Study Plan for
Study 8.3.1.2.2.5

Diffusion Tests in the Exploratory Studies Facility

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Revision 0

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Office of Civilian Radioactive Waste Management
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Prepared by
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YUCCA MOUNTAIN PROJECT

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DIFFUSION TESTS IN THE EXPLORATORY STUDIES FACILITY

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ABSTRACT

The diffusion tests in the Exploratory Studies Facility (ESF) will determine *in situ* the extent to which nonsorbing tracers diffuse into the water-filled pores of the Yucca Mountain tuffs that will be penetrated by the ESF.

Effective diffusion coefficients for nonsorbing ions in aqueous solutions will be measured in this study under *in situ* conditions. The data from this study will help in computing accurately the retardation resulting from diffusion of important long-lived radioactive waste species, such as ^{99}Tc and ^{129}I. In addition to expanding the data base of diffusion coefficients applicable to Yucca Mountain tuff units, the results will also be used to evaluate the reliability of calculations by the diffusive model that forms part of the solute-transport code TRACRN being used to estimate the potential for radionuclide migration at Yucca Mountain.

This study consists of a single activity, which is entitled "Diffusion Tests in the ESF." However, the success of the study requires prototype testing of all non-standard techniques proposed for use in the ESF diffusion tests.

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STUDY PLAN FOR DIFFUSION TESTS IN THE EXPLORATORY STUDIES FACILITY

1.0 PURPOSE AND OBJECTIVES OF STUDY

1.1 Objectives of the Study

1.1.1 Overall Purpose

Investigators at Los Alamos National Laboratory (LANL) are conducting studies as part of the Yucca Mountain Project to evaluate the suitability of Yucca Mountain as the site for a high-level nuclear waste repository and the ability of the mined geologic-disposal system to isolate the waste in compliance with regulatory requirements. This study plan describes LANL plans to collect data to be used to predict rates of solute transport via diffusion through unsaturated rock. The plan involves *in situ* measurements of the effective diffusion coefficients for nonsorbing tracers in Yucca Mountain tuff units in the ESF. Figure 1 illustrates the location of this study plan within the Site Characterization Plan (SCP) Geohydrology Program (8.3.1.2) and its subprogram, the Site Unsaturated-Zone Hydrology Investigation (8.3.1.2.2). The diffusion study is one of nine studies planned to characterize the unsaturated zone beneath Yucca Mountain.

The numbers (for example, 8.3.1.2.2) used throughout this plan refer to specific sections of the YMP SCP. The SCP (DOE, 1988) describes the technical rationale of the overall site-characterization program and provides general descriptions of the activities described in detail in this and other study plans.

The diffusion study was developed in response to the recognition that diffusion into the rock matrix may significantly reduce the rate of transport of radionuclides from the repository through the unsaturated zone to the underlying water table or to the surface. The data from this study will help in computing limits for the retardation resulting from diffusion of chemical waste species such as the long-lived radioactive species, ^{99}Tc and ^{129}I. In conjunction with laboratory measurements of diffusion in tuff samples, these data will help define the statistical basis for the diffusion parameters used in performance assessment modeling. The laboratory measurements will be obtained according to the study plan for Diffusion (8.3.1.3.6.2).

1.1.2 Scientific Rationale and Use of Results

If radionuclides are released into the unsaturated zone from the repository, they may be transported toward the accessible environment by groundwater flow in fracture networks in the rock matrix. In addition to fractures, the rock matrix also contains micropores filled with stagnant water; water and solute transport rates in this pore system are probably insignificant relative to fracture transport rates resulting from the lower hydraulic conductivity and greater likelihood of dead-end pores. Diffusion is the process whereby solutes move in the direction of their concentration gradient. This process can act as a retarding and diluting mechanism by removing waste species from the flowing groundwater in fractures, where their initial concentrations are relatively high, into the stagnant water of the matrix pores, where their concentrations are initially zero (Neretnieks, 1980; Skagius and Neretnieks, 1986).

In the absence of advective transport, the rate at which a solute will diffuse from one location to another is related to the concentration gradient by a constant of

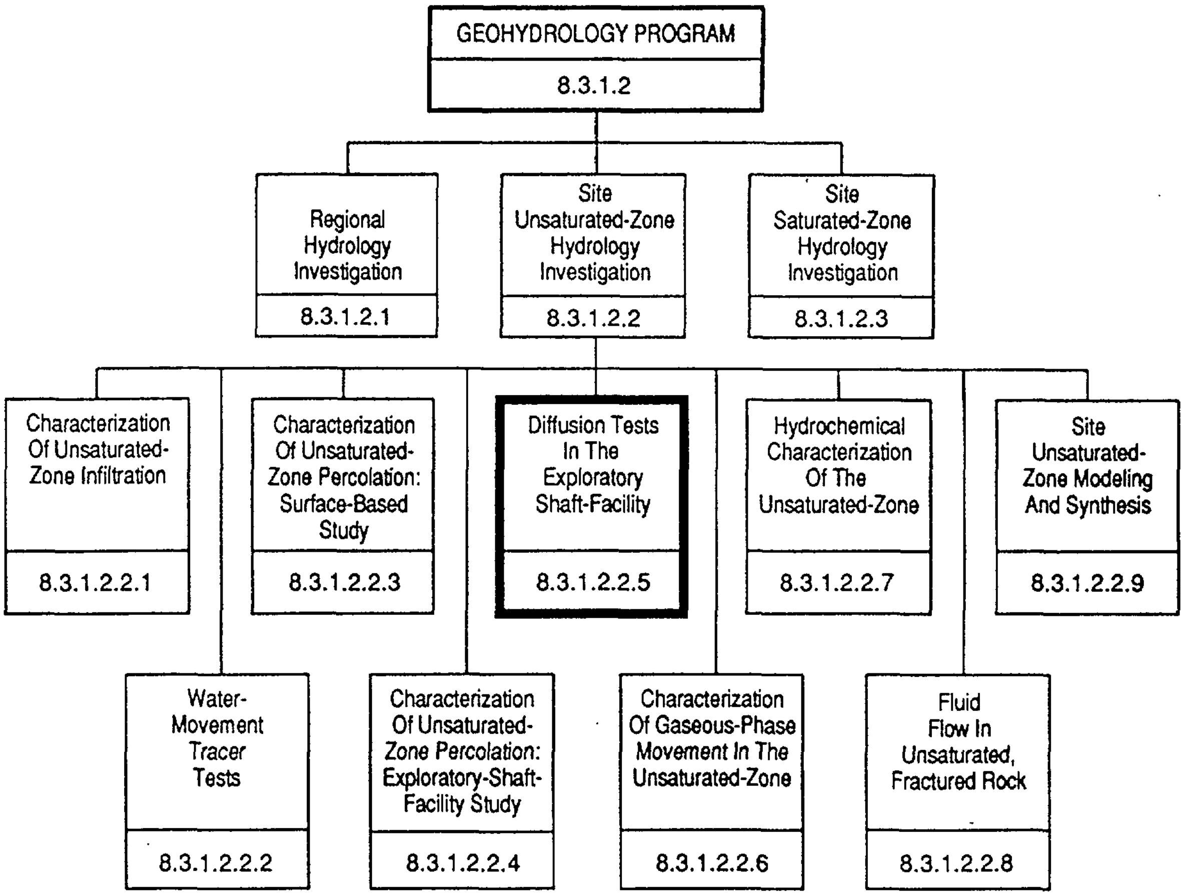

Figure 1. Diagram Showing the Location of the Study Plan Within the Unsaturated-Zone Investigation and Organization of the Geohydrologic Characterization Program.

proportionality known as the diffusion coefficient. Thus, the extent to which diffusion may retard solute transport is a function of the value of this constant for the solute in the rock of interest. Diffusion coefficients for solutes in aqueous solutions are well-known (for example, Robinson and Stokes, 1959). However, apparent or effective diffusion coefficients for the same solutes in porous media are lower by factors of 2 to 100 or more because the solute ions or molecules must follow longer paths of diffusion (Freeze and Cherry, 1979; Birdsell et al., 1988). The value of the effective diffusion coefficient is determined by the saturation of the medium, the tortuosity of the diffusion path, the porosity of the medium, the shape of the pores through which the solute diffuses, and sorption effects. Because some of these factors are difficult to quantify and may be quite variable in a rock, *in situ* measurements of diffusion are useful to the accurate modeling of aqueous transport and retardation of radionuclides in the unsaturated zone at Yucca Mountain.

In addition to expanding the data base of effective diffusion coefficients applicable to Yucca Mountain tuff units, another use of the results will be to evaluate the reliability of modeling calculations. The TRACRN code is being used to help design the *in situ* diffusion tests, and the data that result from the *in situ* tests will help test the diffusive model that forms part of the TRACRN code. TRACRN is the version of TRACR3D

(Travis, 1984) that was baselined for YMP applications and that is being used to perform geochemical transport modeling in Study 8.3.1.3.7.1, Retardation Sensitivity Analyses. Effective diffusivities of aqueous chemical species are being measured in the laboratory with samples of tuff from Yucca Mountain (Study 8.3.1.3.6.2). The effective diffusivity is the effective diffusion coefficient multiplied by the rock capacity factor; for a nonsorbing tracer, the rock capacity factor is equal to the porosity of the rock matrix (Skagius and Neretnieks, 1986). The data from these laboratory experiments will be compared with the *in situ* measurements to help validate the computer codes incorporating the mathematical models and the applicability of the effective diffusion coefficients determined in the laboratory.

The spatial variations of the geologic media and their geophysical properties at Yucca Mountain may result in requests from the performance assessment investigators for effective diffusion coefficients in materials or in locations that differ from those used for the *in situ* determinations. The comparison of laboratory data with field data will aid in establishing the statistical basis on which the effective diffusion coefficients are used for modeling.

1.2 Regulatory Rationale and Justification

1.2.1 Performance Issues

The rationale for the YMP site characterization program is presented in Section 8.1 of the YMP SCP (DOE, 1988). The issue-based strategy was guided by an issue identification procedure to define the activities needed to resolve the issues. The issues were divided into performance issues and design issues; the work in this study plan applies only to performance issues. The key issues and associated information needs that will use the data from this study are the following.

1.2.1.1 Performance Issue 1.1

Performance Issue 1.1 asks, "Will the mined geologic disposal system meet the system performance objective for limiting radionuclide releases to the accessible environment as required by 10 CFR 60.112 and 40 CFR 191.13?" (SCP Section 8.3.5.13; NRC, 1983; EPA, 1985). This issue requires that the geologic setting, engineered-barrier system, shafts, boreholes, and seals be designed so as to limit the cumulative release of radionuclides for 10,000 years following permanent closure of the repository. SCP Table 8.3.1.2-1 (page 10 of 38) indicates that this study plan is responsible for providing diffusivity coefficients in support of this performance issue. Diffusion measurements from this study will be used to satisfy the requirements for the following information needs:

Information Need 1.1.1, "Site information needed to calculate releases to the accessible environment" (SCP Section 8.3.5.13.1).

Information Need 1.1.3, "Calculational Models for Predicting Releases to the Accessible Environment Attending Realizations of the Potentially Significant Release-scenario Classes" (SCP Section 8.3.5.13.3). Parameters needed to satisfy this information need include calculational models of transport of dissolved species in the unsaturated zone, including models developed in Investigation 8.3.1.3.7, Radionuclide Retardation by all Processes Along Flow Paths to the Accessible Environment. The diffusion study will contribute to the supporting data base for Investigation 8.3.1.3.7.

1.2.1.2 Performance Issue 1.2

Performance Issue 1.2 asks, "Will the mined geologic disposal system meet the requirements for limiting individual doses in the accessible environment as required by 40 CFR 191.15?" The results of this study will be used to satisfy the requirements for the site-specific Information Need 1.2.1, "Determination of Doses to the Public in the Accessible Environment Through Liquid Pathways." Parameters needed to satisfy this information need are the same as those required for Information Need 1.1.4 (SCP Section 8.3.5.1.3.4) and include calculational models of transport of dissolved species in the unsaturated zone, including models developed in Investigation 8.3.1.3.7, Radionuclide Retardation by all Processes Along Flow Paths to the Accessible Environment. The diffusion study will contribute to the supporting data base for Investigation 8.3.1.3.7.

1.2.2 Direct Federal Regulatory Requirements

The diffusion measurements from this study will provide supporting information required to evaluate compliance with parts of three federal regulations, 10 CFR 60, 10 CFR 960, and 40 CFR 191, as described below:

Laboratory and *in situ* measurements of effective diffusion coefficients will help to provide reasonable assurance that the requirements set forth by the U.S. Nuclear Regulatory Commission (NRC) in 10 CFR 60 will be met in accord with 10 CFR 60.101(a)(2), which states (NRC, 1983):

"... Demonstration of compliance with such objectives and criteria will involve the use of data from accelerated tests and predictive models that are supported by such measures as field and laboratory tests, monitoring data, and natural analog studies."

The measured diffusion coefficients will serve to quantify the extent to which Yucca Mountain satisfies the favorable siting condition described by the NRC in 10 CFR 60.122(b)(3) (NRC, 1983) and as stated explicitly by the U.S. Department of Energy in 10 CFR 960.4-2-2(b) (DOE, 1984):

"(2) Geochemical conditions that promote the precipitation, diffusion into the rock matrix, or sorption of radionuclides,..."

A performance assessment code, such as TOSPAC (Dudley et al., 1988), will use data from these tests to calculate compliance with the NRC regulation 10 CFR 60.112 (NRC, 1983), which states that the geologic repository system performance following permanent closure shall meet the system performance objective for limiting the release of radionuclide material to the accessible environment as required by radioactivity standards promulgated by the Environmental Protection Agency. These standards were initially set forth in 40 CFR 191.13 (EPA, 1985) and are currently being revised by that agency.

2.0 RATIONALE FOR STUDY

This section provides an overview and justification of the overall study. Section 3 of this plan provides additional technical details for specific tests, analyses, and methods to be used in the study.

2.1 Technical Justification and Overview of Study Approach

2.1.1 Technical Justification

The need for these tests is based on the observation that two of the long-lived fission products in high-level radioactive waste, ^{99}Tc and ^{129}I, are likely to exist under aqueous flow conditions at Yucca Mountain as the nonsorbing chemical species TcO_4^- (Daniels et al., 1982) and I^- (Wolfsberg et al., 1979). Assessment of the performance of a potential nuclear waste repository at Yucca Mountain must address the disposition of these species. Under saturated conditions in fractured rocks, matrix diffusion has been shown to be a significant mechanism for retardation of solute transport (Neretnieks, 1980). Although the conceptual model developed by Montazer and Wilson (1984) is that flow in the unsaturated zone is predominantly through the matrix, there may be saturation and flux conditions under which fracture flow could occur. Therefore, a complete description of the repository performance is likely to require an understanding of the effects of diffusion, either as a retardation mechanism if fracture flow occurs or as a transport mechanism in the absence of fracture flow.

Measurements of diffusion are underway in laboratory studies (see activities described under the study plan for diffusion, Study 8.3.1.3.6.2). However, lithostatic load and *in situ* saturation are important factors in establishing *in situ* equilibrium rock matrix properties (for example, pore geometry). These characteristics may deviate in the laboratory from those obtainable in field studies and may thereby affect the measured diffusion data. *In situ* measurements of effective diffusion coefficients will be undertaken to complement laboratory data in order to expand the data base to be used for the repository performance modeling efforts.

2.1.2 Overview of Approach

The diffusion tests will determine *in situ* the extent to which nonsorbing tracers diffuse into the water-filled pores of the tuffs that the ESF will penetrate. The tuffs are the Topopah Spring welded unit and the vitric and zeolitic zones of the Calico Hills nonwelded unit. Tracers will be introduced into boreholes in each of these tuffs and permitted to diffuse. Bromide will be used as a tracer to quantify the effective diffusion coefficient of a nonsorbing tracer; other tracers, not yet chosen, may be used to simulate the diffusion of ^{99}Tc and ^{129}I in the rock matrix. The emplacement locations will be overcored, and tracer concentrations will be measured as a function of the distance from emplacement. The tracer concentration data will be used to derive the effective diffusion coefficient for each tracer in each of the tuffs in which the tests are performed. The Topopah Spring unit is likely to be highly fractured at the test location. The overcored tuff will be examined to determine whether diffusive transport of nonsorbing species is nonlinear because of fracture boundaries in these unsaturated tuffs. Finally, the *in situ* measurements will be compared with effective diffusivities determined in laboratory measurements of similar tuffs (Study 8.3.1.3.6.2).

2.2 Constraints on the Study

2.2.1 Representativeness of the Site for Repository-Scale Conditions

The purpose of the diffusion tests is to determine effective diffusion coefficients in Yucca Mountain tuffs at and below the repository level under *in situ* conditions. Because the measured coefficients from this study will contribute to the prediction of potential radionuclide releases to the accessible environment, it is therefore important to quantify the extent to which the tested field conditions are representative of the appropriate rock units to be modeled. The matrix conditions most important for controlling the value of the effective diffusion coefficient are mineralogy, total porosity, degree of saturation, pore size distribution, the distribution of water in the pores, and tortuosity (the ratio of the actual length of a flow path between two points to the linear distance between them); not only are average values for these parameters of interest, but also spatial variabilities. Most of these parameters can be directly measured or characterized by standard methods (for example, porosity, saturation, mineralogy, and pore size distribution). In these cases, the best way to evaluate the extent to which field conditions are representative of the tested unit on a repository scale is to measure these values on core samples from the diffusion field site and to compare the results to the distribution function resulting from the same measurements done as part of the Site Unsaturated-Zone Hydrology Investigation (8.3.1.2.2).

2.2.2 Need to Simulate Repository Conditions

A question that then arises is, if a given tuff sample can be shown to be representative of the unit of interest, why is it then not sufficient to measure the effective diffusion coefficient in the laboratory? The answer to this question provides the major rationale for this study. When the tuffs are removed from their underground locations, it is difficult to preserve the integrity of the tuff sample as a result of the coring. In addition, the distribution of water in the pores (affected by factors such as lithostatic load and degree of saturation) cannot be duplicated reliably under laboratory conditions. Even though the value of the lithostatic load on the sample can be reproduced, its effects on pore characteristics cannot be assumed to represent *in situ* conditions because the effects may not be completely reversible. Therefore, these tests will be performed under conditions that resemble as much as possible the long-term repository storage conditions so that the data supplied for performance modeling will accurately represent pre-emplacement conditions.

2.2.3 Effect of *In Situ* Variability of Hydrologic Parameters Determined by Modeling Studies

In situ variability in pore saturation and locations of fractures at the field site also must be considered. An *in situ* study of diffusion in the saturated granite at the Stripa Mine in Sweden was conducted by Birgersson and Neretnieks (1982). They introduced water-soluble tracers into a borehole and used a pump to counter hydrostatic pressure for 3 months while the tracers diffused in a connected pore system; then they overcored the borehole and analyzed the resulting core for tracer concentrations. An *in situ* study of diffusion in the tuffs at the Yucca Mountain ESF would be similar in principle to the Stripa Mine work. The unsaturated conditions, however, eliminate the need for a pump (because capillary suction draws the tracer into the medium) and raise questions about the effects of water that might be used to introduce the tracers into the borehole or to cool the overcore bit. The role of undetected fractures in the immediate vicinity of the tracer test is also of concern.

Pre-experimenting modeling studies were performed to address the effects of variable saturation and fracturing on tracer movement, to evaluate the extent to which tracer movement will be sensitive to the diffusion coefficient of a nonsorbing tracer in unsaturated tuffs at Yucca Mountain, and to estimate the probable range of results. Additional modeling will be conducted following the results of laboratory studies and prototype field work as the controlling parameters become better defined. The results of the modeling done to date are summarized here. The full reports should be consulted for additional details (Birdsell et al., 1987, 1988).

2.2.3.1 Adopted Parameters for Modeling Studies

The schematic of the borehole and the tracer source used in the modeling studies is shown in Figure 2. The tracer source was taken to be 10 mℓ of water containing a nonsorbing tracer such as bromide at a concentration of 1 g tracer/mℓ. The TRACR3D code (Travis, 1984) discussed in the study plan for Retardation Sensitivity Analysis, Study 8.3.1.3.7.1, was used to calculate tracer concentration profiles for times as long as a year in two tuffs. Theoretical details of this code are discussed in Section 3.3 of this study plan. One tuff was assigned porosity, initial saturation, and matrix permeability values characteristic of the Topopah Spring Member of the Paintbrush Tuff at Yucca Mountain. The second had values for these three parameters that were characteristic of the tuffs of Calico Hills. Table 1 summarizes the values chosen for the rock matrix parameters.

Diffusion coefficients for chemical species diffusing through bulk water are normally on the order of 10^{-5} cm^2 s^{-1} (Robinson and Stokes, 1959). The cumulative effects of saturation of the porous medium, the tortuous nature of the diffusion path, and the porosity of the medium decrease the coefficient by about one to two orders of magnitude (Birdsell et al., 1987, 1988; Conca, 1991). Consequently, the effective diffusion coefficient in most rocks is expected to be in the range of 10^{-6} to 10^{-7} cm^2 s^{-1}. In the modeling studies by Birdsell et al. (1987, 1988), the effective diffusion coefficient was generally assigned the value 1×10^{-7} cm^2 s^{-1}. An effective diffusion coefficient of 1×10^{-6} cm^2 s^{-1} was used for comparison in one set of calculations to determine the sensitivity of the results to a larger value for this parameter. Actual diffusion coefficients are expected to fall within the range of these two values.

2.2.3.2 Effect of Introducing Tracer Solution

One question that was investigated in the modeling studies was the effect of introducing the tracer in an aqueous solution. The tuff immediately around the emplacement position would be saturated initially. The modeling studies calculated tracer movement as a function of time into unfractured, porous tuff from a source whose initial saturation and porosity were the same as those of the surrounding matrix. These results were then compared to the case in which the immediate source region was initially saturated by the 10 mℓ tracer solution. For the Topopah Spring tuff, the tracer front traveled 8.2 cm into the tuff from the saturated source region, after a year's time, vs 7.2 cm for the ideal case from a source at the same saturation and porosity as the surroundings. Consequently, introducing a tracer solution drives the concentration 13% farther into the matrix. In the Calico Hills tuff, the tracer front traveled 7.8 cm into the tuff from the initially saturated source region, after one year, vs 7.2 cm for the ideal case; introducing the tracer solution drives the concentration 8% farther into the matrix.

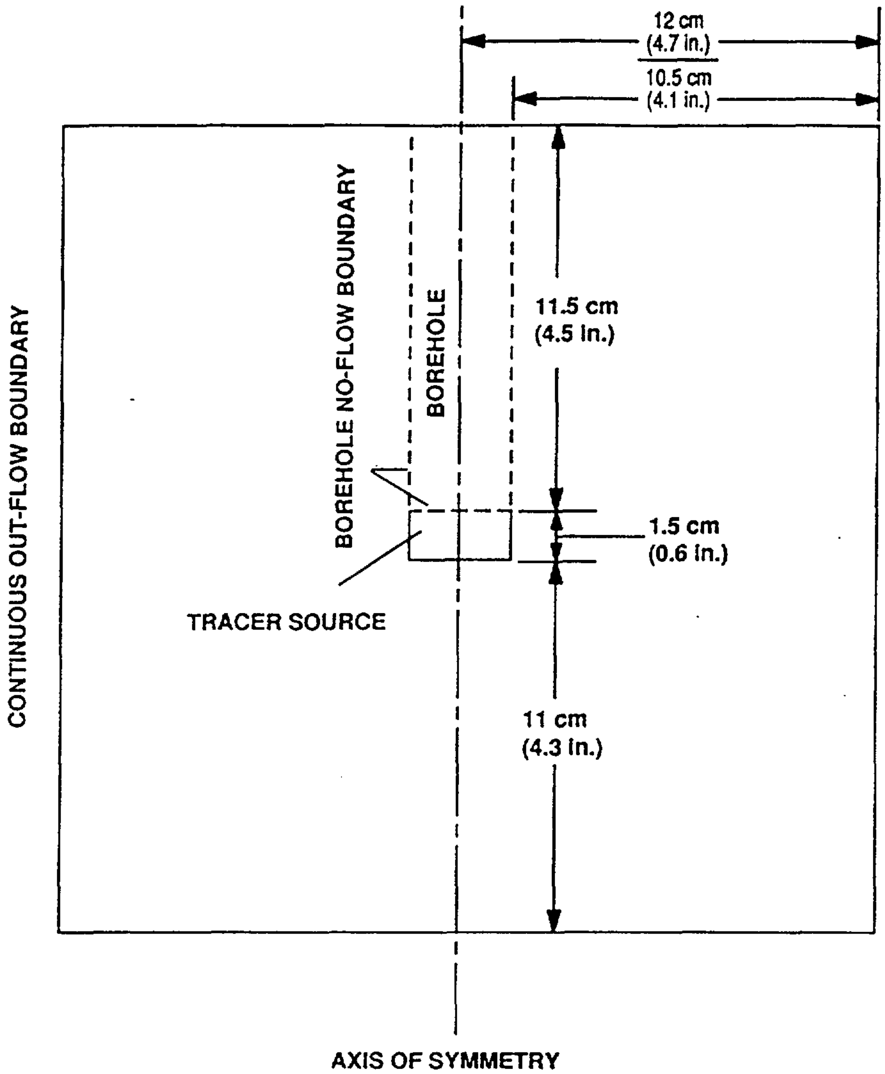

Figure 2. Vertical Cross Section of the Borehole, Tracer Source Region, and Surrounding Matrix Used by Birdsell et al. (1988) for Model Simulations of Tracer Movement Under Assumptions of Pure Diffusion and Diffusion With Advection.

These calculations indicate that the introduction of tracers in an aqueous solution will not have a major effect on the concentration profile curves for Topopah Spring and Calico Hills tuffs after a year's time. However, this effect will be taken into account during the diffusion tests by measuring the porosity and degree of saturation of the rock matrix surrounding the tracer source.

2.2.3.3 Contribution of Advection to Total Tracer Transport

Another effect that must be considered is the possibility of advective transport, as well as diffusion, when the tracer is introduced in an aqueous solution. Calculations provided

TABLE 1

HYDROLOGIC PROPERTIES OF YUCCA MOUNTAIN TUFFS ADOPTED FOR MODELING STUDIES[a]

	Calico Hills Nonwelded Unit	Topopah Spring Welded Unit
Matrix properties		
Permeability, darcy	2.1×10^{-6}	2.0×10^{-6}
Porosity	0.31	0.14
Saturation	0.91	0.65
Fracture properties		
Permeability, darcy	20.7	1.76
Porosity	0.99	0.99
Saturation	0.04	0.04

[a]Birdsell et al., 1988.

comparison of transport under pure diffusion conditions and diffusion combined with advection in both tuffs. Advection was a minor perturbation in the Calico Hills tuff, but the calculation of the results of the *in situ* test in the Topopah Spring tuff is likely to include correction for advective transport. Modeling results for the Calico Hills simulation indicate that after one year, the tracer front has traveled 8.8 cm for the combined advection plus diffusion case, vs a distance of 7.8 cm for the pure diffusion case (Birdsell et al., 1988). Advection drives this concentration 12% farther from the edge of the source than does diffusion alone. After one year, the Topopah Spring simulation predicts that the tracer front will have traveled 10.4 cm from the combined advection plus diffusion case, vs 8.2 cm for the pure diffusion case. Advection drives the tracer front 31% farther from the edge of the source than does diffusion alone.

This modeling calculation shows that the effective diffusion coefficients can still be computed in both units provided the contribution of advection to the test results can be determined. This will require knowledge of the matrix properties. The *in situ* tests must be carried out with a minimum pressure differential between the alcove and the tracer emplacement site to maximize diffusive transport relative to advection.

2.2.3.4 Effect of Fractures on Tracer Transport

Another question that was investigated in these modeling studies was the effect of a nearby fracture on the results. The parameters adopted for the fractures are given in Table 1. Modeling was done with a horizontal fracture 11.5 mm beneath the tracer source. In the Calico Hills tuff, the initial saturation difference between the source and the matrix was too low to force fluid toward the fracture. Consequently, the high permeability of the fracture had little effect on the overall transport after a year's time. The effect of the horizontal fracture in the Topopah Spring tuff was greater than that in the Calico Hills because of fluid flow in the fracture. The effects of the fracture diminished with time. After 6 months, the tracer concentration profiles were shifted only slightly downward and outward near the fracture relative to the computer simulation without a fracture.

Tracer transport from the source into the rock matrix containing a single vertical fracture located radially at different distances from the source region was also modeled. The results predict that the proximity of the fracture to the source region will determine its importance to the experimental results, especially if the fracture diverts flow from the source into the matrix. A fracture that intersects the source region will undoubtedly affect the transport most of all. Consequently, attempts will be made to ensure that the tracer source is injected into a region free of fractures, based on downhole scans of the borehole with a borescope and on examinations of the recovered core. Nonetheless, if fractures are found in the overcored section at the end of the test, the modeling studies indicate that the tracer data can still be analyzed to obtain an estimate of the effective diffusion coefficient.

2.2.3.5 Effect of Cooling Water from Overcoring

If possible, air-drilling will be used to recover intact cores from the region of interest at the end of the experiment. However, in the event that prototype air-drilling is unsuccessful, modeling was conducted to investigate the effect on the established tracer profiles of a water-cooled overcoring bit (Birdsell et al., 1987). At the completion of the yearlong test, the region was overcored so as to remove intact the source region and the surrounding matrix to a radius of 14.5 cm using a 30-cm O.D./29-cm I.D. drill advancing at 1 m/hr. The drilling process was simulated by progressively saturating the 0.5-cm-wide annular space from the top downward in 30-cm increments (that is, every 18 minutes) to a total depth of 11.7 m, which is 1.5 m below the bottom of the tracer source region.

The saturation front set up by the overcoring process forced tracer out of the overcoring region, affecting the concentrations of order 10^{-8} g/mℓ for the Topopah Spring matrix and 10^{-9} g/mℓ for the Calico Hills matrix. Although these low concentrations were affected by the increased saturation, the detectable tracer fronts, defined as concentrations 10^4 times less than the initial injected concentration (or C/C_0 values of 10^{-4}) showed no change after overcoring. Thus, the calculations indicate that the water from such a bit will not alter the test results significantly, as long as the effective diffusion coefficient is on the order of 10^{-7} cm^2/s or less. A water-cooled bit of this diameter may be unacceptable if the tracer has a larger diffusion coefficient because the saturation front is predicted to overlap with the 10^{-4} g/mℓ concentration front for the case in which the coefficient has a value of 10^{-6} cm^2/s.

Additional modeling is planned to address the question of drying effects (if air-drilling is used for the overcoring) and redistribution of water after core recovery.

2.2.3.6 Sensitivity of Predicted Transport Rates to the Value of the Effective Diffusion Coefficient

The modeling studies predict that the experimental design proposed for these tests will be appropriate for determining *in situ* effective diffusion coefficients because the test results will be sensitive to the value of the coefficient. An order of magnitude increase in the diffusion coefficient causes the calculated detectable tracer front to diffuse approximately twice as far in a one-year period.

2.2.4 Potential Impacts of the Tests on the Site

The potential impacts on the site that result from the diffusion tests are of a local scale. Physical impacts include the construction of alcoves at three locations (Topopah Spring Member tuff and the vitric and zeolitic zones of the Calico Hills unit) in the ESF. Each core hole will be approximately 10 m deep and 0.3 m in diameter when the underground phase of the work is complete. No hydrologic impacts will result from the drilling because the drilling fluid will be air. Chemical impacts will be minimal because all of the tracers to be used are planned to be removed in the core that is retrieved. The core holes can be backfilled at the conclusion of these tests to minimize residual impacts on the underground facilities. All work will be performed in a manner consistent with the guidelines given in SCP Section 8.4 (DOE, 1988).

2.2.5 Required Accuracy and Precision, Limits of Methods, and Capability of Analytical Methods to Support the Study

The basic measurements in the diffusion tests are the determinations of the quantities of tracers in segments of the tuff that surrounds the tracer emplacement hole. Selected and alternate analytical methods are discussed in the subsections describing the individual activities in Section 3. These methods were selected on the basis of their precision and accuracy. The accuracy and precision of each of the techniques are discussed in various publications describing the methods and will be defined, as appropriate, in the technical procedures developed for their implementation, as required in the LANL/YMP Quality Assurance Plan. Performance assessment has not decided what accuracy and precision is required for the effective diffusion coefficient to be measured in this study, which will depend upon the solute transport model adopted and upon the results of sensitivity analyses. The results of this study should help define the extent to which diffusion should be considered as a significant retardation mechanism for radionuclide transport.

2.2.6 Time Required vs Time Available to Complete the Study

The studies planned will require approximately 4 years to complete following the successful completion of the prototype testing and availability of alcoves in the ESF. Ideally, the prototype testing will be conducted in the ESF prototype testing facility (to be built within the first few hundred feet of excavation). The diffusion tests will be carried out concurrently with other tests in the underground facilities. Thus, the duration of the tests will not be constrained by the time available.

2.2.7 Potential Interferences from Other ESF Activities

In the present ESF plans, each diffusion test is to be performed in a specifically designed alcove (approximately 6 × 6 m) on the main test level (in the Topopah Spring Member and the vitric and zeolitic zones of the Calico Hills unit), for which the current general arrangement is presented in Figure 3. The arrangement and dimensions of the various openings are expected to change as additional design or operations analyses are completed. The final location and design of the diffusion tests need to take into account three types of ESF activities that have the potential to interfere with the diffusion tests: those generating heat, stress, or changes in water content. These types of interferences are discussed in detail in the SCP Section 8.4.2.3 (DOE, 1988) and are summarized below.

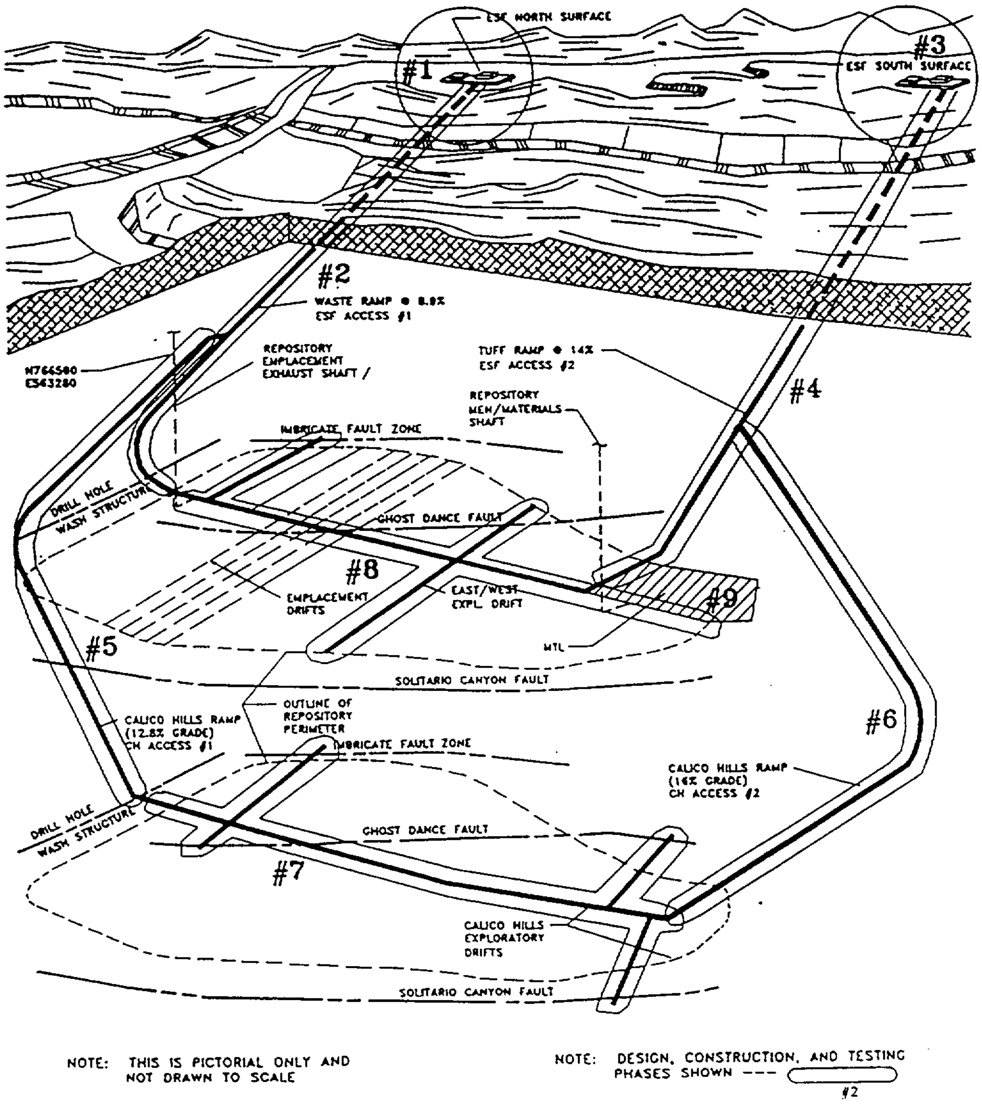

Figure 3. Reference Design Concept for Commencing Study Option #30 (From Exploratory Shaft Test Coordination Meeting Notes, March 8, 1991).

Because fluid viscosity and density vary with temperature, diffusion rates are also a function of temperature. Consequently, the diffusion tests must be conducted in an isothermal environment, outside the zone of influence of temperature changes arising from the mined opening and of the various heater tests planned by SNL and LLNL. Boreholes will be capped to isolate them from temperature fluctuations in the mined openings. Thermal perturbations could arise if the diffusion tests were located within the zone of influence of any of the heater tests planned for the ESF. Relevant SNL experiments include the heater experiment in unit TSw1, canister-scale heater experiment, Yucca Mountain heated block, thermal stress measurements, and heated room experiment, described in SCP Sections 8.3.1.15.1.6.1 through 8.3.1.15.1.6.5.

The engineered barrier system field test, or waste package test, planned by LLNL (SCP Section 8.3.4.2.4.4) also will give rise to thermal perturbations in the surrounding rock. The zones of thermal influence of these tests range from a few meters up to a maximum of 28 m.

Ground motion or changes in the stress state of the rock, for example, from drilling, mining, or blasting activities, could vibrate the diffusion volume to the extent that fracturing could occur during the experiment, thus affecting diffusion paths and rates. As a general rule of thumb, the stress-altered region resulting from blasting activities is estimated to extend about two drift diameters from the drift walls.

Finally, water added during tests or used in drilling or mining activities could move via fractures to the diffusion volume and thereby influence tracer transport rates and paths. Bromide used as a tag for the ESF drilling operations could conceivably interfere with the diffusion tests. However, water used in drilling is estimated to penetrate, in general, less than 10 m (33 ft) into the formation (SCP Section 8.4.2.3.6.2). Tests in which water is to be added include percolation tests, radial borehole test, and hydrologic properties of faults (SCP Sections 8.3.1.2.2.4.2, 8.3.1.2.2.4.4, and 8.3.1.2.2.4.10). The locations of the diffusion test alcoves will be selected to minimize the potential for such interferences.

Testing and observations planned in the ESF during construction, such as the radial borehole test and excavation effects test, will provide data to confirm or better define these estimates. These potential interferences will be minimized by locating the diffusion test alcoves outside the zones of influences of other test activities, and by drilling the injection boreholes to a depth (about 10 m, or 30 ft) sufficient to be outside the zone of stress relief induced by mining the experiment drift.

Another consideration is interference between the short-term (3-month) and long-term (12-month) diffusion tests. The boreholes for each pair of tests will be spaced sufficiently far apart to eliminate the possibility of interference.

3.0 DESCRIPTION OF TESTS AND ANALYSES

All details of the test design described in this study plan should be considered as rough guidelines; one of the objectives of the study is to determine the applicability of the present experimental designs. Final details will be specified in the technical procedures to be prepared upon completion of additional modeling calculations, laboratory tests, and prototype testing prior to initiation of the ESF tests.

3.1 General Approach for Diffusion Tests in the ESF

The diffusion tests will take place in specially-constructed alcoves in the Main Test Levels of the ESF. Three locations for diffusion tests are desired: the Topopah Spring Member, and the vitric and zeolitic zones of the Calico Hills unit. Two boreholes will be dry-drilled vertically downward or subhorizontally in each alcove; each hole will be about 10-cm diameter for the upper 10 m, and about 4-cm diameter for the bottom 45 cm. The bottom of each hole will serve as a source region for the tracer diffusion test. The core removed from the bottom of each hole will be examined for fractures in order to minimize the possibility of fractures intersecting the source region. In addition, the boreholes will be examined for fractures using a downhole borescope.

A 10-mℓ solution containing a suite of tracers will be placed at the bottom of one of the 4-cm diameter holes. One of the tracers will be bromide; the others have not yet been selected. The 10-cm diameter hole will be sealed with an inflatable packer to isolate the bottom of the hole from air pressure and humidity changes in the drift while diffusion occurs during a period of 3 months. The hole will then be overcored, and the bottom portion of the core will be sectioned and analyzed for tracer concentration as a function of position.

The results of the three-month diffusion experiments for each of the tuff units will be used for an initial estimate of the effective diffusion coefficients and to evaluate the extent of advective and fracture flow and the possible need to refine the transport scheme used in TRACRN to model these studies. This knowledge will in turn be used to predict the extent of transport after a longer period of time, which will determine the optimum length of time required for the second set of diffusion tests and the size and type of overcoring needed. Then the diffusion test in each tuff will be repeated in the second borehole for a longer period of time, which will probably be on the order of one year.

In each case, the sample core will be analyzed to determine its matrix porosity, initial saturation, and saturated permeability so that the contribution of advection to transport can be determined.

Prior to initiating the tests in the ESF, plans are to conduct additional sensitivity analyses using TRACRN and to collect preliminary diffusion data, test collection methods, and improve data-analysis methods by conducting preliminary diffusion studies in the laboratory. The field techniques required for this study will be tested and optimized during prototype testing.

3.2 Test Methods

These tests require drilling procedures and apparatus to permit emplacement of the tracer solution in the bottom of the borehole, a method to recover the core into which the tracers have diffused, a technique to section the recovered core, and an analysis procedure for each tracer that is used. Table 2 lists the required measurement parameters. The subsections below summarize the test methods to obtain the required data, as presently conceived. Many of the procedures to be used for these tests were partially developed and tested in prototype tests conducted at Apache Leap in Arizona and in G-Tunnel at the Nevada Test Site (NTS); however, additional prototype testing is needed to ensure that the diffusion tests will gather the information required.

TABLE 2

MEASUREMENT PARAMETERS FOR THE DIFFUSION TESTS

Measured Data Items	Test Method	Derived Parameters	Expected Values	Source of Estimates
Distance of tuff sample from borehole	Ruler	--	0 to 15 cm (0 to 6 in.)	a
Tracer concentrations in tuff samples and source solutions	Analytical chemistry methods	$\frac{C}{C_o}$	0.1 to 100%	b
Diffusion time	Calendar	--	3 to 12 month	a
Porosity	Mercury penetrometry	--	10 to 35%	c
Neutron diffusion and attenuation	Neutron probe	Saturation	50 to 100%	c
Dry mass of a measured geometric shape	Ruler and balance	Dry bulk density ρ_b	2.0 to 2.2 g/cm^3	d
Tracer concentrations in tuffs and equilibrated solutions	Solid-rock column experiments	K_d	~0 to 10 mℓ/g	e
Effective diffusion coefficient	Derived from above data	D_e	10^{-7} to 10^{-6}	f

Source of estimates:
[a]Design parameter.
[b]Birdsell et al., 1988.
[c]Montazer and Wilson, 1984.
[d]Based on grain density of 2.30 g/cm (Daniels et at., 1982, p. 144), together with the range of values for total porosity.
[e]DOE, 1988, Table 8.3.5.13-4 (p. 8.3.5.13-61).
[f]Birdsell et al., 1988 and Conca, 1991.

Detailed technical procedures for the test methods referenced in this section and listed in Table 3 will be written following completion of prototype work and will be finalized at least 60 days prior to initiating the ESF tests. All of the technical procedures listed in Table 3 will become standard procedures. Based upon Tables 2 and 3, Table 4 lists the expected equipment and service needs of the diffusion tests.

The data resulting from the tests will be used in predicting the long-term performance of the site as a nuclear waste repository. The prototype testing, as well as the actual diffusion tests, will be performed in accordance with the Los Alamos National Laboratory (LANL) Quality Assurance Program Plan, LANL-YMP-QAPP (Appendix A). All computer codes will be validated and verified according to Quality Assurance procedures.

TABLE 3

DETAILED TECHNICAL PROCEDURES TO BE USED

DP Number	DP Title	Effective Date
TWS-INC-DP-61	Solid-Rock Column Experiments	3/13/89
TBD[a]	REECo Air-Drilling and Coring Procedure	b
NWM-USGS-GP-10	Borehole Video Fracture Logging	4/12/85
TBD	Downhole Neutron Well-Logging	b
TBD	Downhole Temperature Logging	b
TBD	Tracer Preparation and Injection Procedure	b
TBD	Borehole Overcoring	b
TBD	Technique for Sectioning the Recovered Core	b
TBD	Determination of Porosity	b
TBD	Gravimetric Determination of Water Content	b
TBD	Mineralogic Characterization of Tuff Samples	b
TBD	Analytical Procedures for Determination of Tracer Concentrations in Recovered Cores	b
TBD	Effective Diffusion Coefficient Analysis	b

[a]TBD = to be determined.
[b]These procedures will be written after prototype testing is completed and will be available at least 60 days before the ESF tests are to be initiated.

TABLE 4

INSTRUMENTATION, EQUIPMENT, MATERIALS, AND SERVICES FOR THE DIFFUSION TESTS

Item	Quantity[a]	Description	Procurement Method
Pressure transducers	3	Standard	Tester's Organization purchase order
Air-drilled coreholes, each ~10-m deep, plus overcoring of region of interest	6	To be developed in prototype test	Drilling support contractor
Tracer injection apparatus with double packer	3	Special	Tester's organization design and fabrication
Neutron well-logging tool	1	Standard	Support contractor, purchase or lease
Optical borescope	1	Standard	Support contractor, purchase or lease
Diamond-coated wire or saw blade	1	Standard	Tester's organization purchase order
Ion chromatograph	1	Standard	Tester's organization purchase order
Rock crusher or centrifuge	1	Standard	Tester's organization purchase order

[a]Quantities here include testing needs for Topopah Spring Member and vitric and zeolitic zones of Calico Hills.

3.2.1 Diffusion Tests Setup

Two boreholes will be dry-drilled vertically downward or subhorizontally in each alcove. The approximate dimensions of each hole are illustrated in Figure 4: a 10-cm (4 in.) diameter borehole will be drilled about 10 m (30 ft) to penetrate beyond the zone of stress relief resulting from the excavation of the 6-m diameter alcove. From the bottom of this borehole will be drilled a 4-cm (1.5 in.) diameter hole about 45 cm (18 in.) deep to penetrate beyond the region of stress relief induced by drilling the 10-cm diameter hole.

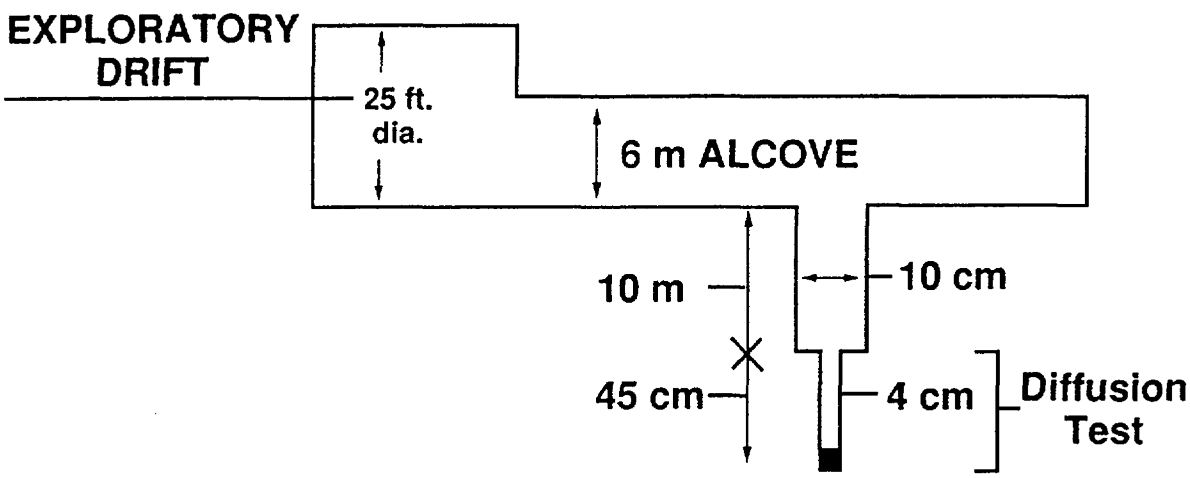

Figure 4. Approximate Dimensions of Boreholes to be Used for Tracer Diffusion Tests in the ESF.

All drilling will be done with air as the bit cooling fluid because water could alter the *in situ* degree of saturation of the rock at the bottom of the hole where the diffusion test is to be conducted. Air drilling technology and dust suppression techniques were developed and tested in Los Alamos prototype drilling tests in USW UZ-1 and USW UZ-6 at the Nevada Test Site (Whitfield, 1985) and the Apache Leap site in Arizona as well as in prototype diffusion work in G-Tunnel at the Nevada Test Site. The air-drilling procedures will be tested and optimized during prototype diffusion testing to be conducted as part of this study. Core from the small-diameter part of the hole will be recovered and stored in Lexan tubing to be used for measurements of porosity, degree of saturation, and mineral composition, for mapping of fractures, and for laboratory studies of diffusion (Study 8.3.1.3.6.2).

Tracer injection methodology will be tested during the prototype phase of this study. Downhole temperature profiles will be monitored to ensure that the borehole has re-established equilibrium temperature conditions. Downhole moisture measurements will be made with a neutron well-logging tool in order to determine when moisture re-equilibration has been obtained. Downhole scanning for the presence of fractures will be done with an optical borescope. If fractures are identified in the recovered core or in the borescope, the hole will be deepened and rechecked. When each hole is not being logged, it will be plugged with a piece of plastic foam and a cap. Prior to tracer injection, the bottom of the hole will be milled and vacuumed to remove dust.

3.2.2 Tracer Selection and Injection

The suite of tracers to be used in the diffusion tests have not been completely defined. The tracers are to serve three purposes: (a) to simulate the behavior of a completely nonsorbing solute, (b) to simulate the behavior of technetium, and (c) to simulate the behavior of iodine.

Bromide appears to be the best choice for the case of the nonsorbing solute, based on results reported in other field studies and laboratory studies (for example, Wolfsberg et al., 1979; Daniels et al., 1982; Birgersson and Neretnieks, 1982; Skagius and

Neretnieks, 1986; Whittemore, 1988). It is chemically stable, nonsorbing, nonvolatile, non toxic, and easy to detect by a variety of cost-effective methods (Whittemore, 1988). Its natural background in the tuffs is sufficiently low as not to interfere with the tracer tests: ground waters extracted from unsaturated YMP tuff cores had bromide concentrations of 0.1 to 0.3 mg/ℓ (I.C. Yang, U.S. Geological Survey, pers. commmun., 1990). A more appropriate measure of the background for the purposes of these tests is the total bromide released from the tuff matrix when it is crushed in preparation for leaching. Crushing and leaching of thirty tuff samples from the unsaturated zone (USW UZ-1 and USW UZN-43) from depths of 20 to 1270 ft showed bromide contents averaging 0.04 μg/g of tuff (Hydro Geo Chem, 1990). At least one additional nonsorbing tracer will be included in the injected solution as a means of checking that the measured tracer concentrations have not been contaminated by the use of bromide to trace water used during ESF construction and as a double check for the assumption of nonsorbing behavior.

Analogues for the two radionuclides, ^{99}Tc and ^{129}I, are of interest because their long half-lives and generally negligible sorption indicate that they are the waste components most likely to migrate the farthest from the repository in the event of a leak. Although an effective diffusion coefficient can be calculated for these species from the bromide results by assuming identical sorption behavior, it would be useful to test the extent to which volatilization (in the case of iodine) and sorption effects affect transport rates. Table 5 lists desired characteristics and alternative tracers which are being considered. The tracers and detection methods will be selected following a literature survey and screening by laboratory tests conducted under saturated and unsaturated conditions.

A tracer injection apparatus has been designed and tested to deliver a 10-mℓ volume of tracer solution to the bottom of a 10-m borehole (Figure 5). The apparatus includes two inflatable packers connected to a nitrogen gas cylinder, which serve as a double-barrier to isolate the region where diffusion is occurring from changes in atmospheric pressure in the drift above. At the bottom of the apparatus is a column with a capacity of 10 mℓ in which the tracer solution is held in place by a check valve. The solution will contain a suite of tracers. To minimize the potential for injection of air bubbles into the matrix along with the solution, the solution will be deaerated prior to use. The apparatus will be inserted into the borehole, the packers will be inflated, and the tracer will be injected when the Teflon plunger is activated by nitrogen pressure.

3.2.3 Sample Collection and Analysis

At the completion of the tracer diffusion period, overcoring will use air-cooled bits if at all possible. The diameter of the overcored hole will be about 30 cm (12 in.). The success of the diffusion tests will depend upon good recovery of intact core for the sections cored from the bottom-most 10 to 20 cm of the small-diameter hole, extending to about 50 cm below the bottom.

In the laboratory, sectioning of the core will be performed dry with a diamond-coated wire or saw blade to preserve the *in situ* tracer concentrations. The proposed geometry of the sections is shown in Figure 6 (Samples labeled with the same number [for example, 2] are expected to have the same tracer concentrations. In the half-disk of core immediately below that shown, the sample numbers 6, 7, 8, 9, and 10 correspond to the locations in the diagram labeled 1, 2, 3, 4, and 5, respectively.). Several methods will be tried for

TABLE 5

SELECTION CRITERIA FOR TRACERS

Tracer 1. Purpose: to simulate the behavior of a completely nonsorbing solute

Desired characteristics:

Nonsorbing, nonvolatile, nonbiodegradable, natural background negligible relative to injected concentration, easy to detect, high precision for detection, water soluble to extent that concentration is still detectable after dilution of initial concentration by two or more orders of magnitude, nontoxic, meets regulatory requirements.

Alternatives:

Inorganic bromide salt (LiBr, NaBr, KBr, $CaBr_2$, $MgBr_2$)
Trifluoromethylbenzoic acids (o-TFMBA, m-TFMBA, p-TFMBA)
Uranine
Cr-EDTA

Tracer 2. Purpose: to simulate the behavior of technetium

Desired charasteristics:

Analogue for technetium, natural background negligible relative to injected concentration, easy to detect, high precision for detection, water soluble to extent that concentration is still detectable after dilution of initial concentration by two or more orders of magnitude, nontoxic, meets regulatory requirements.

Alternatives:

^{95}Tc (half-life, 61 days)
^{99}Tc (half-life, 213,000 years)
Rhenium, as sodium perrhenate ($NaReO_4$)

Tracer 3: Purpose: to simulate the behavior of ^{129}I

Desired charasteristics:

Analogue for ^{129}I, natural background negligible relative to injected concentration, easy to detect, high precision for detection, water-soluble to extent that concentration is still detectable after dilution of initial concentration by two or more orders of magnitude, nontoxic, meets regulatory requirements.

Alternatives:

Inorganic iodide salt (LiI, NaI, KI)
^{125}I (half-life, 60 days)
Iodide salt labeled with ^{129}I to an atom ratio on the order of 10^{-4}

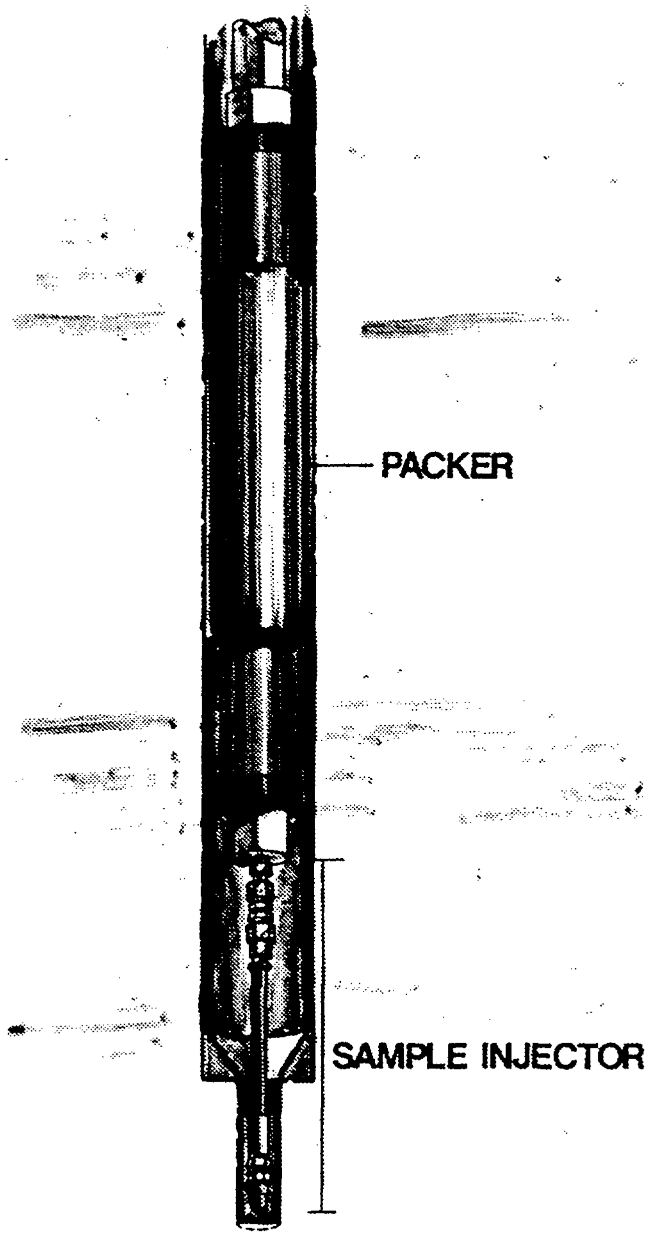

Figure 5. Schematic of the Borehole Packer System and Tracer Injection Apparatus.

extracting the tracer. One method is to crush each section and then leach it with water; another alternative is to use a high-speed centrifuge to extract the water from the intact sample. As complete a recovery as possible is desired in order to calculate a mass balance for the tracer as a check that volatility effects are negligible.

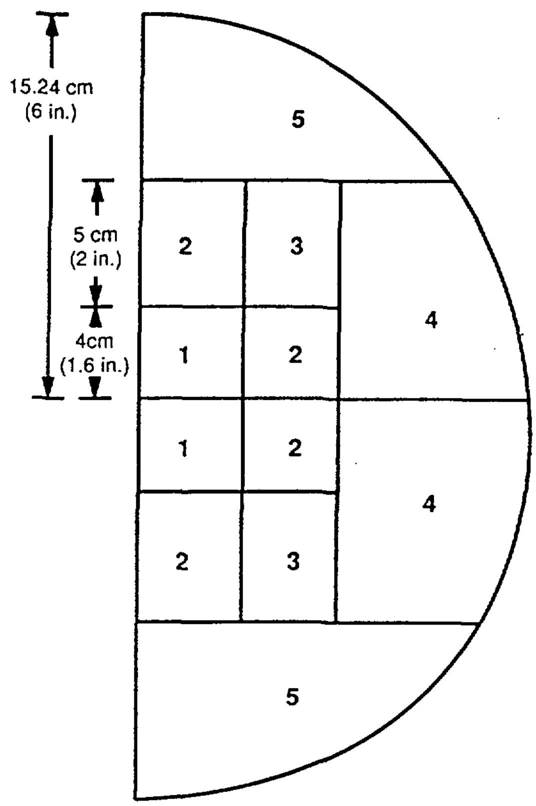

Figure 6. Diagram of Sample Locations in a Half-Disk of Core Immediately Below the Borehole.

The tracers will be assayed in the leachate or in the extracted fluid. For bromide, a wide variety of analytical methods can be used (Whittemore, 1988). Considerations in the selection of a given method depend upon the detection limit, freedom from interferences, and speed, difficulty, and cost of the analysis. Accuracy and precision are especially critical for this study. High-precision methods applicable to low concentrations of bromide in water are ion chromatography, colorimetry, and neutron-activation analysis; these and other methods are reviewed by Whittemore (1988). Of these, ion chromatography is the most convenient and is the method of choice for analysis of the field test samples. Its detection limit for bromide is as low as 1 $\mu g/\ell$ if an anion-concentrator column is used, more than adequate to measure concentrations from initial values down to background (about 0.3 mg/ℓ or less depending upon the extent of dilution by the leaching process).

A review and selection of analytical techniques for the other tracers used in the field tests will be made after the tracers have been chosen, that is, after literature review and laboratory testing have been conducted.

3.3 Diffusion Equations and Measured Parameters

The measured tracer concentrations as a function of distance from emplacement will be analyzed using TRACRN (Travis, 1984) to compute the effective diffusion coefficient for each tracer. TRACRN is a finite-difference, three-dimensional flow and transport code that incorporates geochemical and physical processes and data along with hydrologic and geologic data to do integrated transport calculations (8.3.1.3.7.1). Finite-difference methods are numerical techniques used to solve a system of differential equations when analytical solutions are not possible. In the diffusion test calculation, flow and transport are described by invoking conservation of mass for the liquid phase,

$$\partial_t (\varepsilon \sigma \rho) + \nabla \cdot (\rho \vec{u}) = 0 \qquad \textbf{(1)}$$

conservation of mass for the tracer,

$$\partial_t (\varepsilon \sigma \rho C) + \nabla \cdot (\rho \vec{u} C) = \nabla \cdot (\varepsilon \sigma \rho D_e \nabla C) \qquad \textbf{(2)}$$

and conservation of momentum for the liquid phase, given by Darcy's law,

$$\vec{u} = - (k/\mu) \ (\nabla P + \rho \vec{g}) \qquad \textbf{(3)}$$

where

C = concentration of the tracer, g tracer/g fluid
t = time, s
D_e = effective diffusion coefficient, cm^2/s
$\vec{g}$ = gravitational acceleration, cm/s^2
k = permeability, cm^2
P = liquid pressure, $dyne/cm^2$
$\vec{u}$ = fluid velocity, cm/s
ε = porosity, volume of voids/total volume
μ = fluid viscosity, g/cm/s
ρ = fluid density, g/cm^3
σ = saturation, volume of water/volume of voids

Sorption is not included in the tracer conservation equation, Eq. (2), because the tracers to be used are nonsorbing. To verify the assumption of a nonsorbing tracer, the sorption distribution coefficient K_d will be measured in laboratory experiments for each tracer and each tuff using an intact tuff column flow approach. The porosity and dry bulk density of the tuff in which the experiment is performed will be measured in pieces of tuff removed from the vicinity of the diffusion measurement.

In Eq. (3), both k and P are functions of matrix saturation. Permeability k is expressed as the product of the saturated permeability (k_s) and the relative permeability (k_r), which ranges between 0 and 1 and increases with degree of saturation:

$$k = k_r \ k_s \qquad \textbf{(4)}$$

The liquid and gas pressures are related by:

$$P = P_g - P_c \qquad \textbf{(5)}$$

where P_c, the capillary pressure, varies with saturation. The relative permeability and capillary pressure vary with saturation according to the empirical Eqs. (6) and (7) (Klavetter and Peters, 1986):

$$k_r = \left[1 + (\alpha P_c)^\beta\right]^{(1-\beta)/2\beta} \left\{1 - \left[\frac{(\alpha P_c)^\beta}{1 + (\alpha P_c)^\beta}\right]^{(\beta-1)/\beta}\right\}^2 \tag{6}$$

$$P_c = \frac{g \rho}{\alpha} \left\{\left[\frac{\sigma - S_r}{1 - S_r}\right]^{\beta/(1-\beta)} - 1\right\}^{1/\beta} \tag{7}$$

where S_r is the residual saturation, and α and β will be empirically measured for the materials studied.

When advection is negligible (that is, $\vec{u} = 0$), Eq. (2) simplifies to Eq. (8), provided that the product $\varepsilon\sigma\rho$ is constant.

$$\partial_t = \nabla \cdot (D_e \; \nabla C) \tag{8}$$

No-flow and ambient boundary conditions will be used for modeling the results of the field tests. No-flow boundaries stop both flow and transport at the boundaries of this type (for example, see Figure 2). Ambient boundary conditions set the values of P, σ and C_0 at external boundaries to their initial values. Temperature affects the diffusion coefficient because fluid viscosity and density are temperature-dependent; these effects will be taken into account so that laboratory and field determinations of the effective diffusion coefficient can be compared on a common basis.

3.4 Sensitivity Analysis

The TRACR3D code was used to derive estimates of tracer concentrations that may be obtained in these tests. The purpose of these simulations was to determine the sensitivity of the effective diffusion coefficients, calculated from the data, to the uncertainties in the measurements. The following assumptions were made. The borehole geometry was that shown in Figure 2. The simulations assumed that the water and tracer source were placed in the bottom of the open borehole. The borehole was treated as a well-drained porous medium with a porosity of 0.99, a saturated permeability of 0.1 darcy, and P_c and k_r as defined by Eqs. (9) and (10) , respectively:

$$P_c = 5 \times 10^3 \, (1 - \sigma) \tag{9}$$

$$k_r = \sigma \tag{10}$$

These properties allowed the borehole to drain in approximately two days into the Calico Hills tuff which was assumed to be a homogeneous medium with a porosity of 0.33 and a saturation of 0.91.

At the conclusion of an *in situ* test, the borehole was assumed to be overcored. The resulting core, with a diameter ~30.5 cm (12 in.), was assumed to be cut so as to obtain a disk that extended 5-cm (2 in.) downward from the bottom of the borehole. The disk was cut in half parallel to the symmetry axis. One of the resulting half-disks was cut parallel to a radius of the original right cylinder to form two half-disks, each 2.5 cm (1 in.) thick. Each of these half-disks was subdivided as shown in Figure 6 to produce a total of 24 pieces of core for analysis. The TRACR3D results were integrated over the 10 sample types, of which 5 are shown in Figure 6, and the remainder are located in the half-disk below. The results of the calculations for a diffusion test that lasts 9 months are shown in Figure 7. The abscissa is the $\log_{10}$ of the effective diffusion coefficient, and the ordinate is the $\log_e$ of the relative expected total amount of tracer in the sample divided by the original concentration of tracer in the source. The curves are labeled with the sample numbers from Figure 6.

The effects of uncertainties in the measurements of tracer concentrations are shown in Figure 8. Both axes show $\log_{10}$ of the effective diffusion coefficient. The broken line is the true coefficient, and the other three curves show the lower bounds on the estimated values of the effective diffusion coefficients that could be expected for errors of 15%, 30%, and 50% associated with the individual concentration measurements. The statistical test from which these curves are derived bounds the range of effective diffusion coefficient values that can be rejected with a probability of 0.95 as a function of the true value in a test designed to reject the true value only 5% of the time.

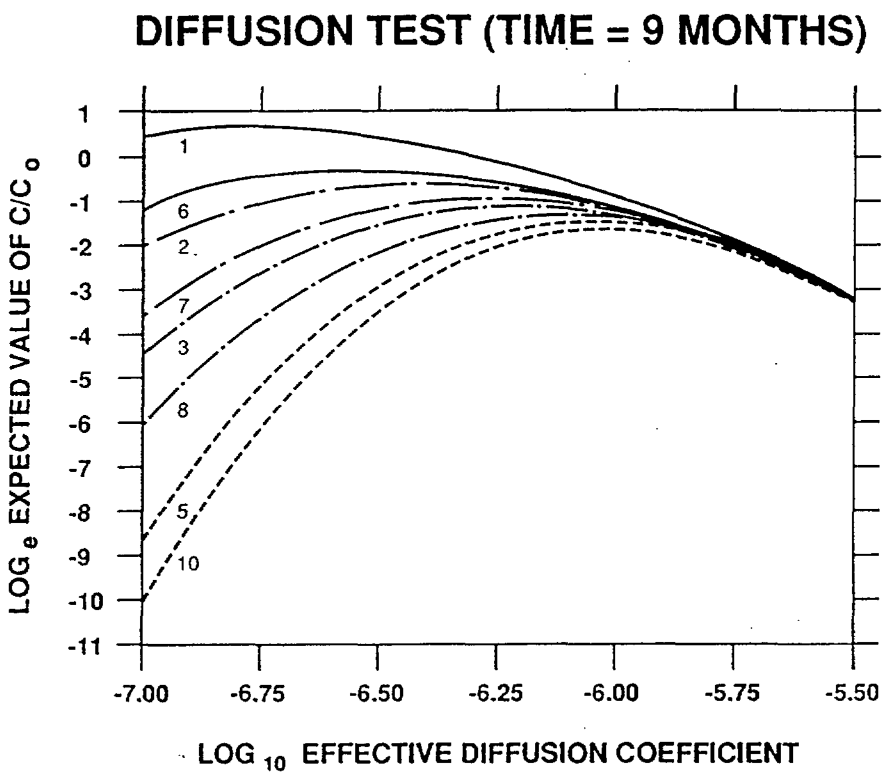

Figure 7. Plot of Expected Values for the Relative Tracer Concentration in Core Sections as a Function of the Effective Diffusion Coefficient. The Curves are Labeled with the Core Section Numbers Defined in Figure 6.

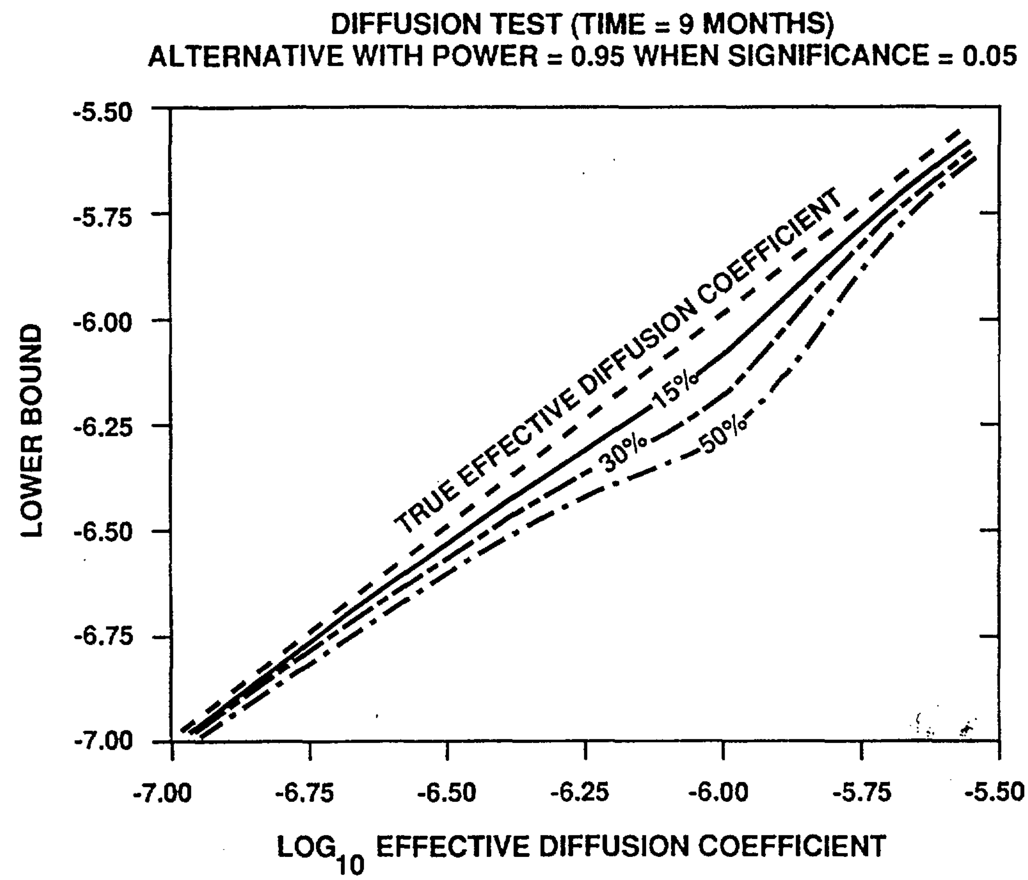

Figure 8. Plots of the Lower Bounds on Values for the Effective Diffusion Coefficient as a Function of the True Value, for Various Errors Associated With the Individual Measurements of Relative Tracer Concentration. The Dashed (Uppermost) Line Indicates the True Value of the Effective Diffusion Coefficient. The Other Curves are Labeled With the Experimental Errors in Percentages.

The bulge in the curves in Figure 8 near effective diffusion coefficient values of 10^{-6} can be explained qualitatively by referring to the curves in Figure 7. The curves at the left side of Figure 7 increase so rapidly that effective diffusion coefficient values can be obtained with very little uncertainty. Around values of 10^{-6}, the curves flatten, so the measured tracer concentrations cannot be used to determine values of the effective diffusion coefficient as precisely as at the extremities. This relative lack of certainty results in the bulges that occur in the curves in Figure 8. Overall, however, the patterns in Figure 7 make different values for the coefficient easy to detect in a homogeneous medium, even with large measurement errors.

Additional modeling studies using TRACRN are to be conducted in order to evaluate the impact of uncertainties in measured parameters on the interpretation of the results.

3.5 Test Representativeness

The comparison of effective diffusion coefficients derived from laboratory measurements (Study Plan for Diffusion, Study 8.3.1.3.6.2) with those determined *in situ* is an important aspect of this site characterization study. The *in situ* measurements will result in data from three locations beneath Yucca Mountain. The spatial variations of the geologic media may result in requests from the performance assessment investigators for effective diffusion coefficients in materials or in locations that differ from those used for the *in situ* determinations. The availability of both laboratory and field data will aid in determining the distribution functions of effective diffusion coefficients used for performance assessment modeling. With these data, modeling of radionuclide transport rates can be made with much greater confidence in the accuracy of the results than would be possible without the data.

4.0 APPLICATION OF RESULTS

4.1 Resolution of Performance Issues

The results of this study will supply quantitative information concerning solute diffusion under *in situ* conditions. The data will be used to calculate radioactive nuclide transport through liquid pathways for repository system performance. Thus, application of results in this study is tied directly to the resolution of the following performance assessment issues and related information needs:

Performance Issue 1.1: Will the mined geologic disposal system meet the system performance objective for limiting radionuclide releases to the accessible environment as required by 10 CFR 60.112 and 40 CFR 191.13? (SCP Section 8.3.5.13; NRC, 1983; EPA, 1985).

Diffusion measurements from this study will be used to satisfy the requirements for the site-specific Information Need 1.1.1, "Site Information Needed to Calculate Releases to the Accessible Environment" (SCP Section 8.3.5.13.1) and Information Need 1.1.3, "Calculational Models for Predicting Releases to the Accessible Environment Attending Realizations of the Potentially Significant Release-Scenario Classes" (SCP Section 8.3.5.13.3).

Performance Issue 1.2: Will the mined geologic disposal system meet the requirements for limiting individual doses in the accessible environment as required by 40 CFR 191.15?

The results of this study will be used to satisfy the requirements for the site-specific Information Need 1.2.1, "Determination of Doses to the Public in the Accessible Environment Through Liquid Pathways." The diffusion measurements from this study will provide supporting information required to evaluate compliance with parts of three federal regulations, 10 CFR 60, 10 CFR 960, and 40 CFR 191, as described in Section 1.2.

4.2 Interfaces with Other Site-Characterization Studies

The results obtained in this study will be used in the following investigations. However, this study plan neither constrains nor is constrained by progress by these other studies and activities. Information will be provided to other studies through the YMP data management system, such as the Site and Engineering Properties Database (SEPDB).

Description of the Unsaturated Zone Hydrologic System at the Site (8.3.1.2.2). This investigation is directed at understanding the fundamentals of unsaturated flow and transport at Yucca Mountain. Diffusion is one of the transport parameters to be characterized in this investigation. Of the nine studies in this investigation, the Diffusion Tests in the ESF (Study 8.3.1.2.2.5) is the only study addressing aqueous transport by matrix diffusion.

Study Plan for Diffusion (8.3.1.3.6.2). The comparison of laboratory measurements of effective diffusivity obtained in the Diffusion Study, with measurements made under *in situ* conditions is an important application of this study. This comparison is expected to help increase the confidence that laboratory measurements result in data that are comparable to those measured under *in situ* conditions.

Radionuclide Retardation by All Processes along Flow Paths to the Accessible Environment (8.3.1.3.7). A goal of this study is to evaluate the significance of physical processes, including matrix diffusion, in affecting radionuclide transport. The information will be used to address Information Need 1.1.3, by developing and testing calculational models of solute transport in the unsaturated and saturated zones capable of predicting time-dependent mass-flux fields in at least two dimensions (SCP Section 8.3.5.13.3). A high level of confidence is desired for this information (SCP Table 8.3.5.10-5). To evaluate matrix diffusion, the retardation study will correlate the results obtained from the laboratory (8.3.1.3.6.2), field (8.3.1.2.2.5), and modeling investigations and activities.

5.0 SCHEDULE AND MILESTONES

5.1 Schedules

A tentative schedule for the work covered in this study is shown in Figure 9. The schedule information includes the sequencing, interrelations, and relative durations of the described activities. Interfaces among the studies and activities described in Section 4.2 are not shown because they neither constrain nor are constrained by progress on the other studies.

5.2 Milestones

Schedule components associated with the single activity comprising this study are listed in Table 6, along with milestone numbers and titles from the master schedule presented in SCP Section 8.5.1.2. Specific dates are not included in the table because the schedule depends upon the ESF construction schedule, which has been revised from that originally stated in the SCP.

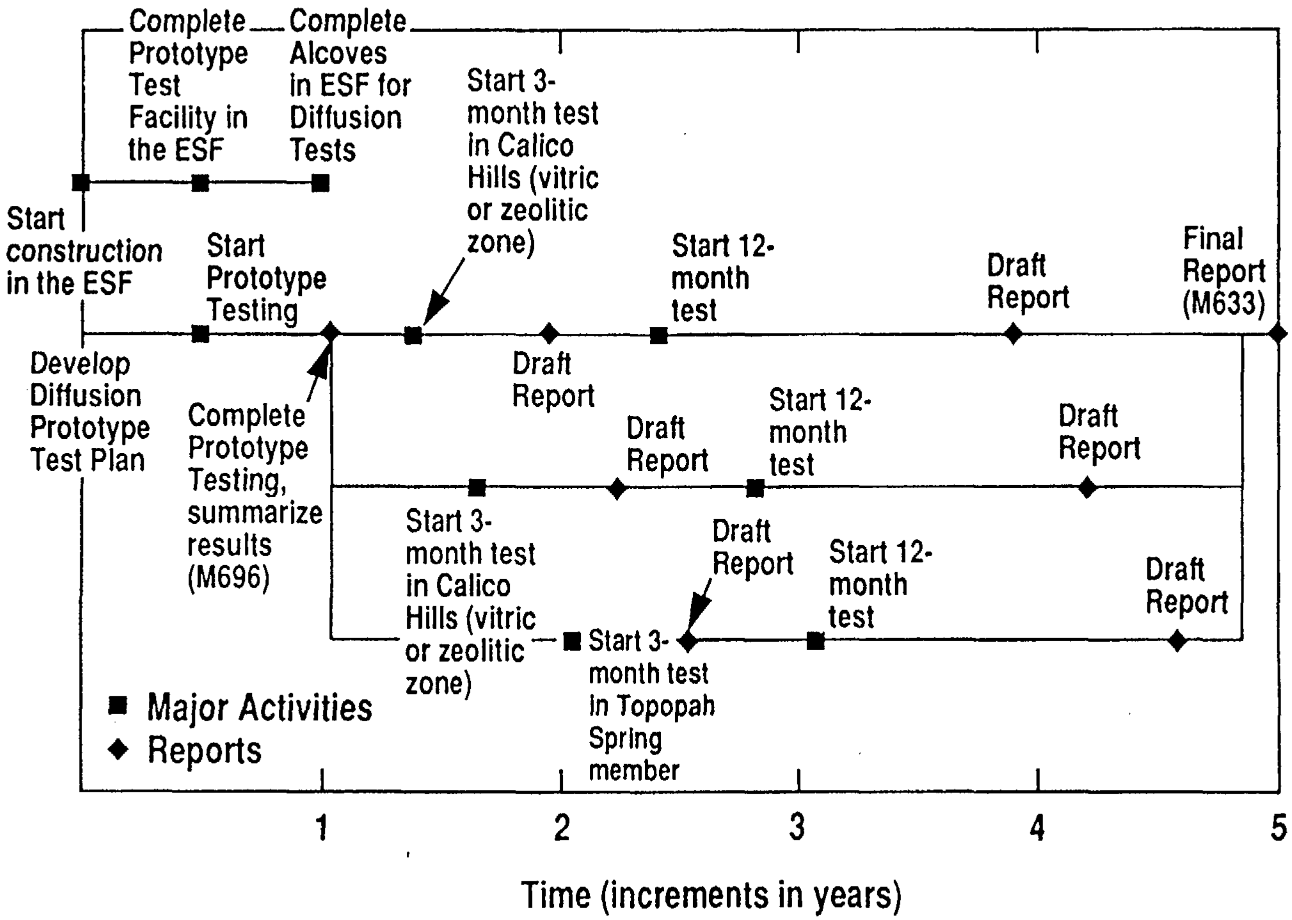

Figure 9. Schedule for the Diffusion Tests in the ESF.

TABLE 6

SCHEDULE FOR THE DIFFUSION TESTS IN THE ESF

Item	Date
Prototype Testing in the ESF	Upon completion of ESF Prototype Facility
Complete prototype testing in the ESF and report results	6 months after start of prototype testing; Milestone M696
Start first 3-month diffusion test in the Calico Hills unit	4 months after completion of prototype testing
Start second 3-month diffusion test in the Calico Hills Unit	4 months after initiation of first Calico Hills diffusion test
Draft report on first 3-month diffusion test in the Calico Hills unit	3 months after completion of first 3-month diffusion test in the Calico Hills unit.
Start 3-month diffusion test in the Topopah Spring Member	4 months after initiation of second Calico Hills diffusion test
Draft report on second 3-month diffusion test in the Calico Hills unit	3 months after completion of the second 3-month diffusion test in the Calico Hills unit
Start first 12-month diffusion test in the Calico Hills unit	9 months after completion of the first 3-month diffusion test in the Calico Hills unit
Draft Report on 3-month diffusion test in the Topopah Spring Member	3 months after completion of 3-month diffusion test in the Topopah Spring Member
Start second 12-month test in the Calico Hills unit	9 months after completion of the second 3-month diffusion test in the Calico Hills unit
Start 12-month test in the Topopah Spring Member	9 months after completion of the 3-month diffusion test in the Topopah Spring Member
Draft report on the first 12-month Calico Hills diffusion test	6 months after completion of the first 12-month Calico Hills diffusion test
Draft report on the second 12-month Calico Hills diffusion test	6 months after completion of the second 12-month Calico Hills diffusion test
Draft report on the 12-month Topopah Spring Member diffusion test	6 months after completion of the 12-month Topopah Spring Member diffusion test
Final Report, M633	6 months after completion of the 12-month Topopah Spring Member diffusion test

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APPENDIX A

QUALITY ASSURANCE SUPPORT DOCUMENTATION

NOTE: A quality assurance grading report for the study's WBS element will be prepared before the start of work in accordance with applicable YMP Office guidance.

TABLE A-1

APPLICABLE NQA-1 CRITERIA FOR SCP STUDY PLAN 8.3.1.2.2.5
AND HOW THEY WILL BE SATISFIED

NQA-1 Criteria	Documents Addressing These Requirements		Date of Issue (Anticipated)
1. Organization	The organization of the Office of Civilian Radioactive Waste Management (OCRWM) program is described in Section 8.6 of the SCP. The LANL QA organization is described in the LANL-YMP-QAPP.		
	TWS-QAS-QP-01.1	Interface Control	03/19/90
	TWS-QAS-QP-01.2	Stop Work Control	02/20/89
	TWS-QAS-QP-01.3	Conflict Resolution	03/04/89
2. QA Program	The LANL QA program is described in the LANL-YMP-QAPP and includes a program description addressing each of the NQA-1 criteria. An overall description of the YMP QA program for site characterization activities is described in Section 8.6 of the SCP. The LANL QA program contains quality implementing procedures (QP) further defining the program requirements.		
	TWS-QAS-QP-02.3	Readiness Review	03/19/90
	TWS-QAS-QP-02.4	Management Assessment	06/05/89
	TWS-QAS-QP-02.5	Selection of Personnel	03/02/90
	TWS-QAS-QP-02.6	Personnel Orientation and Indoctrination	08/17/90
	TWS-QAS-QP-02.7	Personnel Training	08/17/90
	TWS-QAS-QP-02.9	Personnel Proficiency Evaluations	03/02/90
3. Design and Scientific Investigation Control	This study is a scientific investigation. The following QPs apply:		
	TWS-QAS-QP-03.2	Preparation and Technical and Policy Reviews of Technical Information Products	05/09/89
	TWS-QAS-QP-03.3	Preparation and Review of an SCP Study Plan	05/24/89
	TWS-QAS-QP-03.5	Documenting Scientific Investigations	03/10/89

TABLE A-1

APPLICABLE NQA-1 CRITERIA FOR SCP STUDY PLAN 8.3.1.2.2.5
AND HOW THEY WILL BE SATISFIED
(continued)

NQA-1 Criteria	Documents Addressing These Requirements		Date of Issue (Anticipated)
	TWS-QAS-QP-03.7	Peer Review	05/24/89
	LANL-YMP-QP-03.17	Reviews of Software and Computational Data	01/25/91
	LANL-YMP-QP-03.18	Creation, Management, and Use of Computational Data	01/25/91
	LANL-YMP-QP-03.19	Documentation of Software and Computational Data	01/25/91
	LANL-YMP-QP-03.20	Software Configuration Management	01/25/91
	LANL-YMP-QP-03.21	Software Life Cycle	01/25/91
	LANL-YMP-QP-03.22	Verification and Validation of Software and Computational Data	01/25/91
4. Procurement Document Control	LANL-YMP-QP-04.4	Procurement of Commercial-Grade Items and Services	12/10/90
	LANL-YMP-QP-04.5	Procurement of Noncommercial-Grade Items and Services	12/10/90
5. Instructions, Procedures, Plans, and Drawings	Applicable parts of this criterion are covered in Item 6.		
6. Document Control	LANL-YMP-QP-06.1	Document Control	11/16/90
	LANL-YMP-QP-06.2	Preparation, Review, and Approval of Quality Administrative Procedures	10/10/90
	LANL-YMP-QP-06.3	Preparation, Review, and Approval of Detailed Technical Procedures	10/10/90
7. Control of Purchased Items and Services	Applicable parts of this criterion are covered in Item 4.		

TABLE A-1

APPLICABLE NQA-1 CRITERIA FOR SCP STUDY 8.3.1.2.2.5
AND HOW THEY WILL BE SATISFIED
(concluded)

NQA-1 Criteria	Document Addressing These Requirements		Date of Issue (Anticipated)
8. Identification and Control of Samples and Data	TWS-QAS-QP-08.1	Identification and Control of Samples	10/10/89
	TWS-QAS-QP-08.2	Control of Data	08/23/89
9. Control of Processes	This criterion has been determined to be inapplicable to the scope of work of the LANL YMP.		
10. Inspection	This criterion has been determined to be inapplicable to the scope of work of the LANL YMP.		
11. Testing	This criterion has been determined to be inapplicable to the scope of work of the LANL YMP.		
12. Control of Measuring and Test Equipment	The control of instrument calibration and data collection is described in the technical procedures referenced in Section 3 of the LANL-YMP-QAPP. The following QP also applies:		
	TWS-QAS-QP-12.1	Control of Measuring and Test Equipment	02/20/90
13. Handling, Shipping, and Storage	TWS-QAS-QP-13.1	Handling, Storage, and Shipping Equipment	11/03/89
14. Inspection, Test, and Operating Status of Engineered Items	This criterion has been determined to be inapplicable to the scope of work of the LANL YMP.		
15. Control of Nonconformances	TWS-QAS-QP-15.2	Deficiency Reporting	04/03/90
16. Corrective Action	TWS-QAS-QP-16.2	Trending	06/20/89
17. Records	LANL-YMP-QP-17.3	Records Management	01/11/91
18. Audits	LANL-YMP-QP-18.1	Audits	03/01/91
	TWS-QAS-QP-18.2	Surveys	05/30/90
	TWS-QAS-QP-18.3	Auditor Qualification	05/30/90

SP 8.3.1.2.2.5 R0

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