff and Bagtzoglou, 1996).<sup>5</sup> The primary efforts in FY96 have been to extend the breadth of cases considered, refine models, analyze the information already obtained, and document the work in refereed journal articles (Stothoff, 1996)<sup>6</sup>. In particular, efforts were made to (i) simulate the response of AAI to a more exhaustive set of input parameters, (ii) abstract the relationships between simulated AAI and input parameters, (iii) refine the predictive model for colluvial/alluvial depths, and (iv) examine the sensitivity of areal-average AAI to various input parameters.

#### 10.3.3.1 One-Dimensional Simulator Description

The BREATH simulator used for the 1D simulations considers the coupled flow of moisture and energy in a porous medium and is described in detail by Stothoff (1995). All simulations presented herein use similar boundary conditions. At the bottom of the column, the gradients of saturation and temperature are assumed to be zero, allowing gravity drainage of water and advective losses of energy. At the top boundary of the column, the simulator is presented with 10 yr of meteorological input, based on hourly readings from the Desert Rock, Nevada, National Weather Service meteorologic station located approximately 30 miles east of YM (National Climatic Data Center, 1994); procedures for converting the National Weather Service readings into BREATH meteorological inputs are discussed by Stothoff et al. (1995). The meteorological record runs from March 1, 1983 through February 28, 1993. The decade of weather is repeated until the initial conditions are eliminated; all reported results are for the last simulated decade. One decade may be too short a time period to capture the full range of precipitation events in a statistically robust way, however, considerable insight can be gained on the behavior that might be expected from the columns over longer periods of time.

#### 10.3.3.2 Deep-Alluvium Response Function Abstractions

A large number of 1D simulations were performed to systematically examine the impact of representative deep-alluvium hydraulic properties (Stothoff, 1996)<sup>7</sup> and representative meteorological input values<sup>3</sup> on AAI. To make direct comparisons between simulations, surface boundary conditions were

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<sup>5</sup>Stothoff, S.A., H.M. Castellaw, and A.C. Bagtzoglou. 1996. Simulating the spatial distribution of infiltration at Yucca Mountain, NV. *Water Resources Research*. In preparation.

<sup>6</sup>Stothoff, S.A. 1996. Sensitivity of long-term bare-soil infiltration simulations to hydraulic properties in an arid environment. *Water Resources Research*. Submitted for publication.

<sup>7</sup>*Ibid.*

based on the same 10 yr meteorological sequence. To investigate the impact of meteorological input values, one input value (e.g., precipitation, air temperature, etc.) was changed systematically for the entire sequence either by multiplying each hourly value by a constant or adding a constant to each hourly value.

All deep-alluvium simulations with intrinsic permeability  $k$  less than about  $10^{-9}$  cm<sup>2</sup> [equivalent to silty sands (Freeze and Cherry, 1979)] yielded essentially zero AAI. For these simulations, evaporation from the ground surface was sufficient to reclaim any water not running off during precipitation. For simulations with  $k$  having a value of  $10^{-8}$  cm<sup>2</sup> or greater, a scaling parameter  $Y = \ln[(AAI/AAP)k^{1/2}]$ , where AAP is average annual precipitation, was found to be useful in describing the response of AAI to the hydraulic and meteorologic input properties. The scaling parameter accounts for the decrease in AAI with increasing intrinsic permeability observed in the simulations with maximum AAI occurring for  $k$  around  $10^{-8}$  cm<sup>2</sup>. The  $Y$  values obtained from the simulations can be expressed as a first order expansion about the  $Y$  value obtained for a base-case simulation. Over the range of parameters considered,  $Y$  appears to increase as the square of van Genuchten  $m$ , as the square root of air entry pressure, and as the inverse of porosity. As both  $m$  and air entry pressure increase as  $k$  increases for most porous media, AAI should also increase as  $k$  increases for most porous media when parameter correlations are considered.

Considerable additional work is required to verify the precise nature of the relationships between hydraulic properties, meteorologic inputs, and AAI in deep alluvium. It is expected, however, that vegetation may have a strong impact on AAI in deep alluvium, perhaps masking such relationships. To investigate the impacts of vegetation on AAI, future simulations are being planned that will incorporate the effects of representative YM vegetation on infiltration processes.

### 10.3.3.3 Colluvium/Fracture Response Function Abstractions

To estimate spatial distribution of AAI using estimates of hydraulic input, meteorologic input, and colluvium depths, a functional relationship between these variables is extremely useful. A set of empirical relationships was derived for these variables. One relationship characterizes the decay of AAI with increasing colluvium depth and a second relationship uses corrections to the AAI/depth relationship to characterize the impact of AAP and average annual temperature (AAT) on AAI. The relationships incorporate the impact of hydraulic properties through scaling parameters. Ongoing studies are examining the impacts of other meteorologic input.

The development of the shallow-colluvium functional relationships is discussed in detail by Stothoff et al.<sup>8</sup> The functional relationships reduce to

$$\log_{10} \left[ \frac{AAI/AAP}{I_{D0}} \right] = -C_I \left( \frac{\epsilon b}{b_r} \right)^{\sqrt{1/2}} [1 + J_0(T, M)] \quad (10-3)$$

where  $\epsilon$  is colluvium porosity,  $b$  is colluvium depth;  $b_r$  is a scaling depth;  $I_{D0}$  and  $C_I$  are material dependent coefficients;  $T$  is the relative change in AAT [ $T = (AAT - AAT_0)/AAT_0$ ];  $M$  is the change in the base-10 log of the AAP multiplier [ $M = \log_{10}(AAP/AAP_0)$ ];  $AAT_0$  and  $AAP_0$  are base-case values of AAT and AAP; and  $J_0$  is a bicubic function of  $T$  and  $M$ . Arbitrarily choosing  $b_r$  to be 2 cm, regressed values for  $I_{D0}$  range from 0.641 through 1.21 and values for  $C_I$  range from 0.562 through 1.02.  $I_{D0}$  and  $C_I$  have a correlation coefficient of 0.93.

<sup>8</sup>Stothoff, S.A., H.M. Castellaw, and A.C. Bagztoglou. 1996. Simulating the spatial distribution of infiltration at Yucca Mountain, NV. *Water Resources Research*. In preparation.

Several points are significant about the scaling relationships:

- Porosity and colluvium depth act inversely (e.g., small depths and large porosity are similar to large depths and small porosity),
- The coefficients  $I_{D0}$  and  $C_f$  are highly correlated,
- Sensitivity to climate decreases with increasing AAI.

#### 10.3.3.4 Refined Surface-Cover Model

Since infiltration is sensitively dependent on the distribution of the surface cover above bedrock (i.e., alluvium and colluvium) and a detailed map of surface cover depth is not available and may be difficult to measure, an alternative approach for estimating cover depth is followed here. Stothoff et al. (1995) presented a simple mechanistic model combining creep and weathering using a DEM for the underlying elevation controls. Based on cursory field observations, the model performed relatively well on ridgetops and sideslopes but predicted erroneously large alluvium depths in the upland channels. Accordingly, the model was enhanced to take into account erosion and sediment transport by water movement as well as soil creep and passive degradation. As a first step, the model only accounts for one generic particle size rather than considering a distribution of particle sizes. The model does not explicitly calculate erosion by rain splash or long-range transport by gravity (i.e., boulders rolling downhill). It is assumed that spatial variability in alluvium depths arises solely from the variability in surface elevation; all erosion-balance parameters are assumed constant in space. The original cover-balance mathematical model is based on work presented by Beaumont et al. (1992); the enhanced model, incorporating balance equations for overland flow and sediment transport, is based upon work presented by Woolhiser et al. (1990).

Each of the balance equations is solved using the same general finite-volume flow-routing approach. The DEM grid is discretized into square boxes, or nodes, with 1D connections to the nearest eight nodes. Taking advantage of the hyperbolic nature of the equations by assuming that upstream variables uniquely determine fluxes to downstream nodes, the nodes in the grid can be processed in order from highest to lowest elevation in one pass. The resultant predictions are reasonably consistent with field observations of bedrock cover ranging from zero in patches along crestlines, to tens of centimeters on sideslopes, to (in places) more than a meter at the base of some sideslopes above terraces. These trends in cover are also consistent with observations at neutron-probe boreholes (Flint and Flint, 1995). However, the model performs poorly in wash bottoms in large part due to insufficient spatial resolution. Accordingly, within regions having slopes less than 10 degrees and designated Quaternary alluvium by Scott and Bonk (1984) (i.e., terraces and channels), a regressed relationship between alluvium depth and slope is used to estimate the alluvium depth (Stothoff and Bagtzoglou, 1996). The resultant alluvium distribution is the base case spatial distribution of alluvium considered for sensitivity analysis.

#### 10.3.3.5 Sensitivities of Spatial Distributions of Infiltration

Two issues are of particular interest when examining the spatial distribution of AAI. General trends in the spatial distribution of AAI are of interest (i.e., localized zones of high AAI), as is the sensitivity of the areal average AAI to the various input parameters. The first issue is examined by using reasonable values for hydraulic properties, colluvium and alluvium depths, and meteorologic input, in conjunction with the regression formulae developed in section 10.3.3.3, to predict the resultant distribution

of AAI. The second issue is investigated by using first order perturbations to the input parameters and examining the responses in the predicted areal average AAI.

To estimate the spatial distribution of infiltration, the subregional area was subdivided into three classes: deep alluvium, fractured welded bedrock overlain by colluvium, and nonwelded bedrock. Deep alluvium is classified as the area within the Scott and Bonk (1984) alluvium outline with ground slope less than 10 degrees, while the CNWRA 3D GFM (Stirewalt and Henderson, 1995) was used to determine the exposure of bedded nonwelded tuffs (PTn). The remaining area was presumed to consist of welded-tuff bedrock overlain by colluvium. The areas classified as deep alluvium and PTn are about 21 percent and 4 percent of the total subregional area.

Modeling AAI in PTn outcrop areas is problematic for several reasons:

- The layer is thin enough to make the semi-infinite assumption questionable.
- Bedding thicknesses are on the order of meters, making the assumption of homogeneous properties questionable.
- Roughly half of the measured permeabilities are less than  $10^{-10}$  cm<sup>2</sup> (Schenker et al., 1995), thus should yield zero AAI, but some measured permeabilities are in the range of  $10^{-8}$  to  $10^{-9}$  cm<sup>2</sup> and would be expected to yield significant and even quite large AAI.
- Other PTn hydraulic properties are highly variable.

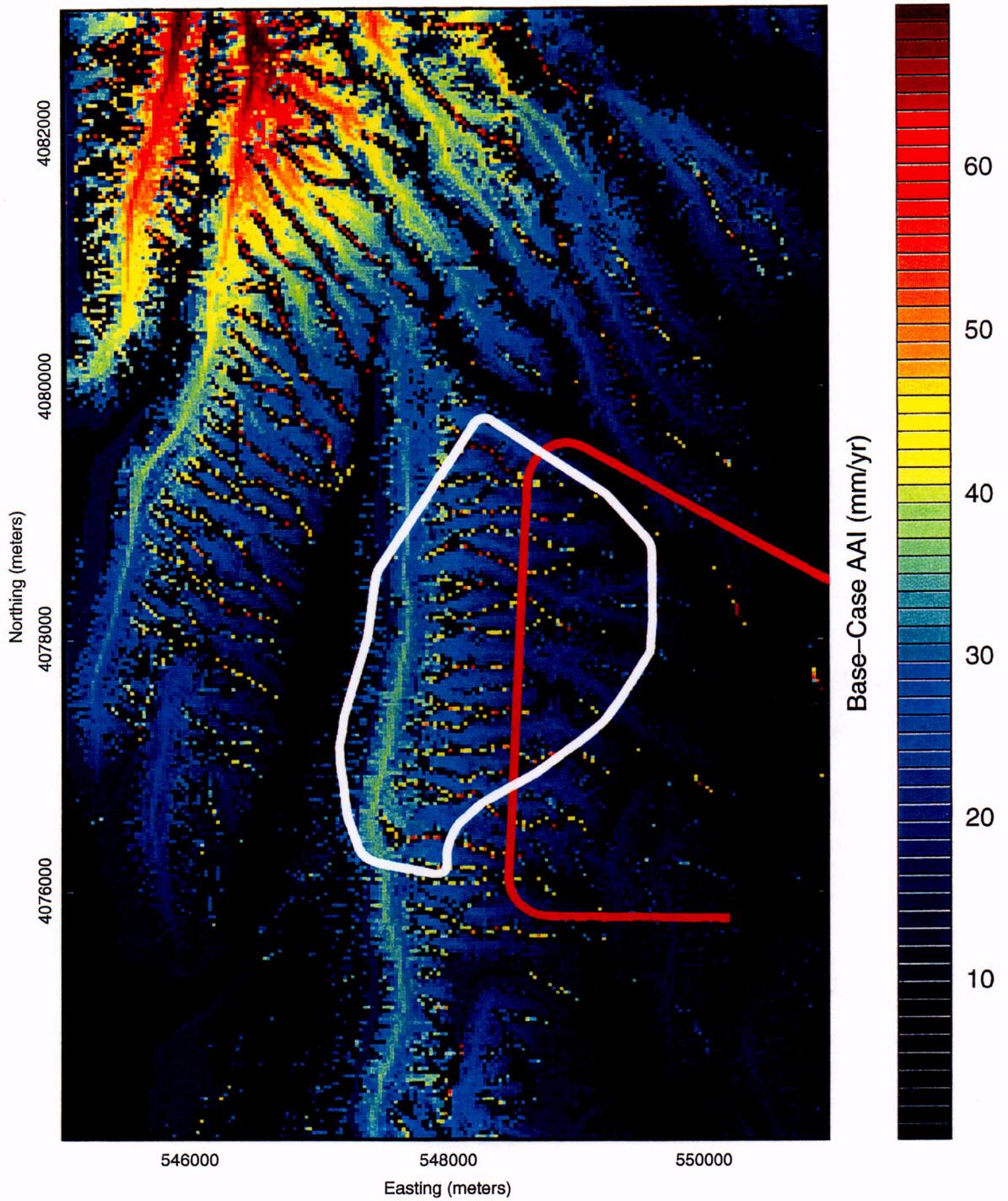
Because of the large uncertainty in PTn response, but relatively small exposure area, the simple approach of assigning a fraction of the AAP as AAI was adopted for PTn outcrops. The base case used 10 percent of AAP for AAI in the PTn outcrops regardless of colluvial cover; the sensitivity of areal average AAI to the PTn was assessed using 0 and 20 percent of AAP.

An estimated spatial distribution for AAI is shown in figure 10-4, based on using base-case surface-cover distribution, base-case reference properties shown in table 10-1, and present day meteorologic conditions. The average AAI over the subregional area for this example is 15.0 mm/yr; within the 3 km E-W×4 km N-S box surrounding the proposed repository footprint, the average AAI is 14.6 mm/yr. Within pixels classified as deep alluvium, PTn, and colluvium/fracture, average AAI is 2.4 mm/yr, 15.4 mm/yr, and 18.6 mm/yr. The largest AAI tends to be on ridgetops and sideslopes. Part of this trend is from enhancement of AAI through systematic meteorological variation; a larger part is from progressive thinning of colluvial thickness with elevation.

Using normalized sensitivity coefficients (Sykes et al., 1985), the sensitivity of areal average AAI to the generic parameter  $\alpha_k$  is

$$S_k = \frac{\alpha_k}{AAI} \frac{dAAI}{d\alpha_k} \quad (10-4)$$

The sensitivity coefficients are calculated by using first order derivatives between a high and low perturbation, normalized by a reference value. In general, sensitivity coefficients will change as the set of base input values change. Accordingly, sensitivity coefficients are calculated for a base-case AAI distribution and a set of alternate AAI distributions where the alternate AAI distributions result from



**Figure 10-4. Example spatial distribution of AAI accounting for depth of alluvium, underlying bedrock, and meteorological effects**

changing the base-case value for a single input parameter. Due to the high correlation between  $I_{D0}$  and  $C_p$ , sensitivity calculations always use an identical value for both parameters.

Values for the input parameters used to calculate sensitivity coefficients are shown in table 10-1. For cases where alternate input parameter values were used to examine sensitivity coefficient variability, the alternate input values are shown as well as the resulting relative change in areal average AAI. Sensitivity coefficients estimated using the perturbations in table 10-1 are shown in table 10-2. The sensitivity coefficients are for the entire region; the calculated areal average AAI values within the 12 km<sup>2</sup> area centered on the repository footprint are generally within 25 percent of the regional values, so that sensitivity coefficients are quite similar.

As can be seen from table 10-1, changing AAP and AAT individually by amounts that might be expected in a pluvial period results in relative increases in areal average AAI of 3.1 and 2.0 for the base-case set of hydraulic properties. For comparison, simultaneously changing both factors by the amount shown in the table results in a relative increase of 4.9.

Several generalizations can be made by examining the sensitivity coefficients presented in table 10-2:

- Areal average AAI is quite sensitive to systematic variation in AAP and AAT.
- Colluvium/fracture system parameters cause the next largest response, with porosity causing larger variation than  $I_{D0}$ .
- Deep-alluvium hydraulic properties cause relatively small variation in areal average AAI due to the small contribution of alluvium to the overall AAI.
- Sizable variation in local AAI within PTn outcrop areas has little impact on areal average AAI due to the small outcrop area.
- As the total AAI contributed by a zone decreases, the sensitivity of areal average AAI to the zonal parameters also decreases.

#### 10.3.4 Progress Toward Development of a Distributed Watershed Model of Solitario Canyon

The low matrix permeability and the general absence of through-cutting fractures in the PTn unit suggest that this hydrostratigraphic unit may act to limit deep percolation reaching the repository horizon. Fast flow paths from the surface to the repository are probably only found coincident with faults such as the Bow Ridge, Sundance, and Ghost Dance that completely transect the PTn and along which hydrostratigraphic units are offset. The reach of Solitario Canyon wash that extends from Little Prow in the north to Plug Hill to the south generally lies below the PTn unit but above and updip from the repository horizon. It has been postulated that focused infiltration (subissue ii) and deep percolation (subissue iii) may occur during extended periods of flow in Solitario Canyon or under conditions where runoff has ceased but water remains ponded in pools or embayments. Although runoff events in Solitario Canyon may be infrequent under present climatic conditions, pluvial conditions will undoubtedly recur during the next 10<sup>5</sup> yr (see section 10.3.1.1) and runoff events may be more frequent and more sustained.

**Table 10-1. Parameter values used for sensitivity coefficient estimation**

PARAMETER	BASE CASE			ALTERNATE BASE VALUE			
	Low	Reference	High	Low	Reference	High	Rel. AAI
Alluvium $k$ (cm <sup>2</sup> )	10 <sup>-8</sup>	10 <sup>-7</sup>	10 <sup>-6</sup>	10 <sup>-7</sup>	10 <sup>-6</sup>	10 <sup>-5</sup>	0.966
Alluvium $m$	0.1	0.2	0.3	—	—	—	—
Alluvium $P_o$ ( $\times 10^5$ Pa)	1	2	5	—	—	—	—
Alluvium porosity $\epsilon_a$	0.1	0.2	0.5	—	—	—	—
AAP fraction in PTn	0.0	0.1	0.2	—	—	—	—
$I_{DO}$ and $C_I$	0.5	0.7	0.9	0.4	0.6	0.8	1.13
Colluvium porosity $\epsilon_c$	0.1	0.2	0.3	0.05	0.1	0.15	2.2
Multiplier for depth $b$	0.5	1	2	0.25	0.5	1	1.7
AAP multiplier	0.67	1	1.5	1	1.5	2.25	3.1
AAT shift (°C)	-3	+3	+3	-6	+3	0	2.0

In areas where alluvial depths exceed 25 to 50 cm, detailed numerical simulations have shown that few wetting pulses are able to reach the fractured tuff units before being dissipated by evaporation (section 10.3.3). These detailed infiltration simulations for YM, however do not yet account for the effects of ponding and flow concentration through overland flow. Accordingly, a study was initiated to simulate rainfall-runoff processes in Solitario Canyon to determine the magnitude and duration of runoff producing storms and locations within the watershed where ponding and channel flow was likely to occur.

The distributed watershed model KINEROS (KINematic runoff and EROSION model) (Woolhiser et al., 1990) was selected as the simulator primarily because it was developed and tested on small watersheds in the arid to semi-arid southwestern United States. The fundamental conceptual model underlying KINEROS assumes that the watershed can be approximated by a cascading network of 1D planar overland flow segments, 1D interception channels, and ponds or detention storage elements. Rainfall excess is computed by subtracting two components from the input rainfall pulse: (i) specified depth of rainfall intercepted by vegetation or other surface condition and (ii) infiltration, as computed by the Smith and Parlange (1978) approximate solution to the Richards equation. KINEROS then uses the kinematic wave equation to route rainfall excess over both the planar overland flow segments and through interception channels. For overland flow, the user may specify either the Manning resistance equation, a laminar flow resistance equation, or the Chezy law. The same options exist for channel segments that may be specified to have either a circular or a trapezoidal cross section. Surface detention is simulated by coupling the conservation equation with a power law depth-outflow relationship that represents a weir or other uncontrolled backwater producing outflow structure. The erosion modeling capability of KINEROS was not used in this study and is not described.

**Table 10-2. Relative change in AAI used to calculate base-case sensitivity coefficients and the AAI sensitivity coefficient values for the base case and cases resulting from systematically changing parameters**

PARAMETER	RELATIVE AAI		SENSITIVITY COEFFICIENT						
	PERTURBATION		Base Case	ALTERNATE BASE VALUE					
	Low	High		$k$	$I_{D0}$ and $C_I$	$\epsilon_c$	$b$	AAP	AAT
$k$	1.11	0.965	-0.014	-0.005	-0.013	-0.007	-0.008	-0.014	-0.008
$m$	0.967	1.24	+0.271	+0.089	+0.239	+0.126	+0.156	+0.339	+0.186
$P_0$	1.20	0.961	-0.121	-0.040	-0.106	-0.056	-0.070	-0.152	-0.083
$\epsilon_a$	1.05	0.975	-0.077	-0.025	-0.067	-0.035	-0.044	-0.096	-0.053
PTn	0.966	1.03	+0.034	+0.035	+0.030	+0.016	+0.019	+0.011	+0.017
$I_{D0}$ and $C_I$	1.27	0.749	-0.914	-0.947	-0.683	-0.348	-0.261	-1.12	-1.19
$\epsilon_c$	2.16	0.556	-1.60	-1.66	-1.40	-1.06	-0.99	-1.63	-1.39
$b$	1.73	0.463	-0.848	-0.878	-0.700	-0.441	-0.585	-0.499	-0.470
AAP	0.289	3.05	+3.33	+3.31	+3.43	+3.38	+2.47	+2.63	+2.44
AAT	2.04	0.609	-0.715	-0.731	-0.760	-0.814	-0.441	-0.442	-1.14

Initial KINEROS simulations were conducted for the small 1.23 km<sup>2</sup> subwatershed in the extreme northern end of Solitario Canyon near Little Prow to determine whether the model was capable of providing the required information on channel recharge. The subwatershed was divided into 28 plane elements with mean length 162 m and 12 channel reaches with mean length 326 m. Channel and overland flow segments had slopes that ranged from 0.08 to 0.21; the mean slope was 0.128. Based on observations made during a reconnaissance level field study, channel cross sections were approximated by trapezoids with one-to-one sideslopes and widths ranging from 0.3 to 4 m. The Manning resistance equation was used for both overland flow planes, channel segments. Manning's  $n$  was 0.101 for the overland flow planes and 0.0165 for the channels. Field reconnaissance conducted after the simulations were completed revealed there is substantial vegetation in channel bottoms and Manning's  $n$  should probably be greater than 0.0165.

In the absence of field measurements of saturated hydraulic conductivity under imbibition, estimates of  $K_s$  for the overland flow planes were based on the results of rainfall simulator studies conducted at Mercury, Nevada (12.7 mm/hr). For the channel bottom, soil texture data were used to develop a  $K_s$  estimate of 61 mm/hr. Other parameters used in the infiltration equation include (i) net capillary drive  $G$  (80 mm for overland flow planes, 63 mm for channels; both derived from rainfall simulator data); (ii) porosity (0.34 for overland flow planes, 0.44 for channels); (iii) rock fraction (set to 0 because  $K_s$  and  $G$  were derived from rainfall simulator data); (iv) microtopography factor, which affects the effective area of infiltration after rainfall ceases (20 mm); (v) maximum saturation (0.94 for overland flow planes, and 0.95 for channels); and (vi) initial soil saturation, which was varied depending on the month during which a shower occurred.

To adequately capture the dynamic response of a small watershed, rainfall intensity data must have a temporal resolution of at least 5 min. Yet there are no recording precipitation gages in Solitario Canyon to provide these data. Hourly precipitation data are available from the Beatty, Nevada, meteorologic station, but it is difficult to disaggregate hourly data. An alternate approach was used wherein two 100-yr sequences of daily precipitation were synthesized using the USCLIMAT model. Each shower in the second 100-yr synthetic sequence, having a rainfall total that exceeded 12.7 mm (0.5 in.), was disaggregated using a method described by Woolhiser and Osborn (1985) and Woolhiser and Econopouly (1986). Showers were sorted by increasing total precipitation and two showers were selected from each of the following percentile ranges: (i) greater than 95 percent, (ii) 70 to 80 percent, and (iii) 50 to 55 percent. Statistics for each of the six selected storms are listed in table 10-3.

The six simulated storms were used for determining the sensitivity of the volume of water infiltrated into the channels of the Little Prow watershed to variations in hydraulic and infiltration parameters. Dimensionless sensitivity coefficients were generally larger for the least intense runoff producing storm (storm 6) than for the most intense runoff producing storm (storm 2), a reflection of the extreme sensitivity of the runoff process when runoff is a small percentage of rainfall. Varying the saturated hydraulic conductivity under imbibition for both channels and overland flow planes had the greatest effect on channel infiltration. Manning's  $n$  on the overland flow planes had little effect on channel infiltration, while increasing  $n$  in the channels increases the flow depth and wetted area for infiltration. Channel infiltration is highly sensitive to the microtopography parameter for overland flow planes for small storms because a small or zero value for the parameter causes much of the water in storage on the surface when rainfall ceases to be infiltrated on the upland areas before it can reach the channel system.

**Table 10-3. Statistics of simulated storms**

Storm Number	Depth (mm)	Duration (min)	Average Intensity (mm/hr)
1	52.0	317	9.84
2	40.6	83	29.3
3	21.6	74	17.5
4	20.8	91	13.7
5	17.5	100	10.7
6	17.5	74	14.2

Subwatershed modeling conducted to date indicates that KINEROS is a reasonable tool for estimating channel recharge in Solitario Canyon, provided that error bands can be established. Actual estimates of channel infiltration in Solitario Canyon will not be provided until better estimates for the key hydraulic and infiltration parameters are obtained. Based on the absence of local rainfall data with high enough temporal resolution, simulation of daily rainfall coupled with disaggregation into showers and shower intensity patterns appears to be the only method that can be used to provide the required precipitation data. Because channel infiltration is highly sensitive to rainfall, the synthetic rainfall sequences must be compared to regional depth-duration statistics. In addition, the spatial distribution of rainfall during a storm may also be important for a watershed the size of Solitario Canyon (approximately 10 km<sup>2</sup>).

#### **10.4 ASSESSMENT OF PROGRESS TOWARD MEETING OBJECTIVES**

Efforts during FY96 have been focused on three of the six subissues identified in the USFIC KTI. In addition, some effort was devoted to assessing ambient flow conditions in the saturated zone. Efforts at improving estimates of AAI and developing an understanding of the processes that may lead to the development and transient behavior of perched water bodies at YM will facilitate evaluation of the DOE assertion that seepage into the drifts will be low. Of the five hypotheses developed by DOE to test this assertion, the three hypotheses that are directly or indirectly addressed by these efforts are: (i) flux that percolates through the repository horizon is substantially less than net infiltration, (ii) rapid fracture flow occurs only within a limited volume of the repository block at any specific time, and (iii) the effect of climate change on seepage can be bounded.

Within this KTI, no general sensitivity analysis was conducted to evaluate the importance of each area of investigation to the overall performance of the repository. There is already ample evidence from TSPAs conducted both by the NRC and the DOE that the performance of the repository is highly sensitive to changes in infiltration and seepage. However, sensitivity analyses were integral parts of the two technical investigations described in sections 10.3.3 and 10.3.4 that addressed shallow infiltration. These sensitivity analyses were conducted primarily to determine which model parameters had the greatest effect on estimates of shallow infiltration.

Progress toward resolution on the effects of climate change on the ambient hydrogeologic regime at YM and on the range of shallow infiltration under current climatic conditions was described in

section 10.3.1. Analytical and empirical methods for determining ambient hydrogeologic conditions in the vicinity of the repository drift and in the saturated zone from beneath YM to the Amargosa Farms region have not yet been fully developed. It is anticipated that continued analyses of the  $^{36}\text{Cl}$  data from the ESF coupled with the development of detailed, drift scale unsaturated flow models will help to bound estimates of seepage into the repository. Understanding of the saturated flow regime beneath YM and its effect on radionuclide dilution will primarily be gained from developing more detailed 3D flow and transport models. During FY97 it is anticipated that the regional-scale flow and transport model developed by DOE as part of the NTS environmental restoration program will be finished and the modeling results will greatly improve understanding of transport and mixing within the YM saturated zone. Results of tracer tests now being conducted at the C-well complex will further improve understanding of transport in the saturated zone.

- Significant progress was made toward resolving technical issues at YM. A draft issue resolution status report on climate change, future precipitation, and water table rise was prepared. Estimates of average annual precipitation under current climatic conditions developed by the NRC and the CNWRA using numerical models are similar in magnitude and areal distribution to estimates developed by the DOE from measured data.
- A quantitative method was developed for bounding the range of climatic and hydrostratigraphic conditions that are necessary for perched water bodies to develop beneath YM.  $^{14}\text{C}$  data from boreholes at YM were used to constrain estimates of recharge rates and durations required to develop and sustain perched water bodies for an idealized YM.
- Estimates of average annual shallow infiltration at YM were developed using BREATH, a 1D two-phase, non-isothermal flow code. The effect of factors such as the thickness of alluvial cover, material properties, and hill slope orientation, on average annual shallow infiltration was assessed for each 30-m square pixel in the YM vicinity. From these analyses, maps were prepared that depict the estimated spatial distribution of AAI. Sensitivities of AAI to variations in material properties and climatic factors were calculated. Studies have been initiated to assess the effect of ponding during rainfall-runoff events in Solitario Canyon on local infiltration rates.

## 10.5 INTEGRATION WITH OTHER KEY TECHNICAL ISSUES

The USFIC KTI has provided general information on the regional saturated flow system to the KTI on Radionuclide Transport. Estimates of shallow infiltration developed in this KTI were supplied to the KTI on Total System Performance and Integration for the audit review of TSPA-95 (TRW Environmental Safety System, Inc., 1995). Boundary conditions from the unsaturated flow model used in the perched water study were provided to the KTI on Thermal Effects on Flow for simulating the effect of repository heating on the development of local perched water bodies above the repository horizon. Interaction with the KTI on Structural Deformation and Seismicity (SDS) has focused on assessing the effect of the geologic structure and the regional contemporary *in situ* stress field in the YM area on saturated zone flow. In addition, information from the GFM developed within the SDS KTI was used in developing the hydrostratigraphic cross sections used in the perched water study.

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# 11 RADIONUCLIDE TRANSPORT

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## 11.1 INTRODUCTION

A fundamental concern in evaluating the suitability of Yucca Mountain (YM), Nevada as a potential repository for high-level radioactive waste (HLW) is the possibility of radionuclide transport through the subsurface from the proposed repository to the accessible environment. Dose calculations of the type recommended by the National Academy of Sciences (NAS) (National Academy of Sciences, 1995) ultimately require an estimate of concentrations of different radionuclides in aqueous, gas, and/or solid phases that occur along the exposure pathway. These concentrations will vary as a function of space and time depending on the processes that control the rate of radionuclide transport through the subsurface and the effects of changes in system chemistry and hydrology. Therefore, processes that control the reduction (or increase) of radionuclide concentration in the groundwater need to be studied in any evaluation of proposed repository performance.

The Radionuclide Transport Key Technical Issue (KTI) is concerned with the processes that may affect radionuclide transport from the proposed repository to the accessible environment. A number of processes, such as sorption, matrix diffusion, dispersion, mineral precipitation, radioactive decay, and dilution may serve to reduce radionuclide concentration during transport, ultimately leading to a reduction in potential dose to man. This is especially true for the longer time periods recommended by NAS (National Academy of Sciences, 1995). On the other hand, existence of fast transport paths can keep the concentration relatively higher. An understanding of the geochemical processes that influence radionuclide transport may be used to offset uncertainties in hydrologic models of the YM system (Simmons et al., 1995). Not understanding the degree to which these processes are affected by changes in system chemistry/hydrology makes it difficult to reasonably bound radionuclide transport. In the U.S. Department of Energy (DOE) Waste Containment and Isolation Strategy (WCIS),<sup>1</sup> matrix diffusion, sorption, and dilution are mentioned as key site attributes that need to be tested in any suitability demonstration for a proposed repository at YM. The attributes include three hypotheses related to matrix diffusion, sorption, and dilution: (i) reduction of radionuclide concentration by depletion and dispersion during radionuclide transport (Hypothesis 10), (ii) a flux in the saturated zone that is much greater than the flux contacting the waste (Hypothesis 11), and (iii) strong mixing within the saturated zone that leads to a dilution of a radionuclide-bearing aqueous phase (Hypothesis 12).

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<sup>1</sup>U.S. Department of Energy. 1996. *Highlights of the U.S. Department of Energy's Updated Waste Containment and Isolation Strategy for the Yucca Mountain Site*. DOE Concurrence Draft. July 1996. Washington, DC: U.S. Department of Energy.

The Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA) have identified subissues to cover data and analysis needs to address the effects of radionuclide transport on overall repository performance:

- Identifying which radionuclides require some form of retardation to meet performance requirements at YM.
- Evaluating geochemical and hydrological controls on radionuclide transport and the potential for dilution at YM, corresponding to DOE WCIS Hypotheses 11 and 12.
- Evaluating conceptual models and mathematical approaches to modeling radionuclide retardation at YM, corresponding to DOE WCIS Hypothesis 10.
- Evaluating the sensitivity of the overall performance of the proposed repository to ranges in parameters controlling radionuclide transport.

The following sections present technical work accomplished during fiscal year (FY) 1996. Work includes evaluation of DOE flow and transport conceptual models using both site specific and natural analog data. Experimental data and models are presented for constraining radionuclide sorption coefficients. Progress in developing geographic information system (GIS) coverages for existing hydrochemical data is also presented. These activities have been designed to establish a basis for subsequent review and evaluation of DOE submittals. It is important to note that some of the information necessary for answering these questions is also needed to address other KTIs. For example, hydrostratigraphy and hydraulic properties are necessary for both the Radionuclide Transport and Unsaturated and Saturated Flow Under Isothermal Conditions KTIs.

## **11.2 OBJECTIVES AND SCOPE OF WORK**

The work under this KTI is intended to lead to resolution of these subissues through the use of quantitative models in evaluating the effects of transport and dilution processes on repository performance under geochemical and hydrologic conditions specific to YM. The complex geochemical and hydrological conditions at YM make it difficult to establish reasonable boundary and initial conditions for modeling of transport processes. The system heterogeneity makes it especially difficult to determine bounding values for radionuclide transport given the possible changes through space and time in key parameters such as pH. Sensitivity analyses can provide some insight as to which parameters have the greatest effect on repository performance, and identify those areas of the KTI that can use bounding calculations in performance assessment (PA).

Both the NRC and the DOE have attempted to include the effects of geochemistry on radionuclide transport in PA calculations (e.g., Wilson et al., 1994; TRW Environmental Safety Systems, Inc., 1995; Wescott et al., 1995). However, there remains sufficient uncertainty in both the hydrological and the transport models used in these efforts that continued study of radionuclide transport is warranted. Therefore, the NRC has elected to conduct a detailed review of a vertical slice of the overall DOE program in the area of radionuclide transport.

FY96 activities for the Radionuclide Transport KTI were designed to:

- Seek resolution with the DOE on data used for neptunium (Np) sorption coefficients ( $K_d$ ). This is related to DOE WCIS Hypothesis 10. PA calculations in DOE Total System Performance Assessment (TSPA) include retardation for all radionuclides in the unsaturated and saturated zones. Preliminary sensitivity analyses (TRW Environmental Safety Systems, Inc., 1995) have identified Np sorption as an important parameter in repository performance. The NRC/CNWRA and the DOE experimental data for Np sorption may be similar enough to allow agreement on the likely magnitude and conservative estimates of sorption coefficients for Np at YM. Ultimately, this type of information will be combined with stratigraphy, flowpath information, and saturation data to address Np transport in the subsurface.
- Provide a basis for critical evaluation of conceptual models of flow and transport used by the DOE in TSPA calculations. This is related to DOE WCIS Hypotheses 10 and 11.
- Identify critical radionuclides for which retardation is likely to be necessary for performance requirements to be met. This is related to DOE WCIS Hypothesis 10. An evaluation of key radionuclides has already been done by the DOE (Kerrisk, 1985) and the NRC/CNWRA (Jarzempa and Pickett, 1995) under the existing Environmental Protection Agency (EPA) regulations based on inventory and initial geochemical considerations. Because of the NAS recommendations for a new EPA standard, identifying key radionuclides will require input from the KTI on TSPA and Integration and the Support Development of the EPA Standard KTI.
- Identify, acquire, and evaluate available hydrochemical data to bound flow and the potential for dilution and mixing within the YM system. This is related to DOE WCIS Hypotheses 11 and 12. The DOE on-line databases will be searched for electronic forms of site specific data to supplement existing GIS databases at the CNWRA. The search of DOE data will focus on concentrations of geochemical tracers. The tracer information can be used to evaluate the extent of mixing between aquifers in the YM region and perhaps establish boundary conditions for flow models being developed in the Isothermal Flow KTI.

## 11.3 SIGNIFICANT TECHNICAL ACCOMPLISHMENTS

### 11.3.1 Chlorine-36 at the Yucca Mountain Site and Evaluation of Conceptual Models

It is important to evaluate DOE conceptual models of flow and transport using, to the extent possible, available site specific data (DOE WCIS Hypotheses 10 and 11). Radionuclide transport in groundwater of the unsaturated zone at YM is demonstrated by analyses of natural and bomb-pulse  $^{36}\text{Cl}$ . A review was conducted of a Los Alamos National Laboratory (LANL) report released in April 1996 (Fabryka-Martin et al., 1996) on studies of  $^{36}\text{Cl}$  extracted from rock samples collected in the Experimental Studies Facility (ESF). The data appear to have been collected with care and data quality seems to be high. The data set reveals a fairly coherent pattern of relatively low values of  $^{36}\text{Cl}/\text{Cl} < 1,500 \times 10^{-15}$  all along the ESF. The prevailing interpretation of these data is that they represent natural cosmogenic  $^{36}\text{Cl}$  and imply maximum groundwater travel times ranging from 50,000 to 550,000 yr. In addition, five zones

ranging in width from a single sample to a discontinuous zone spanning 130 m have elevated  $^{36}\text{Cl}/\text{Cl}$  ratios to  $3,800 \times 10^{-15}$ . These high ratios in the rock are reasonably interpreted to indicate some component of bomb-pulse  $^{36}\text{Cl}$  generated within the last 50 yr. All these samples with elevated  $^{36}\text{Cl}/\text{Cl}$  were collected from features such as fault gouge, joints, or fractures. Four of the five elevated  $^{36}\text{Cl}/\text{Cl}$  zones were located in zones in the vicinity of projections from surface expressions of mapped faults, but only one of these four was collected from a fault. Collectively the elevated  $^{36}\text{Cl}/\text{Cl}$  data demonstrate short  $^{36}\text{Cl}$  transport times (less than 50 yr) from the ground surface to the depth of the ESF (280 m). An estimate of mass of  $^{36}\text{Cl}$  transported through these rapid paths is not available at this time. Surface infiltration in fault zones and rapid groundwater flow in various (but not all) fractures is also indicated. The  $^{36}\text{Cl}/\text{Cl}$  data indicate the importance of through-going fractures in radionuclide transport; if it is determined that significant mass can be transported through fast paths from the repository to the groundwater table, then DOE conceptual models should be designed to take into account the importance of fracture transport.

### 11.3.2 Using Uranium Transport at Peña Blanca Natural Analog to Constrain Radionuclide Transport

Technical activities related to this effort were centered on two fronts: interpretation of uranium transport at the Nopal I uranium deposit at the Peña Blanca natural analog site, and followup laboratory analyses of samples from Nopal I. The journal article was submitted to the NRC and is intended for publication in the journal *Applied Geochemistry* (Pickett et al., 1996).<sup>2</sup> The article made use of data and analyses initiated under the former Geochemical Analogs Research Project and continued under the Radionuclide Transport KTI. A summary of the results from this study and their relationship to subissue resolution is presented below.

Data from Nopal I have been used to identify key processes and bound parameters in hydrologically unsaturated tuffs. Understanding which processes are most critical in radionuclide transport in a field-scale site is an important step in developing conceptual transport models appropriate to hydrologic and geochemical conditions at YM. This effort focuses on bounding conceptual models of radionuclide transport, the third subissue of this KTI, and addresses DOE WCIS Hypothesis 10.

Pickett et al. (1996)<sup>3</sup> used uranium-series isotopic data from rocks surrounding the Nopal I deposit to deduce information on the salient features of uranium (U) transport behavior at the analog site. Geologic, geochemical, and hydrologic features of Nopal I that make it an appropriate analog for the proposed HLW repository at YM have been detailed elsewhere (Percy et al., 1994). Uranium-series analyses provide information on the relative distribution of natural radionuclides as a function of time. At the Nopal I site, radioactive disequilibria among three nuclides in the  $^{238}\text{U}$  chain ( $^{230}\text{Th}$ ,  $^{234}\text{U}$ , and  $^{238}\text{U}$ ) in tuffs and fracture-filling materials surrounding the U ore deposit reveal a complex, multistage, history of U mobility over the past few hundred thousand years. Apparent episodicity in U transport behavior may have implications for attempts to model long-term radionuclide transport at the proposed repository.

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<sup>2</sup>Pickett, D.A., J.D. Prikryl, W.M. Murphy, and E.C. Percy. 1996. Uranium-series disequilibrium investigation of radionuclide mobility at the Nopal I uranium deposit, Peña Blanca District, Mexico. *Applied Geochemistry*. In press.

<sup>3</sup>*ibid.*

Uranium distributions around the deposit (Pearcy et al., 1995; Pickett et al., 1996)<sup>4</sup> demonstrate an apparent horizontal component of transport (i.e., assuming a vertically aligned ore body) on the scale of tens of meters in hundreds of thousands of years; the vertical component is likely to have been greater. Concentrations of U in solids filling discrete fractures are higher relative to the surrounding, generally fractured, tuff. This implies that discrete fractures may have accommodated more U transport than the bulk rock. Uranium was transported the greatest distances from the ore deposit along mappable mesofractures. While calculations have suggested that the microfracture network surrounding one such mesofracture contains about five times the amount of U as the mesofracture itself (Pearcy et al., 1995), the generally microfractured tuff is not apparently itself a conduit for distal transport. Furthermore, among the matrix traverses (i.e., those through generally fractured tuff rather than along mapped mesofractures), correlations between outcrop-scale fracture density and U concentration gradients suggest greater transport in more fractured tuff. The majority of both solids from mineralized fractures and samples representative of the bulk rock exhibit  $^{230}\text{Th}$ - $^{234}\text{U}$ - $^{238}\text{U}$  disequilibria relationships requiring a multistage U transport history (Pickett et al., 1996).<sup>5</sup> In particular, while  $^{234}\text{U}/^{238}\text{U}$  ratios greater than unity imply addition of water-mobilized U within the past few hundred thousand years,  $^{230}\text{Th}/^{234}\text{U}$  ratios significantly greater than unity require a subsequent U removal event (Osmond and Ivanovich, 1992). The history of U mobility at the Nopal I site, as suggested by the U-series data, is (i) removal of U from the deposit and transport and addition of U to rocks outside the deposit; (ii) a period of at least 200,000 yr following or accompanying U transport; and (iii) partial U removal from rocks outside the deposit (figure 11-1). Patterns of activity ratio variations with distance, as well as local deviations from the patterns, imply smaller-scale episodic behavior superimposed on this overall pattern. Sequential extraction experiments on Fe oxide-rich fracture infillings reveal distinct histories for different phases/sites within the rocks. Most notably, uranium-series distributions demonstrate that U sequestered in secondary phases, chiefly Fe oxides and oxyhydroxides, is incorporated into the minerals over time through either coprecipitation or dissolution/reprecipitation.

The key results of this study and implications for KTI resolution are three-fold. First, radionuclide mobility at the Nopal I site and, by analogy, YM is sensitive to changes in geochemical and hydrologic conditions. U transport behavior at Nopal I has been complex and episodic over the past few hundred thousand years, with significant recorded U transport events at least as young as 9,000 yr. The period recorded by the uranium-series features of the rocks has been dominated by oxidizing hydrochemical conditions; this is supported by caliche ages as old as 54 ka (Pearcy et al., 1995) and by preliminary U/Pb ages of around 3 Ma on uranophane. Nevertheless, significant (and possibly cyclic) shifts in the mobility of U have been possible. At Nopal I it has not yet been determined what caused these shifts, but environmental variations due to climate change may be important. The most important effect of climate change would be on the flux of water through the unsaturated zone, and the episodicity of transport at Nopal I suggests that such changes can alter transport. Because of the strong analogy between conditions at Nopal I and YM, the demonstrated timing, episodicity, and complexity of transport at Peña Blanca suggest that such conditions can be expected at YM and are likely to be important to radionuclide transport at the proposed repository. To what extent repository performance will be affected remains to be determined. This study suggests that key parameters (e.g.,  $K_d$ ) in modeling transport behavior at YM

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<sup>4</sup>Pickett, D.A., J.D. Prikryl, W.M. Murphy, and E.C. Pearcy. 1996. Uranium-series disequilibrium investigation of radionuclide mobility at the Nopal I uranium deposit, Peña Blanca District, Mexico. *Applied Geochemistry*. Submitted to NRC.

<sup>5</sup>*Ibid.*

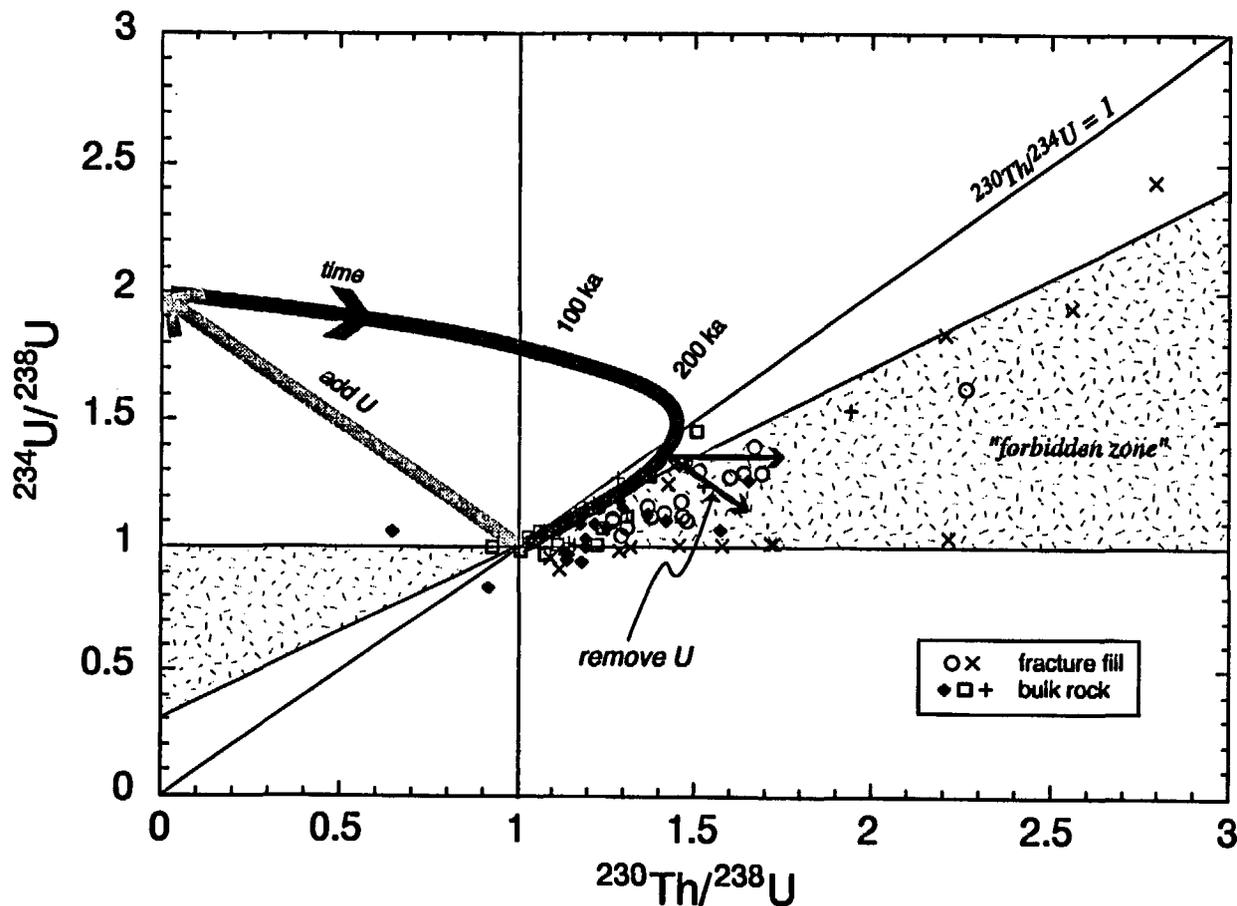


Figure 11-1.  $^{234}\text{U}/^{238}\text{U}$  versus  $^{230}\text{Th}/^{238}\text{U}$  plot of Nopal I traverse bulk rock samples, with preferred model for evolution. Symbols denote separate traverses away from the ore deposit. The crosses and circles represent samples of minerals filling mesofractures; the other symbols are for samples from traverses through generally microfractured tuff. Note the different axis scales. The model assumes an initial rock at or near secular equilibrium (i.e., both ratios equal to one) to which high- $^{234}\text{U}/^{238}\text{U}$  aqueous U is added, followed by significant time evolution (note time labels on curve), and finally by partial U removal with or without U isotope fractionation. Clearly, not all rocks would have followed the same path, and U addition and removal likely occurred in a more continuous or episodic manner. The "forbidden zone" reflects combinations of the two activity ratios that require multistage histories.

should have sufficiently broad bounds to account for such potential variations in geochemistry. Second, with respect to distance, fracture transport is dominant over matrix tuff transport and hydrology. The importance of transport along fracture pathways at YM has been demonstrated by  $^{36}\text{Cl}$  evidence for rapid transport (Fabryka-Martin et al., 1996). For the unsaturated zone at Nopal I, this is supported by observation of rapid near-surface water infiltration following storms. Finally, incorporation of aqueous U into fracture filling minerals suggests that sorption is not fully a reversible process. In constructing process-level models, it is important to consider other geochemical processes such as mineral growth or dissolution that may affect potential radionuclide remobilization. Furthermore, distribution of U among minerals at Nopal I may be useful in assessing  $K_d$ 's used in PA at YM, at least in a relative sense.

New laboratory analyses of Nopal I samples have been centered on the use of gamma spectrometry for more rapid, non-labor-intensive, non-destructive analysis of decay-series radionuclides. Many analyses were conducted and detailed study of data reduction procedures are planned to allow maximum utility of the gamma spectra. In addition to ease of analysis compared to alpha spectrometry, these data provide information on mobilization and transport at Nopal I of other radionuclides of potential interest to PA of the proposed HLW repository at YM, including  $^{226}\text{Ra}$ ,  $^{231}\text{Pa}$ ,  $^{227}\text{Ac}$ , and  $^{210}\text{Pb}$ .

### 11.3.3 Geochemical Parameters Controlling Radionuclide Sorption

Under the current DOE WCIS, Hypothesis 10 calls for reduction in radionuclide concentration through depletion and dispersion. Testing this hypothesis requires a means of constraining processes that contribute to the depletion and retardation of radionuclide transport. An important mechanism for retarding the migration of radionuclides such as Np, U, and Pu is sorption onto minerals present along groundwater flow paths. A quantitative understanding of actinide sorption behavior is complicated by the possible dependence of sorption on geochemical parameters, including aqueous solution properties (e.g., pH, ionic strength, radionuclide concentration, complexing ligands) and sorptive phase characteristics (e.g., composition, surface area, sorption site density, surface charge). The dependence of sorption on various parameters makes it difficult to describe and predict actinide retardation and transport in geochemical systems of variable and composite mineralogic composition and changing aqueous speciation, but it is possible to determine reasonable bounds.

Batch experiments were conducted at the CNWRA to investigate the sorption of U(6+) and Np(5+) on the minerals quartz, clinoptilolite, montmorillonite, and  $\alpha$ -alumina over wide ranges of experimental conditions. These minerals were selected because their mineralogic and surface characteristics, that could potentially influence radionuclide sorption behavior, are distinct from each other. In addition, quartz, clinoptilolite, and montmorillonite are abundant mineral phases at the proposed HLW repository at YM. The experiments were designed to evaluate the possible effect on radionuclide sorption of pH, radionuclide concentration, radionuclide aqueous speciation, ionic strength, and solid-mass to solution-volume ratio (M/V). Results of these experiments, as well as data from published literature, were used in determining what various geochemical parameters are key to understanding radionuclide sorption behavior. The data were also used to develop and parameterize surface complexation models for describing and predicting radionuclide sorption onto mineral substrates. The results of these interpretations were

summarized in two peer-reviewed articles (Pabalan et al., 1997;<sup>6</sup> Bertetti et al., 1997<sup>7</sup>) submitted to the NRC and intended for publication by Academic Press as part of the book *Metals in Geomedia: Sorption Processes and Model Applications* (E. Jenne, ed.).

The results of selected sets of experiments are plotted in figures 11-2 to 11-10 as a function of pH. Although radionuclide sorption data are typically plotted in terms of percent sorbed, a useful representation is as a distribution coefficient,  $K_d$ , that may be defined as

$$K_d \text{ (ml/g)} = \frac{\text{equilibrium amount sorbed}}{\text{equilibrium amount in solution}} \times \left( \frac{V}{M} \right) \quad (11-1)$$

where  $V$  is the volume of experimental solution (ml) and  $M$  is the mass of solid (g). The use of  $K_d$  provides a means of normalizing sorption results with respect to the sorbent concentration (or  $M/V$  ratio) and of taking into account the decrease in solution concentration of the radionuclide due to sorption.

### *Uranium(6+) Sorption*

As an example of the importance of geochemical conditions on sorption behavior, figure 11-2 shows data on U(6+) sorption on common minerals as a function of pH taken from both the literature and from the CNWRA experiments. Data in the figure demonstrate that U(6+) sorption on these minerals is strongly affected by solution pH. Although the minerals used in the experiments have different mineralogic and surface properties, U(6+) sorption on these minerals is similar with respect to dependence on pH. In all cases, U sorption is at a maximum at near neutral pH (~6.0 to ~6.8) and decreases sharply towards more acidic or more alkaline conditions. Differences in experimental conditions (e.g., pH,  $PCO_2$ , surface area), however, can lead to large differences in  $K_d$ , as shown by the silica sorption data presented in figure 11-2.

Pabalan et al. (1997)<sup>8</sup> showed that there is a close correspondence between the pH dependence of U(6+) sorption and the predominance field of the U(6+) hydroxy aqueous complexes. U(6+) sorption occurs in the pH range where the U(6+) hydroxy complexes are important. At low pH values where the uranyl cation  $UO_2^{2+}$  is predominant, U(6+) sorption is typically weak for common minerals, except for those cation exchangers such as montmorillonite and clinoptilolite where U(6+) sorption through an ion exchange mechanism can be important. Aqueous carbonate complexation plays an important role in reducing radionuclide sorption at higher pH (Pabalan et al., 1997).<sup>9</sup> For example, at higher  $PCO_2$ , the

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<sup>6</sup>Pabalan, R.T., D.R. Turner, F.P. Bertetti, and J.D. Prikryl. 1997. Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>7</sup>Bertetti, F.P., R.T. Pabalan, and M.G. Almendarez. 1997. Studies of neptunium(V) sorption on quartz, clinoptilolite, montmorillonite, and  $\alpha$ -alumina. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>8</sup>Pabalan, R.T., D.R. Turner, F.P. Bertetti, and J.D. Prikryl. 1997. Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>9</sup>*Ibid.*

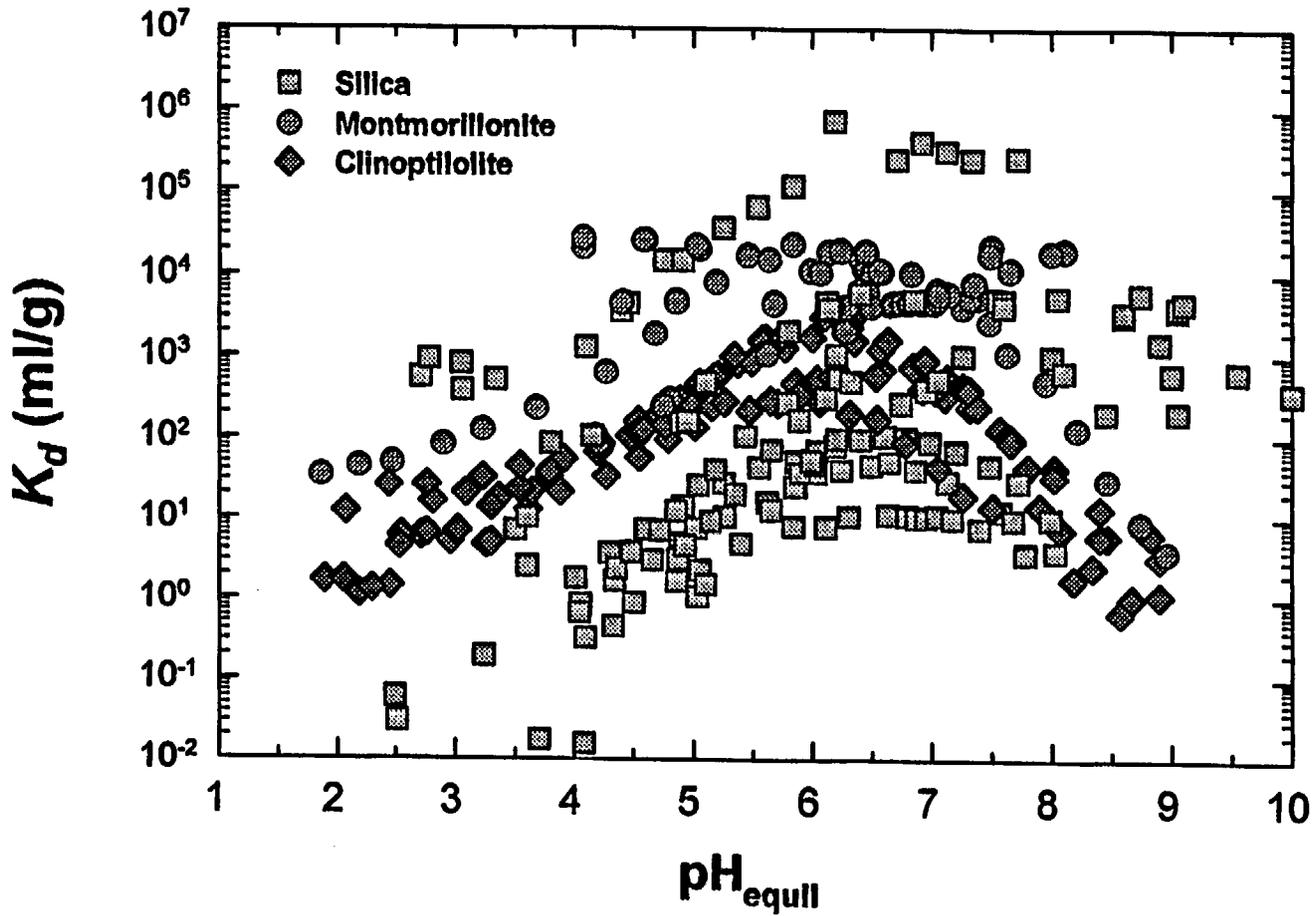


Figure 11-2. Uranium(6+) sorption (expressed as  $K_d$  in ml/g) on common rock-forming minerals. Results are taken from literature (Zachara and McKinley, 1993; McKinley et al., 1995) and from batch experiments conducted at the CNWRA for a range in geochemical conditions ( $\Sigma U$ ,  $PCO_2$ ,  $M/V$ ). Note the similarities among the different minerals in strong pH dependence of U(6+) sorption behavior, and the wide range in  $K_d$  observed for a given mineral.

predominance field of the mononuclear U(6+) aqueous hydroxy species  $[\text{UO}_2(\text{OH})_x^{2-x}]$  becomes reduced in a manner similar to the reduction in U(6+) sorption envelope (i.e., the maximum is lowered and the high pH side is shifted to lower pH). This is due to the increased importance of the U(6+) aqueous carbonate complexes at higher  $\text{PCO}_2$ .

For the U(6+)-H<sub>2</sub>O-CO<sub>2</sub>-mineral systems considered,  $K_d$  decreases with increasing initial U concentration particularly in the intermediate pH range (Pabalan et al., 1997).<sup>10</sup> The effect is greater at higher initial U concentrations due to the nonlinearity of the sorption isotherm except at low U concentrations. The  $K_d$ , which is the slope of the isotherm at a fixed U solution concentration, is larger at lower solution concentrations and approaches a constant value at low enough solution concentrations where the isotherm is linear. In addition to the CNWRA results, decreasing sorption with increasing initial U concentration has also been observed for the U(6+)-ferrihydrite system (Waite et al., 1994). In the presence of excess sorption sites, the nonlinear trend in sorption with increasing U concentration may also be influenced by the formation of polynuclear aqueous complexes (O'Day, 1994). Likewise, the decrease in the proportion of sorbed U(6+) associated with an increase in initial U concentration has been used as evidence against formation of polynuclear U(6+) surface complexes (Waite et al., 1994). Experimental results also indicate that solution ionic strength has little influence on U(6+) sorption, at least over the range in ionic strengths considered here (Pabalan et al., 1997)<sup>11</sup> and where the ion exchange sorption mechanism is negligible.

Changes in sorption behavior for a given mineral as a function of solid-mass to solution-volume (M/V) ratio can appear to be significant when data are plotted in a typical manner of percent U sorbed versus pH (Pabalan et al., 1997)<sup>12</sup> (figure 11-3a). The apparent M/V effect, however, is mostly eliminated if the results are plotted in terms of  $K_d$ , a ratio of equilibrium concentrations in the solid versus in solution (figure 11-3b), although there is significant uncertainty in the data at both high and low pH. Plotting data in terms of  $K_d$  instead of percent U sorbed makes comparison of different sets of experimental data easier (figure 11-4).

Based on expert elicitation, DOE PA calculations use probability density functions for U sorption coefficients that range from 0 to 30 ml/g (TRW Environmental Safety Systems, Inc., 1995), but there is no clear link to the effects of geochemical conditions on U sorption. Based on CNWRA experiments, U(6+) sorption on quartz,  $\alpha$ -alumina, clinoptilolite, and montmorillonite expressed in terms of  $K_d$  is similar with respect to pH dependence. However, the  $K_d$  values for the different minerals vary over three orders of magnitude. This variation is an artifact of representing sorption data using  $K_d$ , which normalizes the amount of U(6+) sorbed to the sorbent mass and not to the number of available sorption sites. Surface areas measured by gas adsorption (e.g., N<sub>2</sub>-BET) methods are a relative index of the number of sorption sites on the mineral surface (Davis and Kent, 1990). Thus, it is more useful to represent sorption data normalized to the specific surface area of the mineral sorbent. Figure 11-5 presents the results of the CNWRA batch experiments on U(6+) sorption on quartz,  $\alpha$ -alumina, clinoptilolite, and montmorillonite shown previously in figure 11-4 and replotted in terms of  $K_a$  (ml/m<sup>2</sup>), where  $K_a$  is  $K_d$  normalized to the

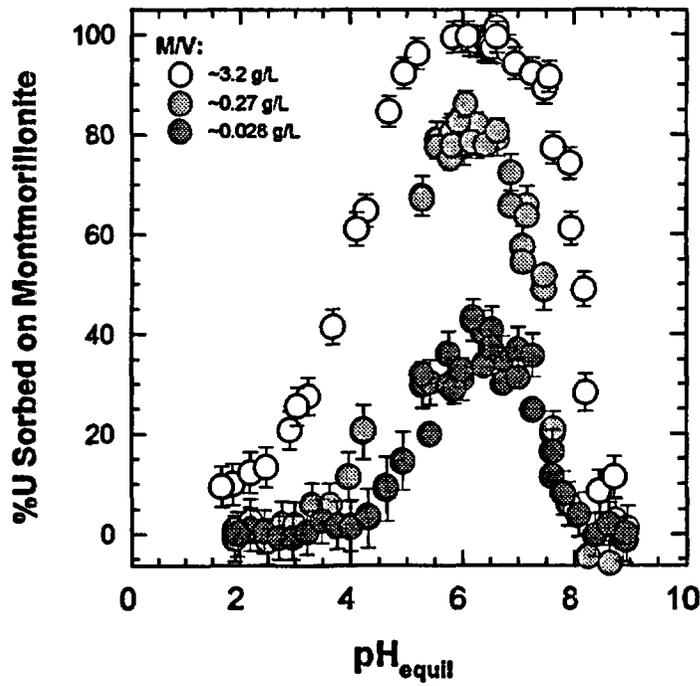
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<sup>10</sup>Pabalan, R.T., D.R. Turner, F.P. Bertetti, and J.D. Prikryl. 1997. Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>11</sup>*Ibid.*

<sup>12</sup>*Ibid.*

a)



b)

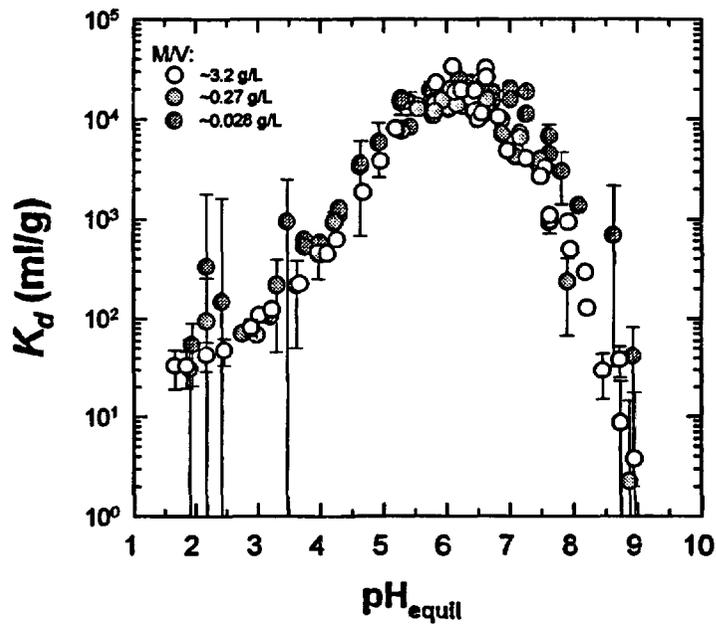


Figure 11-3. a) Uranium(6+) sorption on montmorillonite as a function of M/V expressed as percent U(6+) sorbed versus pH. Note the increasing percent sorbed with increasing M/V. b) Uranium(6+) sorption on montmorillonite as a function of M/V expressed as  $K_d$  versus pH. The effect of M/V is largely removed.

## U(6+) Sorption Results

( $\Sigma U_i \sim 2.4 \times 10^{-7} \text{ M}$ ;  $PCO_2 = 10^{-3.8} \text{ atm}$ )

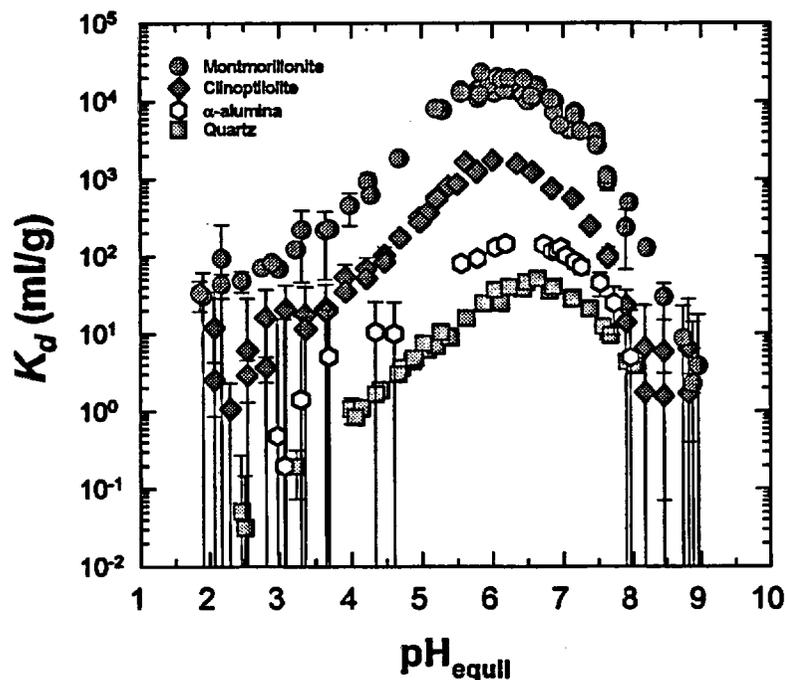


Figure 11-4. CNWRA experimental results for U(6+) sorption on montmorillonite, clinoptilolite,  $\alpha$ -alumina, and quartz expressed as  $K_d$

mineral's  $N_2$ -BET specific surface area ( $S_a$  in  $m^2/g$ ) (i.e.,  $K_a = K_d/S_a$ ). The  $S_a$  used in the normalization are 0.03, 97, 0.23, and  $10.1 \text{ m}^2/g$  for quartz, montmorillonite,  $\alpha$ -alumina, and clinoptilolite, respectively. Surface area normalized sorption data for clinoptilolite and montmorillonite are indistinguishable, whereas surface area normalized sorption data for quartz and  $\alpha$ -alumina are almost coincident (figure 11-5). The  $\alpha$ -alumina  $K_a$  are lower than those of quartz due to the higher initial U concentration of the  $\alpha$ -alumina experiments.

The results plotted in figure 11-5 appear to indicate that quartz and  $\alpha$ -alumina sorb more U(6+) per unit area than either clinoptilolite or montmorillonite. However, surface areas determined by  $N_2$ -BET methods most likely overestimate the amount of sorption sites on layered silicates such as montmorillonite and zeolitic minerals such as clinoptilolite. For example, it is believed that surface complex formation of U(6+) on montmorillonite occurs on the hydroxylated edge sites of the mineral (Zachara and McKinley, 1993). Wanner et al. (1994) estimated that only about 10 percent of the  $N_2$ -BET measured  $S_a$  is accounted for by the crystallite edges of montmorillonite. Assuming that the "effective" surface area ( $S_{a,e}$ ) for montmorillonite and clinoptilolite is equivalent to 10 percent of the measured  $S_a$ , sorption data for montmorillonite and clinoptilolite can be recast in terms of  $K_{a,e}$ , where  $K_{a,e} = K_d/S_{a,e}$ . For nonlayered and nonporous minerals such as quartz and  $\alpha$ -alumina,  $K_a = K_d/S_a$ . Figure 11-6 plots  $K_{a,e}$  values for quartz, clinoptilolite, and montmorillonite. As shown in the figure, U(6+) sorption on these minerals, which have distinct mineralogic and surface properties, is essentially equivalent when recast in terms of  $K_{a,e}$ .

## U(6+) Sorption, $K_a$ (ml/m<sup>2</sup>)

( $\Sigma U_1 \sim 2-4 \times 10^{-7}$  M;  $PCO_2 = 10^{-3.5}$  atm)

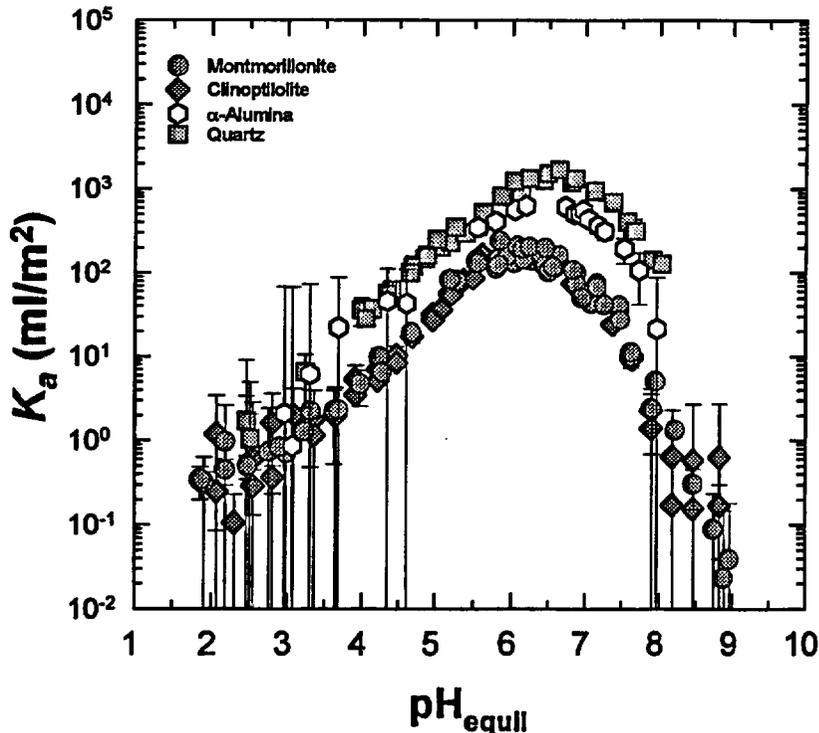


Figure 11-5. U(6+) sorption results shown previously in figure 11-4 and normalized to the measured  $N_2$ -BET surface area ( $S_a$ ). Note similarity in U(6+) sorption on quartz and  $\alpha$ -alumina and in U(6+) sorption on clinoptilolite and montmorillonite.

To test the usefulness of normalization to effective surface area as a relative measure of sorption effectiveness, Pabalan et al. (1997)<sup>13</sup> compiled literature data on U(6+)-sorption for  $TiO_2 \cdot xH_2O$ , montmorillonite, amorphous  $SiO_2$ , and kaolinite and recast them in terms of  $K_a$ , versus pH. The literature data showed good agreement with the CNWRA results for  $K_a$ , versus pH. Good correspondence between the  $K_a$ , for different minerals and different experimental sets, indicates that  $S_a$ , and  $K_a$ , may be useful parameters for comparing and estimating U(6+) sorption on various sorbents.

In all U(6+)- $H_2O$ - $CO_2$ -mineral systems examined by Pabalan et al. (1997),<sup>14</sup> the experimental results show an unambiguous link between the aqueous speciation of U(6+) and its sorption behavior. Uranium(6+) sorption is most affected by geochemical parameters that influence the formation of U(6+)-hydroxy complexes in the aqueous phase. Geochemical conditions such as low pH and carbonate

<sup>13</sup>Pabalan, R.T., D.R. Turner, F.P. Bertetti, and J.D. Prikryl. 1997. Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>14</sup>*ibid.*

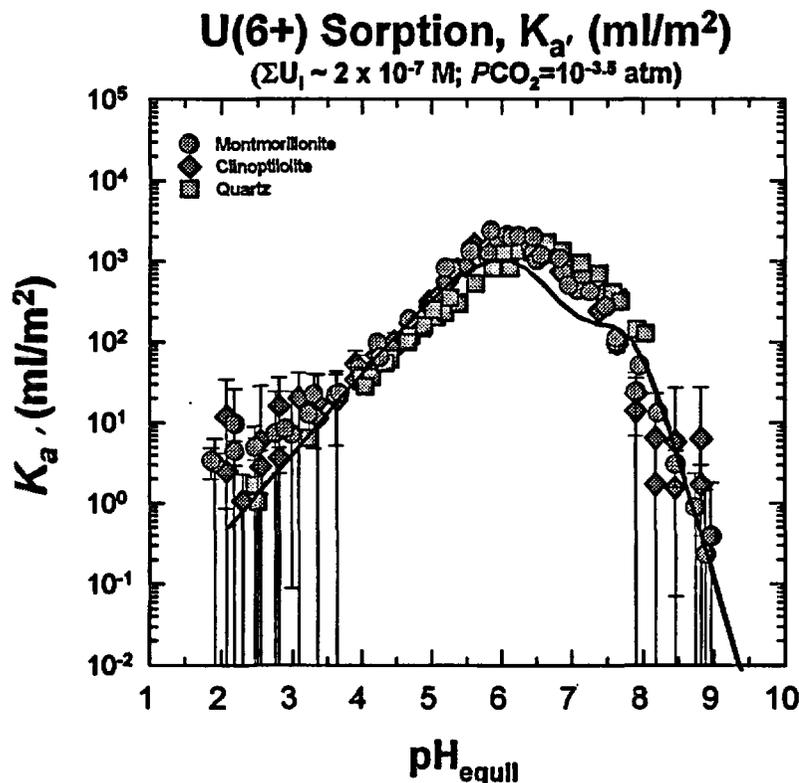


Figure 11-6. U(6+) sorption results shown previously in figure 11-4 and normalized to the effective surface area ( $S_e$ ).  $S_e$  was assumed to be 10 percent of measured  $N_2$ -BET surface area for montmorillonite and clinoptilolite. Note similarity in pH dependence and  $K_a$  for all minerals. The solid line shows the calculated pH dependence of mononuclear aqueous uranyl-hydroxy [ $UO_2(OH)_x^{2-x}$ ] complexes for  $\Sigma U = 2.1 \times 10^{-7}$  M, 0.1 M  $NaNO_3$ ,  $PCO_2 = 10^{-3.5}$  atm (see text for discussion).

complex formation that inhibit the formation of U(6+)-hydroxy complexes suppress U(6+) sorption. The similarity in the pH-dependence of U(6+) sorption on quartz,  $\alpha$ -alumina, clinoptilolite, montmorillonite, amorphous silica, kaolinite, and titanium oxide suggests that U(6+) sorption is not sensitive to the surface charge characteristics of the sorbent as compared to the effect of changing the total number of available sites. The experimental and modeling results demonstrate that changing M/V has little influence on U(6+)  $K_a$ , except at very low M/V ratios. Ionic strength effects are minimal for surface complexation reactions, although these effects can be important if ion exchange is the predominant sorption mechanism and ionic strength effects on the activity of aqueous complexes can indirectly influence sorption behavior.

#### *Np(5+) Sorption*

Neptunium-237 has been identified as a radionuclide of concern with respect to disposal of HLW, especially at longer time frames (~10,000 yr) (Wilson et al., 1994; TRW Environmental Safety Systems, Inc., 1995; Wescott et al., 1995), because of its long half-life ( $2.14 \times 10^6$  yr), suspected high radiotoxicity, and reportedly low sorption characteristics. For example, DOE TSPA calculations (TRW Environmental Safety Systems, Inc., 1995) uses sorption coefficients for Np that range for 0 to 15 ml/g based on expert elicitation, while Rogers and Meijer (1993) report that for Np,  $K_d = 0.65 \pm 0.15$  for devitrified tuff (figure 11-7). Numerous uncertainties remain with respect to the magnitude of Np sorption

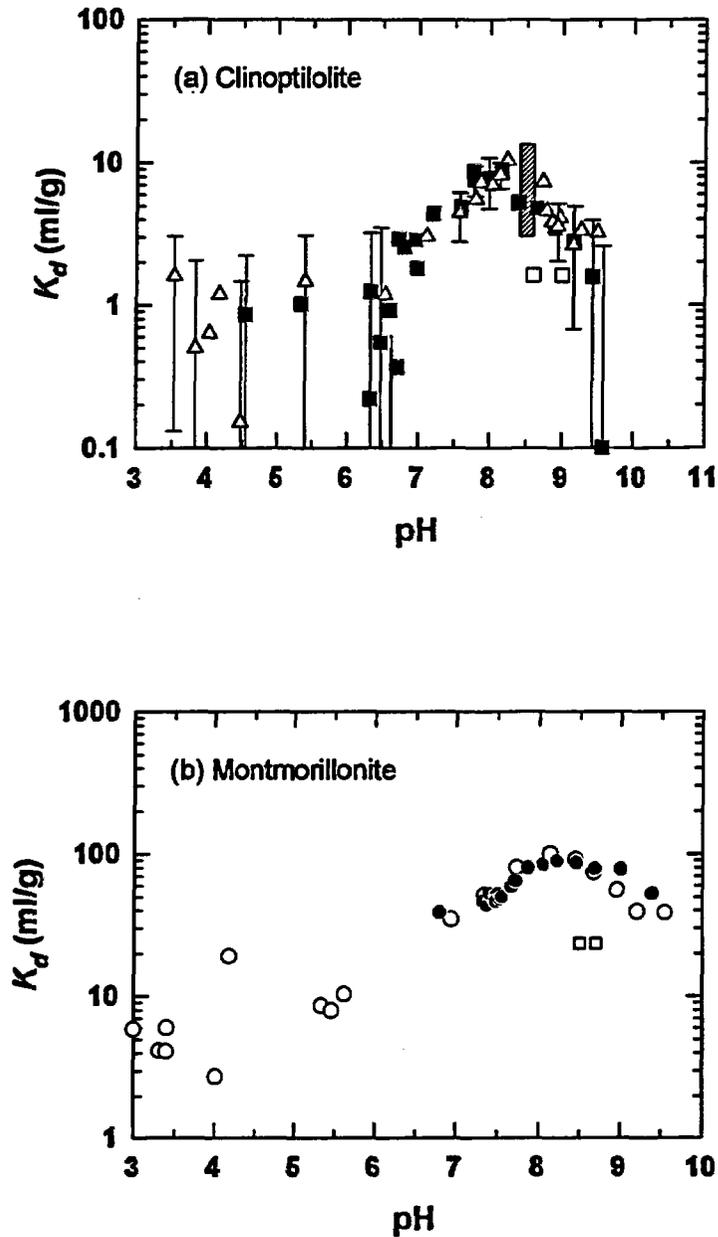


Figure 11-7. Sorption of  $Np(5+)$  on (a) clinoptilolite and (b) montmorillonite under conditions in equilibrium with atmospheric  $PCO_2$ , and with initial  $Np(5+)$  concentration of  $1 \times 10^{-6}$  M. Square and triangle symbols in (a) represent data from experiments with a matrix of 0.1 and 0.01 M  $NaNO_3$ , respectively. Open and closed circles in (b) represent data from forward and reverse experiments, respectively. For comparison, DOE data (Rogers and Meijer, 1993; Triay et al., 1993) are plotted in (a) for  $Np(5+)$  sorption onto clinoptilolite and clinoptilolite-rich tuff (open square symbols and hatched box, respectively), and in (b) for  $Np(5+)$  sorption onto montmorillonite (square symbols).

under the oxidizing conditions and in bicarbonate-rich groundwaters relevant to the proposed HLW repository at YM. For example, reported  $K_d$ s for Np sorption on quartz vary significantly and are dependent on the initial Np concentration, mineral impurities present, and activity of  $\text{CO}_2$  (e.g., Nakayama et al., 1988; Triay et al., 1993).

Using experimental procedures developed for U(6+) sorption, Bertetti et al. (1997)<sup>15</sup> reported the results of experiments conducted at the CNWRA to investigate Np(5+) sorption on quartz, clinoptilolite, montmorillonite, and  $\alpha$ -alumina (figure 11-8). Like U(6+), Np(5+) sorption is similar on different minerals with respect to pH dependence. In the presence of  $\text{CO}_2$  (figure 11-7), Np(5+) sorption reaches a maximum and decreases toward lower or higher pH. The Np(5+) sorption maximum is typically at a higher pH (~8 to 8.5 in the presence of  $\text{CO}_2$ ) and typically much lower (i.e.,  $K_d$  is lower) than for U(6+) sorption.

At a given pH, the Np(5+)  $K_d$  for the different minerals vary by over two orders of magnitude. As with U(6+), when normalized with respect to surface area, the differences between minerals are reduced when Np(5+) sorption is expressed as  $K_a$  (figure 11-9). Differences are also evident between sorption on nonlayered and nonporous minerals quartz and  $\alpha$ -alumina compared to sorption on clinoptilolite and montmorillonite. Similar to U(6+) sorption,  $K_a$  data appear to indicate that quartz and  $\alpha$ -alumina sorb more Np(5+) per unit area than clinoptilolite and montmorillonite (figure 11-9). When normalized to an "effective" surface area as discussed previously, however, Np(5+) sorption expressed as  $K_a$ , on these minerals is essentially equivalent (figure 11-10). The apparent scatter of data points at low pH is a result of larger uncertainties in the experimental data at low sorption values.

Neptunium(5+) aqueous speciation is dominated by  $\text{NpO}_2^+$  at pH below seven in the absence of  $\text{CO}_2$ . However, near pH~7, Np hydrolysis becomes significant and the amount of the Np(5+) hydroxy species  $\text{NpO}_2\text{OH}^0(\text{aq})$  increases with increasing pH throughout the pH range under study. This increase in stability of Np(5+) aqueous hydroxy complex is mimicked by an increase in Np(5+) sorption with increasing pH under  $\text{CO}_2$ -free conditions (figure 11-10). Under atmospheric  $\text{PCO}_2$  conditions, the stability of the neutral hydroxy species reaches a maximum near pH 8.5 and decreases with further increases in pH. Although the neutral hydroxy complex does not become a predominant species in an Np(5+)- $\text{H}_2\text{O}$ - $\text{CO}_2$  solution, a comparison of Np(5+) sorption data and aqueous speciation indicates that the pH dependence of the stability of the  $\text{NpO}_2\text{OH}^0(\text{aq})$  species is distinctly similar to the pH dependence of Np(5+) (Bertetti et al., 1997).<sup>16</sup>

The pH dependent trends in observed U(6+) and Np(5+) sorption behavior are similar for many common minerals, including clinoptilolite, quartz,  $\alpha$ -alumina, montmorillonite, iron oxyhydroxide, and kaolinite even though these minerals have different mineralogic and surface charge characteristics. This similarity suggests that actinide sorption is not sensitive to the surface charge properties of the sorbent as compared to the effect of changes in the surface area or number of sorption sites. On the other hand, actinide sorption is strongly dependent on pH. For conditions where solutions are at low  $\text{PCO}_2$  or  $\text{CO}_2$ -free conditions, sorption increases with increasing pH over the entire pH range studied. For experiments

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<sup>15</sup>Bertetti, F.P., R.T. Pabalan, and M.G. Almendarez. 1997. Studies of neptunium(V) sorption on quartz, clinoptilolite, montmorillonite, and  $\alpha$ -alumina. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

<sup>16</sup>*Ibid.*

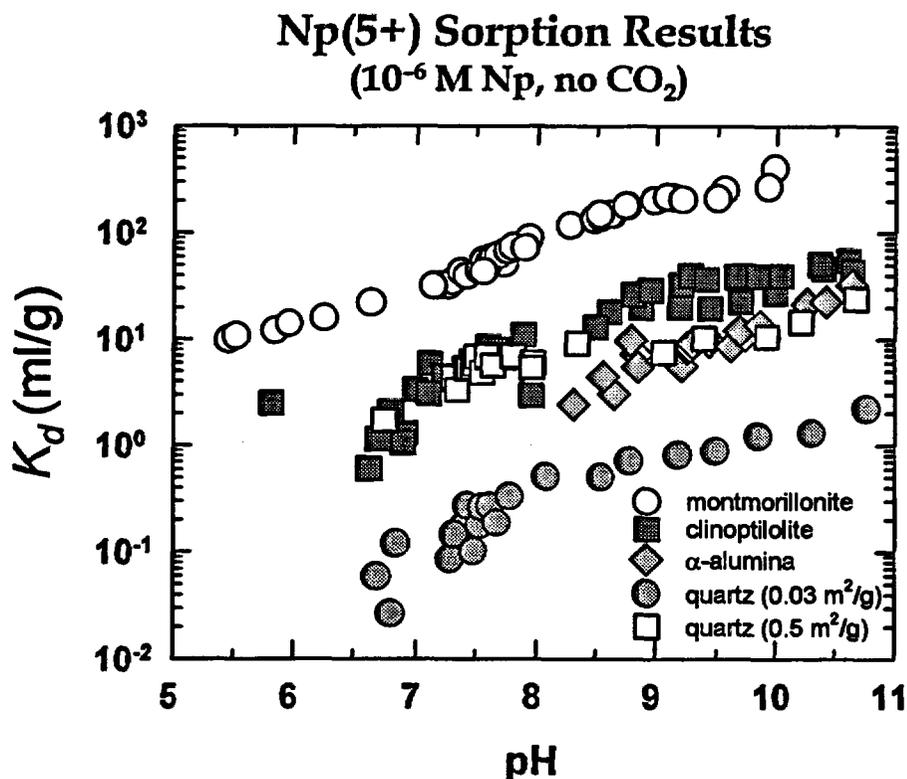


Figure 11-8. CNWRA experimental results for Np(5+) sorption on montmorillonite, clinoptilolite,  $\alpha$ -alumina, and quartz expressed as  $K_d$

with solutions in equilibrium with atmospheric  $\text{PCO}_2$ , a distinct sorption maximum is observed for all minerals. The data also suggest that the magnitude of actinide sorption is the same for different minerals if normalized to the number of available sites using an "effective" surface area.

Observations of data from Bertetti et al. (1997)<sup>17</sup> and Pabalan et al. (1997)<sup>18</sup> indicate a common pattern for actinide sorption that is related to the formation of hydroxy complexes in solution. This pattern suggests that modeling approaches that are capable of accounting for changes in solution chemistry (e.g., surface complexation models) are required for successful description and prediction of sorption of U, Np and other actinides on mineral surfaces over wide ranges of geochemical conditions. The methodology developed here provides a basis for evaluating conceptual models, sorption coefficient bounding limits, and probability distribution functions used by DOE in radionuclide transport calculations.

<sup>17</sup>*Ibid.*

<sup>18</sup>Pabalan, R.T., D.R. Turner, F.P. Bertetti, and J.D. Prikryl. 1997. Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters. *Metals in Geomedia: Sorption Processes and Model Applications*. E. Jenne, ed. New York, NY: Academic Press. In Press.

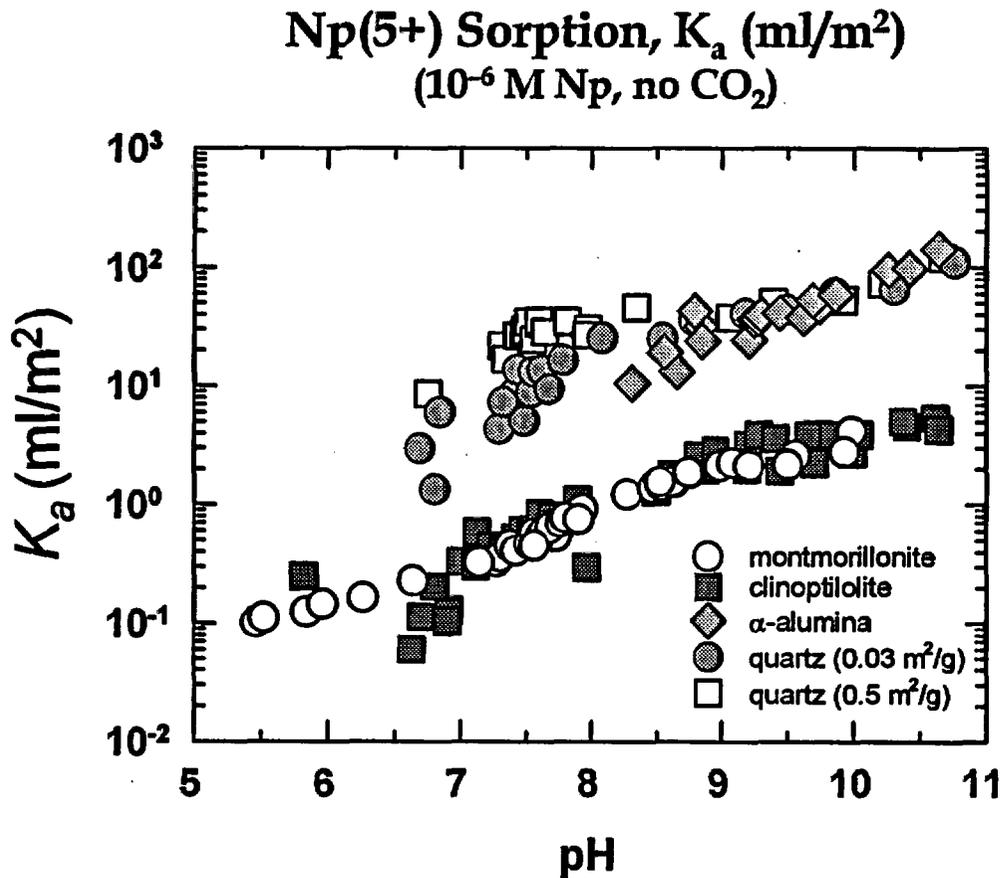


Figure 11-9. Np(5+) sorption results shown previously in figure 11-7, and normalized to the measured N<sub>2</sub>-BET surface area ( $S_a$ ). Note similarity in Np(5+) sorption on quartz and  $\alpha$ -alumina and in Np(5+) sorption on clinoptilolite and montmorillonite.

#### 11.3.4 Evaluating Saturated Zone Mixing Using Existing Hydrochemical Data

A key assumption in the DOE WCIS (Hypothesis 12) with regard to radionuclide transport is the dilution of radionuclide contaminated water upon mixing with the regional groundwater flow system. To address issues related to mixing at the YM site, geochemical information such as water chemistry and mineralogy can be used to provide constraining values for dilution factors used in PA. To allow for effective use, analysis, and interpretation, these data should be evaluated, compiled, and logged in a GIS database that can be related to the geologic, hydrologic, and geographic framework of the YM area. This approach is a necessary part of developing an understanding of the regional groundwater flow system at YM. The effort also serves as a baseline to extend both conceptual models of the current system and predictions of the future performance of the proposed repository.

Under the Radionuclide Transport KTI, the Structural and Seismicity KTI, and the Igneous Activity KTI, geologic and hydrologic GIS coverages including surface geology, structure, and hydrostratigraphy are being developed at the CNWRA for YM and the surrounding regions using the

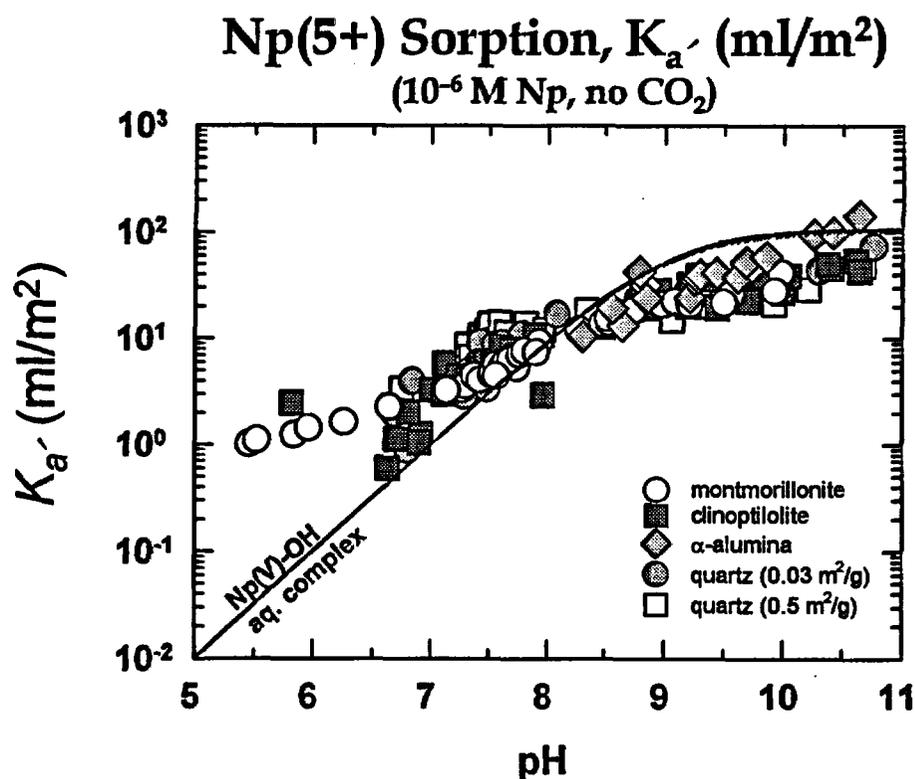


Figure 11-10. Np(5+) sorption results shown previously in figure 11-7 and normalized to the effective surface area ( $S_a'$ ).  $S_a'$  was assumed to be 10 percent of measured N<sub>2</sub>-BET surface area for montmorillonite and clinoptilolite. Note similarity in pH dependence and  $K_a'$  for all minerals. The solid line shows the calculated pH dependence of aqueous neptunyl-hydroxy (NpO<sub>2</sub>OH<sup>0</sup>) complex for  $\Sigma\text{Np}=1\times 10^{-6}$  M, 0.1 m NaNO<sub>3</sub>, no CO<sub>2</sub> (see text for discussion).

Arc/Info (Version 6.1) software package. A similar hydrochemical database would augment and benefit from these coverages and enable aspects of these databases to be incorporated in conceptual models of hydrologic flow. In this manner, the geographic location of specific samples can be traced and associated data supplied. The PC-based GIS software package ArcView (Version 2.0b) provides a convenient means of displaying and combining different Arc/Info coverages and creating different coverages by importing spatially distributed hydrochemical and geochemical data. The display and analytical capabilities associated with the ArcView software provides a means of handling large datasets, with identification of hydrochemical signatures for different aquifers and trend analyses providing a strong basis for bounding conceptual models of the regional hydrologic flow system at YM. The ability to consider hydrochemical information in a geologic, structural, and hydrostratigraphic framework will allow more effective assessment of complex and interactive systems and processes.

Baseline geology and structure are essential in developing conceptual models of the hydrologic flow system in the YM region. Digital Arc/Info coverages were developed by the U.S. Geological Survey (USGS) at an original scale of 1:250,000 (D'Agnesse et al., 1995). In greater detail, Frizzell and Shulters (1990) compiled a map of the surface geology at the Nevada Test Site (NTS) at an original scale of

1:100,000. This map has been digitized in Arc/Info and converted to ArcView GIS shapefile format at the CNWRA.

Based on the hydrostratigraphy, Winograd and Thordarson (1975) identified six aquifers and five aquitards within the YM region. From the bottom of the hydrostratigraphic section these hydrogeologic units are

- Lower clastic aquitard of Precambrian to Lower Cambrian quartzite, shale, and siltstone
- Lower carbonate aquifer of middle Cambrian to Devonian limestone and dolomite
- Upper clastic aquitard of Devonian to Mississippian argillite and quartzite
- Upper carbonate aquifer of Pennsylvanian to Permian limestone
- Local aquitards of Cretaceous granitic stocks, dikes and sills
- Tuff aquitard of Oligocene to middle Miocene interbedded, nonwelded to welded tuffs
- Lava-flow aquitard of upper Miocene lava flow and interflow breccia
- Bedded tuff aquifer of upper Miocene ash-fall and reworked tuff
- Welded tuff aquifer of upper Miocene to middle Pliocene nonwelded to densely welded tuffs
- Lava flow aquifer composed of upper Pliocene basaltic and rhyolitic flows
- Valley fill aquifer of upper Pliocene to Holocene alluvial, fluvial, and lacustrine deposits.

Winograd and Thordarson (1975) note that the surface and subsurface extent of the principal hydrogeologic units vary from basin to basin due to the complex structural and erosional history of the rocks. According to Winograd and Thordarson (1975), the interbasin flow of groundwater is not significantly influenced by the topographic boundaries of the individual basins but rather by the presence and relative positions of the lower carbonate aquifer and the upper and lower clastic aquitards. Figure 11-11 divides the geology of Frizzell and Shulters (1990) into the hydrostratigraphic units of Winograd and Thordarson (1975). For clarity, and due to the different nomenclature adopted by Frizzell and Shulters (1990), the Tertiary units have been divided here into a single aquifer and a single aquitard.

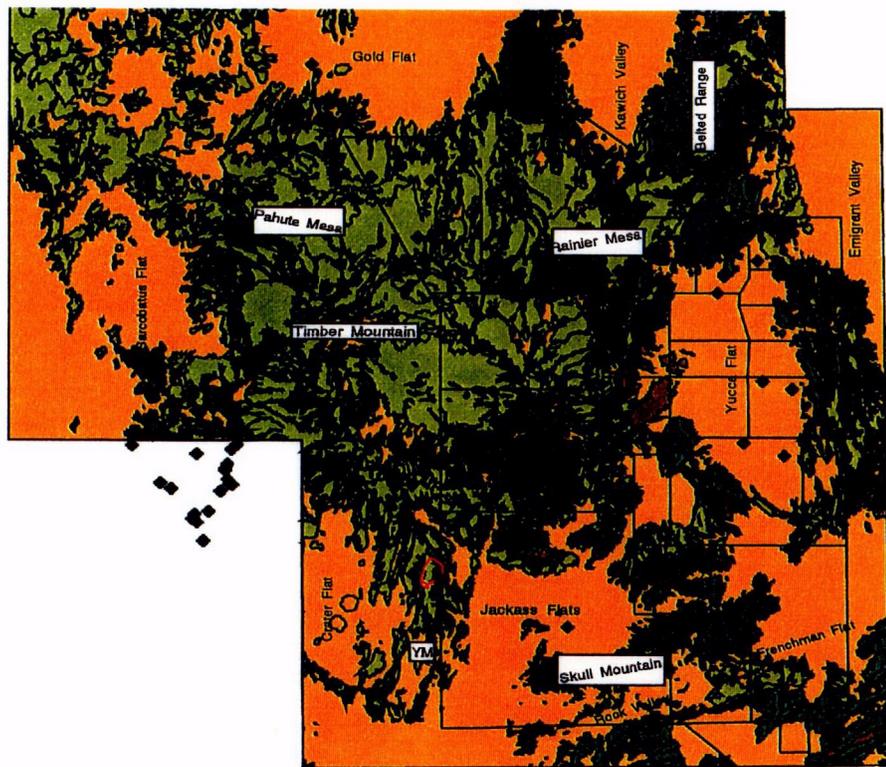
To use hydrochemistry as a means to constrain fluid flow and mixing, it is necessary to develop chemical fingerprints of water in different aquifers. Winograd and Thordarson (1975) also identified five distinct hydrochemical facies in the regional groundwater system:

- Ca-Mg-HCO<sub>3</sub> facies typical of waters discharged from perched springs and regional springs in the carbonate units
- Na-K-HCO<sub>3</sub> facies typical of waters in the tuff aquifer
- Ca-Mg-Na-HCO<sub>3</sub> facies typical of waters in east-central Amargosa Desert and Ash Meadows
- Na-SO<sub>4</sub>-HCO<sub>3</sub> sodium sulfate bicarbonate facies typical of waters discharged at Furnace Creek Wash and Nevares Springs in Death Valley
- a playa facies high in Total Dissolved Solids (TDS), typical of waters discharged by evapotranspiration at Franklin Lake Playa (Alkali Flat).

Waters sampled from the lower carbonate aquifer at the NTS are of the calcium magnesium sodium bicarbonate type which lead Winograd and Thordarson (1975) to infer downward flow of water from the tuffaceous units into the Paleozoic carbonate aquifer.

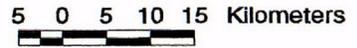
The water facies of Winograd and Thordarson (1975) are based on a relatively small dataset of hydrochemical analyses. An additional, more comprehensive source of water chemistry data is found in the USGS report of Perfect et al. (1995). This report includes spreadsheet files with major and minor

# Map of the Aquifers and Aquitards in the Nevada Test Site in Southern Nevada



- Legend**
- YM Yucca Mountain
  - ◆ Well and Spring Locations
  - ▭ Proposed Repository Outline
  - ▭ Nevada Test Site Boundary

- Valley Fill Aquifer
- Welded Tuff Aquifer
- Tuff Aquitard
- Upper Carbonate Aquifer
- Upper Clastic Aquitard
- Lower Carbonate Aquifer
- Lower Clastic Aquitard



Frizzell and Shulters (1990)

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Figure 11-11. Geology coverage generated using ArcView (Version 2.0b) based on the geologic map of Frizzell and Shulters (1990) (original scale of 1:100,000). The units of Frizzell and Shulters (1990) were assigned to the hydrostratigraphic framework of Winograd and Thordarson (1975) and an additional coverage has been developed that includes the sample locations for charge-balanced water chemistry analyses from Perfect et al. (1995).

Q-11

element analyses compiled over several decades for the region surrounding YM. One file contains the raw data for more than 4,700 wells and springs from USGS and the DOE reports and the USGS National Water Information Service database. A second file included with the report contains data that have been edited to remove duplicate entries, make the data chemically consistent, and calculate whether or note the reported analysis is charge balanced. The editing philosophy used by Perfect et al. (1995) is described in the report. Based on this editing, the number of charged balanced analyses reduces to about 1,800 although this reduced database still includes multiple analyses taken over an extended time at a single sampling point. Figure 11-11 shows the locations of those wells and springs where balanced hydrochemical analyses are available. Some of the hydrochemical data of Perfect et al. (1995) lie outside the current geologic coverage as shown in figure 11-11, particularly in Oasis and Amargosa Valleys. Additional geologic coverages (e.g., D'Agnese et al., 1995) are becoming available, however, to expand the area covered by CNWRA GIS database. These analyses can be used with a geochemical equilibrium code such as MINTEQA2 (Allison et al., 1991) to calculate water saturation with respect to different minerals such as calcite and gypsum. These saturation levels can provide an additional signature to identify different aquifer waters, and can also provide some information regarding groundwater evolution along flow paths.

Using only a GIS database cannot limit all types of uncertainties in PA modeling, such as uncertainties in mathematical models. A GIS database for hydrochemical information can, however, provide the best means for developing conceptual models of fluid flow and mixing, and one of the only means of calibrating, baselining, and validating a numerical model. The hydrochemical information can be used in either a qualitative sense such as defining regional or local trends in groundwater flow or quantitatively in geochemical modeling (Murphy and Pabalan, 1994). Relevant regional scale groundwater patterns can be analyzed by first using hydrochemical facies information and tracers to delineate plausible flow paths, and then using conservative tracers and isotopic data to constrain mixing between end-member solutions. The ability to tie the data to a geographic and geologic framework specific to the YM site is an important aspect of making the most out of the available data. As more data become available, it may also be possible to develop three-dimensional (3D) representations of the information, further increasing the value of the database.

### 11.3.5 Development of Preferred Pathway Model

Prior to the discovery of recent water at depth in the unsaturated zone at YM [e.g., Fabryka-Martin et al. (1996) using  $^{36}\text{Cl}$ , Yang et al. (1996) using tritium, and  $^{14}\text{C}$ ], it was generally held that due to the high matrix potential, any water in fractures would be drawn quickly into the matrix. The preferred conceptual model (TRW Environmental Safety Systems, Inc., 1995) had water flowing through the matrix except in those rare situations where high infiltration rates caused saturated conditions. Having accepted the concept of matrix flow as predominant flow mechanism, it was reasonable to then consider chemical interactions between the aqueous species and the solid through which the solution flowed. Batch sorption experiments were used to simulate the interaction between dissolved radionuclides and the solid matrix. The sorption coefficients from those experiments were converted to retardation factors used in PA models simulating the waste isolation characteristics of a geologic repository (e.g., TRW Environmental Safety Systems, Inc., 1995). If transport of radionuclides is not predominantly through the matrix, then a  $K_d$  approach to retardation based on matrix sorption only is not conservative.

The latest DOE total system performance analysis (TRW Environmental Safety Systems, Inc., 1995) used a Monte Carlo approach in which  $K_d$ s were selected from distributions generated by expert elicitation (Wilson et al., 1994). In addition to this abstraction, the TSPA modeled individual flow paths

composed of part matrix and part fracture. The proportion of the path in each regime was based on a distribution, again generated by expert elicitation (TRW Environmental Safety Systems, Inc., 1995; Chapter 7). The level of abstraction in the TSPA-95 made the comparison to site-specific characteristics difficult.

With the discovery of bomb-pulse water at the proposed repository horizon, investigators at LANL (Los Alamos National Laboratory) have begun sensitivity analyses to determine if alternative conceptual models or adjustments to parameter ranges using existing conceptual models are necessary to explain recent observations (Fabryka-Martin et al., 1996). In their analyses, LANL investigators chose to look at the effects of varying infiltration, fracture density, fracture aperture, and van Genuchten parameters through the nonwelded Paintbrush tuff that overlies the Topopah Spring tuff. They concluded it was not necessary to abandon the existing conceptual model, but found that the lower infiltration rates were inconsistent with the bomb-pulse observations. The code used in the analysis was FEHM, a dual continuum model, that simulated one-dimensional steady-state conditions.

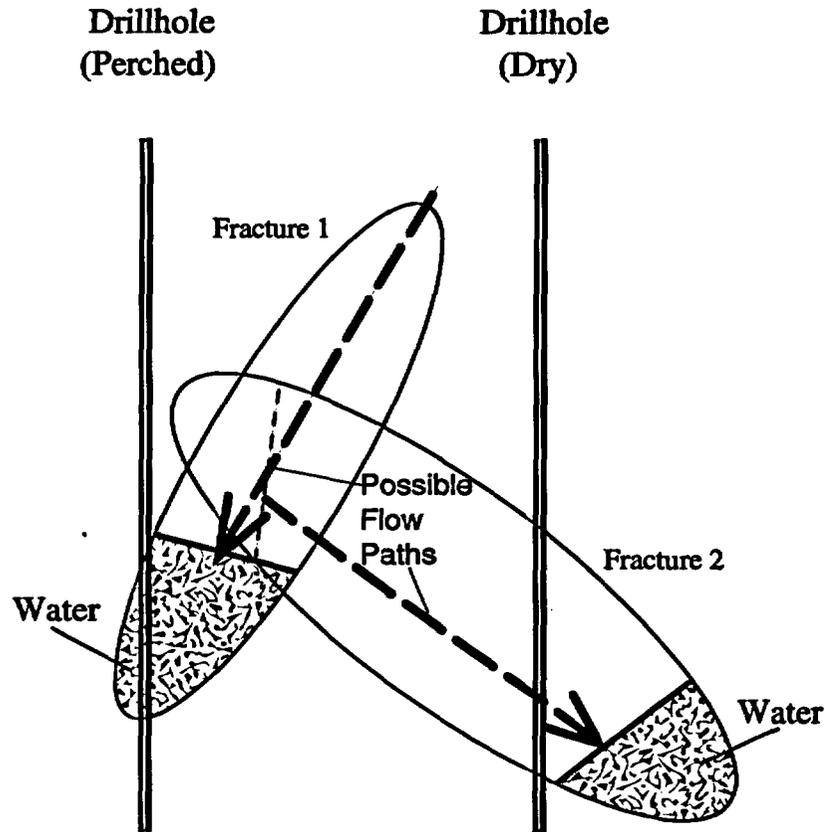
To test whether the current conceptual model of radionuclide transport proposed by the DOE is conservative, the Radionuclide Transport KTI team is developing an alternative conceptual model of flow and transport in the unsaturated zone. Both models will be evaluated using site-specific data to determine if alternative conceptualizations supported by the same site data could result in significant differences in radionuclide mobility.

#### *Alternative Conceptual Model*

The Topopah Spring tuff was chosen as the repository horizon because of its well-drained character. It is proposed that portions of the flow system in the unsaturated zone at YM, like the Topopah Spring, can be approximated by a 3D network of fractures represented as intersecting disks of various sizes and orientations. Previous studies (Long et al., 1985; Dverstorp et al., 1992) have modeled flow in these features when they are totally filled with water or under unsaturated conditions (Rasmussen, 1987). In the current model, the fractures are partially filled with water analogous to a plumbing system that contains traps.

The rate of flow in fractures is considered to be so much greater than that in the matrix, as a first approximation, flow in the matrix can be disregarded. Geochemical evidence of fluid collected from the unsaturated zone and from perched water bodies presented by Yang et al. (1996) is consistent with a model where little interaction occurs between the fractures and matrix. The fact that perched water exists at YM is further evidence for relatively fast and substantial flow in fractures and relatively slow imbibition into the matrix (Striffler et al., 1996). Otherwise, drill holes would not fill with water during the time-scale of observation (months to years). Evidence suggests there are several examples of perched water or at least wet portions of the drillholes in and around YM (Striffler et al., 1996).

The flow of water in this system is envisioned to be intermittent in response to the sporadic rainfall events that occur in the desert. The water flows as rivulets, similar to flow on a smooth surface such as glass, down a single disk-shaped fracture and fills the bottom of the fracture to the level where the fracture intersects another disk-shaped fracture. At this point water flows into the second fracture trickling down to fill the bottom of it (figure 11-12). This process continues to the third, fourth, and more fractures, until the amount of water added to the system equals the capacity of these "traps" first filled to hold water.



**Figure 11-12. Schematic diagram of a conceptual model for flow through intersecting fracture planes**

This flow system can also be envisioned as a series of buckets of various sizes. Pouring water in the first bucket fills it to its capacity at which point water spills over into the next and so on. To make the model more realistic, the buckets are "leaky" allowing the water to move into the matrix (figure 11-13). Consequently, in the time between rainfall events, the buckets lose water to the matrix at different rates depending on the hydraulic conductivity of the matrix and the head of each bucket. (Note that Darcy's law applies only to the individual fractures. In the series of fractures, the head in one fracture does not influence the head in the next.) The longer the time between rainfall events, the greater the capacity of the buckets to hold new water from the next event.

Each bucket is considered a reaction vessel, where processes such as sorption/desorption, precipitation/dissolution, and dilution occur. By considering the surface area contacted by the water, the length of time the water is in contact with the fracture surface and the hydraulic conductivity of the matrix, it is possible to estimate the rock to water ratio for each fracture with its surrounding matrix. Geochemical modeling, which requires masses of reactants to be input, is particularly amenable to this conceptual model.

Besides duration between rainfall events, the amount of rain in each event can affect the distribution of groundwaters of various ages. For example, the intersection of two disks may be toward the top of the disk first to fill. If sometime in the distant past a large rainfall event occurred, water could have filled the first disk and flowed into the second. Subsequent rainfall events might not have been so

### "Leaky Bucket" Model

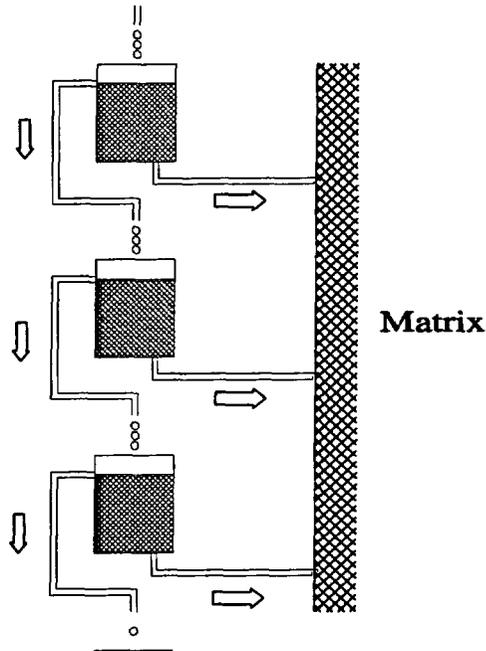


Figure 11-13. Schematic diagram of conceptual model of fracture controlled flow system with diffusion of water into the matrix.

extreme, in which case, new water would not be added to the second disk. As a result, the ages of water in the fractured system need not be a function of depth. There are examples of reversals of groundwater ages with depth at YM. This is interpreted to be lateral flow, possibly via fractures (Liu et al., 1995).

By generating various 3D fracture systems with different characterization parameters and then determining the effects on flow and transport, one may be able to identify those parameters most important in site characterization activities for modeling the repository performance. The types of fracture parameters necessary to model repository performance could include parameters such as fracture intersection length, intersection orientation, difference in height between fracture intersection and bottom of fracture, etc. Likewise, the effects on flow and transport are to be determined, but they could include possible age distribution of water in fracture systems containing traps or perched water, channeling in fracture systems resulting in more direct pathways to the groundwater table, and rock to water ratios important to geochemical modeling.

It should be noted that these simulated fracture systems can be compared with site data. For example, Sweetkind et al. (1996)<sup>19</sup> describe the fracture character of the Paintbrush Tuff nonwelded

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<sup>19</sup>Sweetkind, D.S., E.R. Verbeek, J.K. Geslin, and T.C. Moyer. 1996. Fracture Character of the Paintbrush Tuff Nonwelded Hydrologic Unit, Yucca Mountain, Nevada (Draft Report).

hydrologic unit. This study provides information on fracture density, orientation, length, intersection, and aperture.

Another important aspect that can be addressed when one considers the flow system, not as an equivalent porous medium, but as a system of pipes, is the flux through the unsaturated zone. If it is assumed that fractures are necessary for perched water, then the intersection of the wet portion of a fracture or fractures can be assumed to constitute a perched water body, and one can determine the flux into the fracture by assuming as a first approximation flux into the matrix equals flux into the fracture. By determining the hydraulic conductivity of the matrix in the lab, the head of water at the fracture borehole intersection, and the volume of water in the fracture from a pump test, one can determine the flux into the matrix. Results of this calculation could then be considered in light of age determinations of the groundwater in the fracture/perched zone. Inconsistency in the flux calculation and age could be used to adjust assumptions (e.g., fracture flux  $\neq$  matrix flux or when a trap is flushed, new water pushes the old water to the next trap).

Past arguments against discrete fracture models stated they were too computationally intensive for ready inclusion in a system code PA. However, the system code picks numerous pathways, models the flow and transport along those pathways, and then adds the contributions from all (TRW Environmental Safety Systems, Inc., 1995). This is not different from the modeling envisioned using the 3D disk-shaped fracture model proposed here. The advantage of this model is that it does not require steady-state conditions and is not computationally intensive. Furthermore, fracture properties presented as distributions for each rock unit are being collected at the site and are amenable to inclusion in Monte Carlo simulations. Finally, the geochemistry of the system, where water sits in traps for various periods of time, is well described by batch tests in the lab.

### 11.3.6 Conclusions

The technical objectives of the Radionuclide Transport KTI have been designed to address DOE WCIS Hypotheses 10, 11, and 12. The conceptual model necessary to describe uranium transport at Nopal I requires large, throughgoing fractures to control transport over large spatial scales. This conceptualization is consistent with the importance of fractures in providing fast flow and transport paths for relatively young waters, as indicated by YM-specific  $^{36}\text{Cl}/\text{Cl}$  ratios. In addition, a hydrologic conceptual model has been developed that attempts to take into account the interactions between fractures and provide a framework for future geochemical modeling. Evaluation of conceptual models of transport used by DOE is a critical part of testing DOE WCIS hypotheses on radionuclide transport (Hypothesis 10) and dilution (Hypothesis 11). DOE and NRC PA transport calculations should continue to be designed to address the importance of fracture transport. Work undertaken as part of the Radionuclide Transport KTI has also identified similarities in Np and U sorption behavior between a number of minerals (quartz, montmorillonite, clinoptilolite) that are abundant at YM. When sorption coefficients are normalized to effective mineral surface area, sorption behavior is demonstrated to be strongly affected by changes in pH and  $\text{PCO}_2$ , but relatively insensitive to mineral substrate and changes in solid-mass to solution-volume ratios. This suggests the possibility of developing sorption response curves for PA that are a function of key geochemical parameters (e.g., pH and  $\text{PCO}_2$ ) and provide support for chemically reasonable limits on sorption coefficients. The results from the sorption experiments will be used to assess sorption coefficients for U and Np used by DOE in PA calculations. Work conducted under the Radionuclide Transport KTI has also begun the process of assembling existing hydrochemical data in a geographic framework to constrain flowpaths and mixing in the saturated zone (DOE WCIS Hypothesis 12).

## 11.4 ASSESSMENT OF PROGRESS TOWARD MEETING OBJECTIVES

The four subissues identified in the Implementation Plan for the Radionuclide Transport KTI develop broad areas covering data and analysis needs to address the effects of radionuclide transport on overall repository performance. The research undertaken during FY96 moved toward addressing several of these subissues.

- Review of current DOE research in  $^{36}\text{Cl}$  has provided a basis for critical evaluation of conceptual models of groundwater flow at YM that may be used by the DOE in future PA calculations and viability assessments (DOE WCIS Hypothesis 10).
- Transport studies conducted on samples from the Nopal I U deposit, Peña Blanca district, Mexico, have provided constraints on hydrologic and geochemical controls on radionuclide transport under hydrologically unsaturated conditions in fractured tuff. U transport at Nopal I is controlled by oxidizing hydrochemical conditions and radionuclide mobility at YM may similarly depend upon transient hydrological conditions. Research also identified the importance of considering radionuclide transport through fractures in unsaturated tuffs. This is consistent with a growing consensus that fractures will provide fast pathways for hydrologic flow and transport through the unsaturated zone at YM. Incorporation of aqueous U into fracture minerals at Nopal I suggests that retardation is not a simple reversible process. This work has helped establish a basis from which to critically evaluate conceptual models that may be used by DOE in future PA calculations and viability assessments (DOE WCIS Hypothesis 10).
- NRC/CNWRA research focused on identifying the sensitivity of radionuclide sorption ( $K_d$ ) to different geochemical parameters based on the CNWRA experimental results and sorption results reported in the available literature. The results of this research are simplified approaches to data interpretation and sorption modeling for U and Np. Establishing a methodology to account for the effects of key geochemical parameters on radionuclide sorption coefficients is an important means for evaluating conceptual models, bounding limits, and probability distribution functions used by DOE in radionuclide transport calculations (DOE WCIS Hypothesis 10).
- Available hydrochemical data are being combined into a GIS coverage and tied to coverages of geology and structure. This will enable hydrochemical information to provide boundaries to flow and the potential for dilution within the YM system. The hydrochemical data will also provide a potential means for calculating sorption as a function of water chemistry and groundwater evolution through rock-water interaction along the flow paths. Accounts have been established with the DOE Automated Technical Data Tracking System that has been searched for additional site-specific data related to retardation. This has provided an important step in using existing data to constrain regional groundwater flow and saturated zone mixing (DOE WCIS Hypothesis 12).

Subissues pertaining to the sensitivity of overall performance of the repository to variations in parameters controlling radionuclide transport and the identification of radionuclides requiring some form of retardation to meet performance requirements were not addressed during this FY. Activities designed to address these issues are planned for FY97 under the TSPA and Integration KTI.

## 11.5 INTEGRATION WITH OTHER KEY TECHNICAL ISSUES

The Radionuclide Transport KTI has relied on GIS information provided by the KTIs on Structural Deformation and Seismicity and Igneous Activity to develop hydrochemical coverages for saturated zone dilution analysis. Information on the regional flow system from the KTI on Unsaturated and Saturated Flow Under Isothermal Conditions was used to identify general flow trends. Sensitivity analyses using sorption models and conceptual transport models will be used to support a sorption module for the TSPA and Integration KTI. The Radionuclide Transport KTI will not be supported by CNWRA for FY97, and therefore no changes in inputs or outputs have been identified.

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