Rec'd w/ltr dtd. 9/1/92

Acc. # 9209100217

U.S. DEPARTMENT OF ENERGY

OCRWM

YUCCA MOUNTAIN

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT

CONTROLLED
NO. 1
THIS IS A
RED STAMP
COPY

Retardation Sensitivity Analysis

8.3.1.3.7.1

Prepared by

Los Alamos National Laboratory

9209100238

YUCCA MOUNTAIN PROJECT

T-AD-088
12/89

CONTROLLED
NO. 1
THIS IS A
RED STAMP
COPY

Study Plan Number 8.3.1.3.7.1

Study Plan Title Retardation Sensitivity Analysis

Revision Number 0

Prepared by: Los Alamos National Laboratory

Date: July 1992

Claudia M Newbury 8/11/92
Director, Regulatory and Site Evaluation Division / Date

R.C. Spence 8/8/92
Director, Quality Assurance Division / Date

STUDY PLAN FOR
RETARDATION SENSITIVITY ANALYSIS

K. Birdsell, K. Eggert, and G. Zyvoloski
Los Alamos National Laboratory

ABSTRACT

The Retardation Sensitivity Analysis study will provide analyses on the effects that geochemical, geophysical, and coupled processes, as well as particulate transport have on radionuclide transport from the candidate repository site to the accessible environment at Yucca Mountain. A conceptual geochemical/geophysical model of the Yucca Mountain site will be developed based on available geochemical, hydrologic, and other site characterization data, and on the analyses done under this study. Computational models summarizing the processes in the conceptual model will be constructed. These computational models will be used to perform integrated transport calculations to estimate radionuclide migration rates from the repository to the accessible environment and to determine the sensitivity of such transport calculations to retardation processes and parameters embodied in the modes. Model validation will also be an integral part of this study.

This study will identify the processes having the most significant effects on transport. These results will be used to guide site characterization activities concerned with gathering geochemical data. By interacting with the geochemistry program, data will be incorporated into sensitivity analyses to provide quantitative direction as to areas where further characterization is required or to indicate where characterization is sufficient. Also by identifying the processes that are most significant, the information may be used to restrict the scope of characterization efforts to those processes and parameters that most significantly affect transport. Results of integrated transport calculations will be incorporated into the total system performance assessments. These results can be used to evaluate the effectiveness of Yucca Mountain's geochemical barriers, to estimate potential radionuclide breakthrough to the accessible environment, and to evaluate assumptions used in the modeling of total system performance assessments.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF VARIABLES

$a_{\alpha j}$ = stoichiometric coefficient of component j in species C_α [-]
$\bar{A}$ = energy per unit volume [E/L^3]
$A_{x,c}$ = chemical activity of components at concentration X or c [-]
$b_{\alpha j}$ = stoichiometric coefficient of component j in species S_α [-]
B_k = the rate of appearance of colloid particles in a size category per unit solution volume [$L^{-3}\,T^{-1}$]
C = solute concentration in transporting fluid [M/M fluid]
c_α = concentration of species α in the aqueous phase [M/L^3]
D = molecular diffusivity of a species in the transporting phase [L^2/T]
$\bar{D}$ = hydrodynamic dispersion of a species in the transporting phase [L^2/T]
$d_{s\ell}$ = liquid phase thermal diffusion coefficient [LT]
d_{sg} = vapor phase thermal diffusion coefficient [LT]
E = Young's modules [M/LT^2]
E_k = rate at which colloidal particles disappear from a particular particle size category per unit solution volume [$L^{-3}\,T^{1}$]
F = arbitrary function [-]
g = acceleration caused by gravity [L/T^2]
h_ℓ = specific enthalpy of liquid [E/M]
h_g = specific enthalpy of vapor [E/M]
H = Biot's physical constant [M/LT^2]
I = ionic strength [-]
k = permeability [L^2]
K_{c_α} = equilibrium formation constant of species c_α
K_d = equilibrium sorption coefficient [L^3/M]
K_{s_α} = equilibrium formation constant of species s_α
L = a typical length scale [L]
M = molecular weight [M/mole]
n_{aq} = number of species in aqueous phase
n_s = number of species in solid phase
N_c = total number of components
P = fluid pressure [M/LT^2]
ΔP = change in pore pressure [M/LT^2]
q_e = energy source term [E/L^3T]
R = relative permeability [-]
s_α = concentration of species α in the solid phase [M/L^3 fluid]

S = degree of phase saturation of pore space [-]
$\dot{S}$ = phase source rate [M/L^3 T]
$\dot{S}_{c_\alpha}$ = source/sink term [M/L^3 T] for species α attributable to aqueous phase complexation
t = time [T]
T = temperature [θ]
T_j = total concentration of component j [M/L^3]
ΔT = change in temperature [θ]
$\vec{u}$ = phase velocity vector [L/T]
u = x-displacement [L]
v = y-displacement [L]
V_α = valence of species α
w = z-displacement [L]
$\bar{x}$ = location vector [L]
X_j = concentration of component j [M/L^3]
α = coefficient of thermal expansion [θ^{-1}]
ϵ = strain tensor [-]
ϕ = medium porosity [-]
δ = activity coefficient
σ = stress tensor [M/LT^2]
ρ = phase density [M/L^3]
ρ_m = density of rock matrix [M/L^3]
κ = effective bulk thermal conductivity [E/L θ]
μ = dynamic viscosity of fluid [M/LT]
ξ = arbitrary property axis for colloids
υ = Poisson's ratio
υ_{k_j} = change in colloid property axis with time ($\partial\xi/\partial t$)
λ = ln 2/half-life of solute [T^{-1}]
τ_c = constrictivity [-]
χ = colloid number concentration

Subscripts

g = gas phase
ℓ = liquid phase
i = arbitrary phase
k = colloid particle type
α = αth species of radionuclide

Units

[E] = units of energy
[θ] = units of absolute temperature
[L] = units of length
[M] = units of mass
[T] = units of time

STUDY PLAN FOR RETARDATION SENSITIVITY ANALYSIS

1.0 PURPOSE AND OBJECTIVES

1.1 Objectives of the Study

The purpose of this study is to provide analyses of the effects of geochemical processes on radionuclide transport between the repository and the accessible environment. The primary reason for these analyses is to identify the most sensitive processes and to help guide geochemical site characterization. These analyses will be performed in sufficient detail to test and add justification to assumptions regarding the effects of site geochemistry on the transport calculations that will be the basis of total system performance assessment. Further, the analyses will serve as vehicles for compiling and summarizing the effectiveness of the natural geochemical barriers for inhibiting radionuclide migration. Finally, through sensitivity analysis, this study will aid in determining the point at which the site geochemistry is sufficiently characterized.

The specific objectives of this study are as follows.

- Construct computational models for radionuclide transport and retardation at Yucca Mountain that summarize conceptual models of the effects of site geochemical processes on retardation and that may be used to assess the relative effects of geochemical processes on transport.
- Use the models to perform integrated calculations to assess radionuclide transport between the repository and the accessible environment.
- Demonstrate the sensitivity of transport calculations to retardation processes assumed or demonstrated to be active at the Yucca Mountain site.
- Determine the sensitivity of transport calculations to the parameters of the conceptual retardation models.
- Use the models to develop characterization experiments for the purpose of gathering required site geochemical data and for validating, to the extent possible, conceptual and computational models.

1.2 Regulatory Rationale and Justification

The results of this study will be used to satisfy Investigation 8.3.1.3.7 (DOE, 1988) and to partially guide the geochemical characterization needs described in Site Characterization Plan (SCP) Section 8.3.1.3. The results will also be used to test assumptions for the total system performance assessments used to resolve Issue 1.1. Results from the integrated transport calculations will be used to resolve Issues 1.1 and 1.8, and Information Needs 1.1.3, 1.1.4 and 1.1.5. This study is performed under WBS 1.2.3.4.1.5.1 [formerly WBS 1.2.3.4.1.7.A (Cederberg, 1986)].

1.2.1 General

SCP Section 8.3.1.3 requires that "... the data collected in order to describe the present and expected geochemical characteristics provide the information required by the design and performance issues." SCP Investigation 8.3.1.3.7 requires description of "radionuclide retardation by all processes along flow paths to the accessible environment." To ensure that the geochemical data gathered during site characterization are sufficient for this purpose, the most sensitive processes and parameters must be identified and characterized. The rationale and justification for the activities described below are that these activities will provide the analyses that, when combined with laboratory and field studies, will identify those sensitive processes and parameters.

Figure 1 (SCP Figure 8.3.1.3-2) shows how this study fits into the geochemistry program. The study provides sensitivity analyses of individual transport mechanisms and integrates these mechanisms into a geochemical/geophysical model of radionuclide transport at Yucca Mountain.

In addition, the retardation sensitivity analysis will support total system performance assessment calculations. The total system performance assessment (Issue 1.1) is a probabilistic analysis of transport of radionuclides to the accessible environment. To develop meaningful probability distributions for releases, these analyses must be simplified through the use of assumptions regarding, in part, transport processes and the interaction of radionuclides with the geochemical environment. These assumptions must be tested through detailed analyses and laboratory and field testing. In guiding the geochemical characterization activities, the analyses performed in the activities below will provide a detailed study of the assumptions regarding transport and geochemistry based on mechanistic models. Integrated transport calculations, based on the geochemical/geophysical model developed under the study, will evaluate the retardation capacity of the mountain and provide quantitative estimates of radionuclide releases to the accessible environment in support of Issue 1.1.

1.2.2 Performance Allocation

Performance allocation was used by the Yucca Mountain Site Characterization Project (YMP) to establish the issue resolution strategies (IRS) for performance and characterization issues in the YMP Issues Hierarchy. A general discussion of the performance allocation process is presented in Section 8.1 of the YMP SCP. The IRS for the geochemical program is presented in SCP Section 8.3.1.3.

In addition, a preliminary performance allocation for the total system performance (Issue 1.1) is provided in SCP Section 8.3.5.13. Tables 8.3.5.13-17 of the SCP summarize the primary processes and conditions relied upon for total system performance for the classes of scenarios to be considered. Several of the primary processes require assessment of transport with adsorptive retardation. Further, the input parameter list for SCP Investigation 8.3.5.13.3 (Information Need 1.1.3) requests both conceptual and calculational models from Investigation 8.3.1.3.7. Therefore, the tie to the performance allocation process may be found in the IRS for the geochemical program (SCP Section 8.3.1.3) and in the input parameters of Information Need 1.1.3 (SCP Study 8.3.5.13). Table 1 (part of SCP Table 8.3.1.3-2) shows the performance measures or parameters associated with the models developed under this study as part of the site geochemistry program.

1.2.3 Tie to Regulations

SCP Section 8.3.1.3, which calls for geochemical characterization, is a subissue of Key Issue 1, "Will the mined geologic disposal system at Yucca Mountain isolate the radioactive waste from the accessible environment after closure in accordance with the requirements set forth in 40 CFR Part 191 (EPA, 1986), 10 CFR Part 60 (NRC, 1987), and 10 CFR Part 960 (DOE, 1987)." As such, SCP Section 8.3.1.3 will provide information on the geochemical characteristics needed for the performance assessments and license application content as required by 10 CFR 60.112, 60.122, and 60.21, respectively, and the siting guidelines of 10 CFR 960.

The activities of this study serve to guide geochemical characterization by helping to identify the most significant effects of geochemistry on radionuclide transport. Further, by assembling the transport model necessary for that purpose, the study will also provide integrated calculations of the effects of site geochemistry on radionuclide transport to the accessible environment. Therefore, these activities will help to ensure that the geochemical data developed during site characterization will be sufficient for design and performance assessment needs.

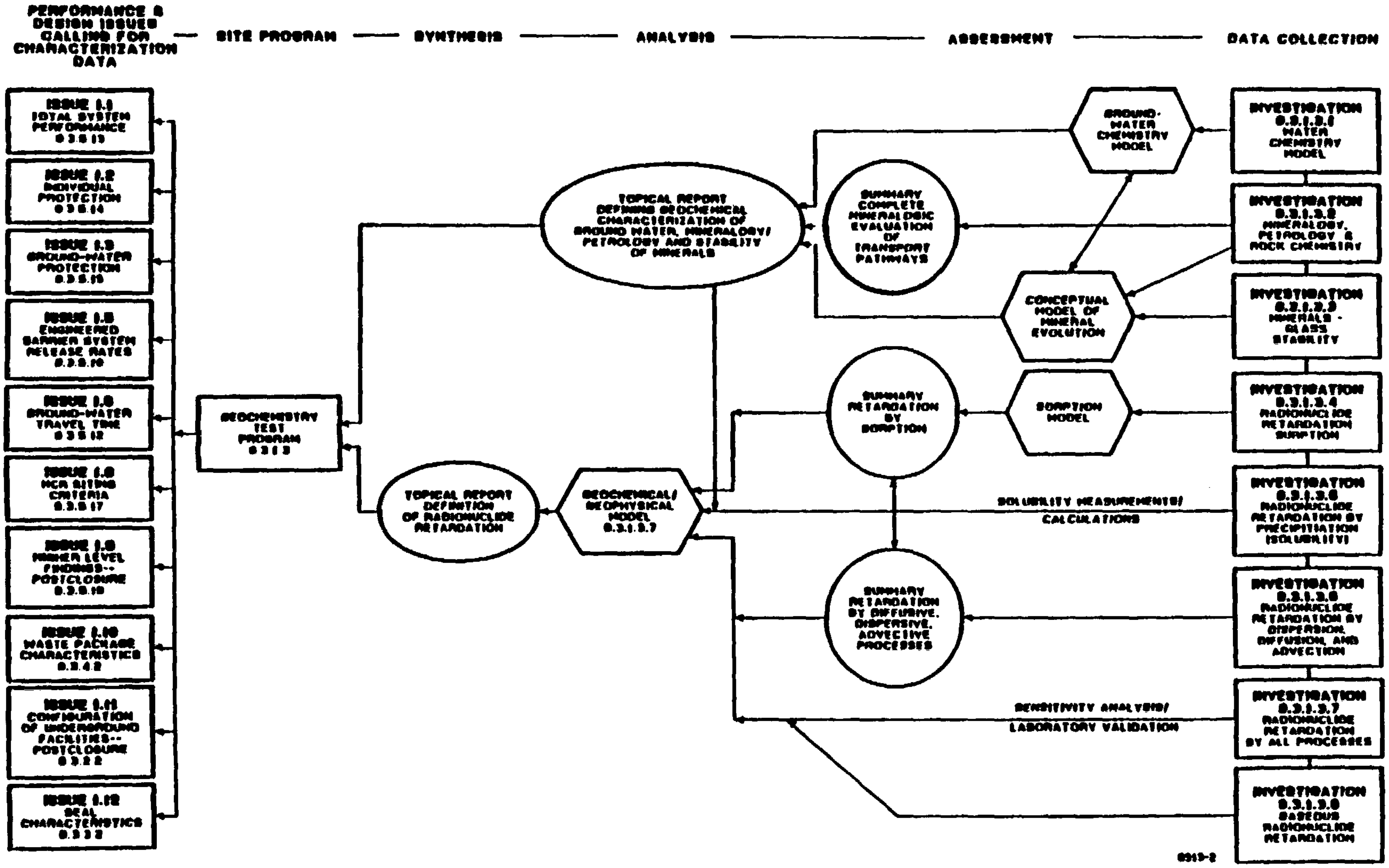

Figure 1. Logic Diagram for Geochemistry Program 8.3.1.3
Source: SCP Figure 8.3.1.3-2

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 1 of 6)

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis				Studies or Activities to Reduce Uncertainty
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis	Need to reduce uncertainty	
RETARDATION MODEL	Radionuclide mobility is substantially retarded by (1) sorption, (2) solubility, and (3) dispersion/diffusion/filtration.	High--mechanisms of transport and retardation are only generally known.	Retardation is largely bypassed by flow field characteristics (i.e., rapid along fractures). One retardation process dominates. Retardation processes in the natural situation are too complex to model reliably.	NA	NA	NA	NA	8.3.1.3.7--retardation, all processes
Liquid Pathway	Predominant release pathway is in the liquid phase; movement is downward and laterally from the repository. Retardation provided by chemical and physical processes.	Low to medium--current hydrologic data support downward movement. Current data base is not extensive enough.	Rapid groundwater movement bypasses chemical and physical retardation processes.	NA	NA	NA	NA	NA

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 2 of 6)

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis				Studies or Activities to Reduce Uncertainty
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis	Need to reduce uncertainty	
Sorption	Sorption is an element-specific function of water composition, solids, redox condition, pH, temperature, rock texture, and hydrologic properties.	Medium to high--some uncertainty over site-specific conditions for individual element behavior	Site specific behavior for specific radionuclides is too complex to predict with confidence. Sorption "barrier"bypassed by physical conditions, rapid fracture flow, and colloidal transport.	Geochemical retardation	High	High	High	8.3.1.3.4.3--sorption models 8.3.1.2.3.1.7--C-hole reactive tracer test
• Sorption as a function of substrate, water chemistry, and sorbate concentration. (continued)	Sorption is controlled by these parameters.	Medium to high--some certainty exists in site conditions	Sorption cannot be modeled as a function of these parameters.	*Subset of sorption model element; overall ranking given with sorption element above.*				8.3.1.3.2.1--3-D mineral distribution 8.3.1.3.4.1.1--sorption as a function of solid phase composition 8.3.1.3.4.1.2--sorption as a function of sorbing element concentration 8.3.1.3.4.1.3--sorption as a function of groundwater composition 8.3.1.3.4.1.5--statistical analysis

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 3 of 6)

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis		
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis
• Sorption as a function of substrate, water chemistry, and sorbate concentration. (concluded)						
• Sorption on particulates and colloids	Sorption on particulates/colloids expected to be minor, and filtration would further reduce effects.	Low--mobile particulates not expected in the far field	Particulate transport may be possible in a flow field dominated by rapid fracture flow.	Subset of sorption model element; overall ranking given with sorption element above.		
• Microbial activity	Not thought to be a significant transport mechanism.	Low--microbial activity below, consistent with existing filed data	No credible alternative	Subset of sorption model element; overall ranking given with sorption element above.		

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 4 of 6)

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis				Studies or Activities to Reduce Uncertainty
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis	Need to reduce uncertainty	
Solubility	Solubility limits levels of radionuclides through far field and solubility limited by equilibrium thermodynamic relations and/or precipitation rates.	Medium to high--in element thermodynamic data and in site chemical environment	Radionuclide concentrations not limited by thermodynamic relations due to colloid formation; thermodynamic data unavailable; nucleation unfavorable. Sorption processes dominate; saturation is not approached.	Geochemical retardation	Medium (saturated zone) High (unsaturated zone)	Low to medium--sorption expected to control radionuclide concentrations	Medium	8.3.1.3.5--retardation by precipitation
• Precipitation (aqueous speciation and solubility modeling)	Radionuclide concentrations in the far field are limited by solubility/precipitation constraints.	Medium to high--limited data on actinides under site conditions.	Solubility/precipitation relationships cannot be modeled reliably.	Subset of solubility model element; overall ranking given with solubility element above.				8.3.1.3.5.1--dissolved species concentration limits
• Colloid formation and stability	Colloid formation is limited under far field site conditions for most radionuclides, and filtration would limit transportation.	Medium--some uncertainty exists about behavior under site conditions.	Colloids form for some radionuclides and transport is possible for rapid groundwater movement along fractures	Subset of solubility model element; overall ranking given with solubility element above.				8.3.1.3.5.2--colloid behavior 8.3.1.3.7.2--applicability of laboratory data to repository transport

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 5 of 6)

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis			
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis	Ne re unce
Dispersion/diffusion/ filtrations	Retardation of radionuclide transport by physical processes along pathways for matrix-dominated flow field and for some conditions of fracture flow	High--flow mechanism is not well established at the site; data on physical retardation mechanisms is very sparse.	Flow is dominated by rapid fracture-flow pathways and retardation mechanisms are bypassed. Data on physical retardation mechanism cannot be obtained for reliable quantification.	Geochemical retardation	Medium (saturated zone) High (unsaturated zone)	Low to medium--sorption expected to control radionuclide concentrations	Mod
WATER CHEMISTRY MODEL	Groundwater chemistry is a controlling factor in retardation by sorption and solubility. Groundwater composition controlled by water-rock interactions trends toward equilibrium.	Low to medium--some uncertainty exists in groundwater composition and thermodynamic modeling of rock-water interactions.	Kinetics of rock-water interactions are too slow to alter composition of recharge water, and flow is dominated by rapid fracture flow. Thermodynamic modeling, therefore cannot model groundwater composition and evolution predictably.	Groundwater chemistry contribution to retardation factors	High	High	H

TABLE 1

PERFORMANCE MEASURES AND PARAMETERS ASSOCIATED WITH GEOCHEMICAL MODELS FOR RETARDATION SENSITIVITY ANALYSIS STUDY (page 6 of 6

Current Representation		Uncertainty and Rationale	Alternative Hypothesis	Significance of Alternative Hypothesis		
Model Element	Current Representation			Performance measure, design or performance parameter	Needed confidence in parameter or performance measure	Sensitivity of parameter or performance measure to hypothesis
Saturated zone	Saturated zone groundwater composition is controlled by rock-water interactions along flow paths with no unexpected changes in groundwater chemistry along pathway to accessible environment.	Low--current data are adequate to explain saturated zone groundwater composition.	No credible alternative	Saturated zone residence times and retardation process. (If fluid flow is controlled by rapid fracture flow through the unsaturated zone, retardation in the saturated zone must be included in performance assessment of releases to the accessible environment.)	High--direct evidence of residence times in saturated zone and origins of water is required.	Medium--some compensation for chemical conditions is possible.
Unsaturated zone	Unsaturated zone groundwater composition is surface recharged, modified by rock-water interaction.	High--very few data are available.	Unsaturated zone water composition reflects deep sources in the saturated zone (i.e., former stands of groundwater table, upwelling leading to perched water).	Unsaturated zone water residence times and fluid chemistry as affected by dissolution of waste and retardation processes.	High	High

2.0 RATIONALE FOR SELECTED STUDIES

2.1 Technical Rationale and Justification

Three activities are described for this study:

- sensitivity analyses using a geochemical transport model of Yucca Mountain and integrated geochemical transport calculations (SCP Section 8.3.1.3.7.1.2),
- analysis of physical/chemical processes affecting transport (SCP Section 8.3.1.3.7.1.1), and
- transport models and related support (SCP Section 8.3.1.3.7.1.3).

This section provides the rationale for each of these activities. Briefly, the purpose of these activities is to identify the extent to which geochemical and physical processes affect calculations of transport to the accessible environment. The three activities of the study will proceed in parallel. The overall goal is to represent the processes affecting radionuclide transport at Yucca Mountain in a computational model capable of providing guidance to characterization and performance assessment activities and to demonstrate an understanding of the effects of geochemical and physical processes on radionuclide transport to the accessible environment.

The activities are presented in a different order here than in SCP Section 8.3.1.3.7.1 to better emphasize the development of this study. For clarification, Table 2 shows the correspondence between the subactivities presented in this study plan and those presented in the SCP. The primary focus of this study is to develop a geochemical model of Yucca Mountain and to use the model to perform integrated transport calculations of radionuclide releases from the repository to the accessible environment. The first activity serves this purpose. It serves to integrate processes, including those presented in the second activity of this study, and data, as they are gathered, into conceptual and computational models of radionuclide transport at Yucca Mountain. Transport calculations performed based on these models form sensitivity analyses which will be used to evaluate the significance of various retardation processes on radionuclide transport at Yucca Mountain. Parametric sensitivity analyses (Section 3.2.1.2) are included under this activity because they can be used to efficiently evaluate the relative contributions of various parameters to radionuclide migration rates and to uncertainty in retardation model calculations. Once model sensitivities are identified, unnecessary complexity in the total systems models can be reduced.

The second activity is concerned with identifying the geochemical and physical processes that most significantly affect transport. Less traditional transport processes (i.e., alternative conceptual models) are considered under this activity. However, the conceptual model described above will be modified as needed to incorporate significant processes identified under this second activity. The effects of colloidal transport and geochemical, physical, and coupled processes on radionuclide migration will be considered under this activity.

The third activity will provide verification, validation, and support for the computational codes and models developed as part of this study. A part of this validation effort is directed toward the design of experiments for characterization activities intended to minimize or quantify uncertainties.

2.1.1 Sensitivity Analyses Using a Geochemical Transport Model of Yucca Mountain and Integrated Geochemical Transport Calculations

Work under this activity will construct a computational model of the geochemical transport system at Yucca Mountain that represents, to the extent possible, the conceptual model of the effects of

TABLE 2

CORRESPONDENCE BETWEEN SUBACTIVITIES PRESENTED IN THE SITE CHARACTERIZATION PLAN AND STUDY PLAN 8.3.1.3.7.1

SCP Activity	Study Plan Section
Analysis of Physical/Chemical Processes Affecting Transport (8.3.1.3.7.1.1)	
Geochemical Processes Affecting Transport	Sect. 3.2.2.2
Physical Processes Affecting Transport	Sect. 3.2.2.3
Particulate Transport	Sect. 3.2.2.1
Heat-load Effects	Sect. 3.2.2.4
Coupled Phenomena	Sect. 3.2.2.4
Geochemical/Geophysical Model of Yucca Mountain Integrated Geochemical Transport Calculations (8.3.1.3.7.1.2)	
Construction of Geochemical/Geophysical Model	Sect. 3.2.1.1
Integrated Radionuclide Transport Calculations	Sect. 3.2.1.1
Transport Models and Related Support (8.3.1.3.7.1.3)	
Code Verification	Sect. 3.2.3.2
Model Validation	Sect. 3.2.3.3
Sensitivity Analysis	Sect. 3.2.1.2

site geochemistry on radionuclide transport. The conceptual model of site geochemistry will consist of the integration of site mineralogy and petrology, background water chemistry, models of radionuclide sorption and solubility, and other geochemical processes affecting transport to the accessible environment. The conceptual model will be continuously updated as new data are gathered, as validation exercises (Section 3.2.3.3) are evaluated, and as the significance of processes identified in the second activity of this study (Sections 2.1.2 and 3.2.2) are evaluated.

The computational model consists of flow, transport, and geochemical processes affecting transport. Initially this study will employ the traditional convective-dispersive equations for transport of dissolved radioactive, sorptive species as embodied in the TRACRN code (Section 3.2.1.1). The model will be used to make calculations of retardation of radionuclides as groundwater transport carries them through the units between the repository's underground facilities and the accessible environment.

The calculations will accomplish two goals. First, at intermediate stages, model calculations will supply sensitivity analyses of the effects of retardation on transport. The calculations will also address the effects of the spatial distribution of hydrologic parameters, geochemical parameters, and mineral assemblages on retardation of radionuclides. The analyses will integrate processes identified as having an effect on retardation and, by indicating the units that need further characterization, will help to ensure that geochemical characterization activities are efficiently applied to repository performance assessments. Models will also be used to design and interpret geochemical characterization experiments.

Second, calculations with the model will help to summarize existing knowledge of the overall retardation effectiveness of the geologic units between the repository and the accessible environment. As described in detail below (Section 3.2.1.1), the model will initially consist of a computational computer program that combines spatially distributed data for the units underlying the repository with the equations of flow and transport. The model uses a numerical solution that allows incorporation of the three-dimensional structure of sorbing units beneath the repository in the transport calculation. Therefore, the model provides a means for integrated representation of the effects of geochemistry on transport.

It must be stressed that the development of the geochemical transport model under this activity is evolutionary. Additional or alternative processes identified in the following activity (Sections 2.1.2 and 3.2.2) may be added to or deleted from the conceptual model as their significance to transport is shown. These processes may not be added to the computational code TRACRN itself, but their contributions to transport will be assessed as part of this study.

Alternative methods for performing the analysis of processes could include direct extrapolation of empirical data to repository conditions or analysis of natural analogues. However, simple extrapolation techniques cannot predict the geochemical interactions that may be expected to occur over the 10,000 yr required of repository performance. Further, computational techniques will be required to determine the response of the geochemical system to scenarios that will be analyzed as part of the total system performance assessment. Natural features that are representative analogues of a repository at Yucca Mountain have not been reported. At this time, the primary value of natural analogues is as a source of data for partial validation of models of geochemical processes. Therefore, it appears that calculational modeling of transport phenomena, supported by laboratory and field characterization, provides the best method of assessing the effects of geochemical processes on radionuclide transport over the performance period of the repository.

2.1.2 Analysis of Physical/Chemical Processes Affecting Transport

The rationale for this activity is to partially guide geochemical characterization activities by investigating processes that may have a significant effect on transport and that thereby provide information that may be used to restrict the scope of geochemical characterization to those processes and parameters that most affect radionuclide transport. The activity will help to determine the most appropriate computational representations for these processes and will use them to assess the sensitivity of these processes to radionuclide transport by calculating their relative contributions to radionuclide transport to the accessible environment. Therefore, two levels of sensitivity analysis will be performed: quantification and integration of the important contributing processes and parametric sensitivity analysis.

In this task, the approach for identification of important physical and geochemical processes will be to model alternative processes, either individually or as part of a larger computer model being developed as part of the first activity in this study (Sections 2.1.1, 3.1.1, and 3.2.1). Currently, four broad categories of processes are being studied: (1) transport of radionuclides in the form of colloids; (2) effects of geochemical processes on transport; (3) effects of physical processes on transport, in particular, the effects of fracture flow in the unsaturated zone and of dispersive and diffusive behavior on transport; and (4) effects of coupled processes, in particular, the effects of regional stress and heat on transport and geochemistry. Once a process has been shown to have a significant effect on transport, the sensitivity of radionuclide transport calculations to parameter changes in the process model will be assessed, and the results will be incorporated into the geochemical conceptual model.

2.1.3 Transport Models and Related Support

The purpose of this activity is to provide documentation, verification, validation, and software support for the transport codes to be applied to the retardation sensitivity analyses. This activity will ensure that the codes applied in this study will be compatible with the guidance put forth in NUREG-0856 (Silling, 1983) and the LANL YMP software quality assurance (QA) requirements.

Most of the codes to be used in this study are modified versions of existing computer programs. The codes were chosen, in part, because the codes' users either developed the existing computer program or work directly with the codes' developers. The codes have extensive support at Los Alamos National Laboratory. A description of their capabilities is given in subsequent sections (Sections 3.2.1.1, 3.2.1.2, 3.2.2.1 and 3.2.2.4). They contain state of the art numerical procedures and are of a small class of codes that meet our requirements for accurate physics and computational efficiency. Some effort is required to bring these codes into compliance with QA standards that conform to NUREG-0856. This compliance will be accomplished by generating YMP versions of these codes. Software support will be limited for the purposes of this activity to the YMP versions of the codes.

Most of the effort under this activity will be concerned with the verification of the YMP versions of the codes and the validation of the conceptual models used in this study. Much of the verification work performed on earlier versions of the codes is usable; however, because all the codes require significant modification for the YMP problem, additional verification activities are necessary. Model validation makes up a significant portion of the study effort as the project moves toward licensing. Because much of the evaluation of the effectiveness of the geochemical retardation barrier will be predicted based upon modeled results, validation of the models used for these results is required.

2.2 Constraints on the Study

2.2.1 Sensitivity Analyses Using a Geochemical Transport Model of Yucca Mountain and Integrated Geochemical Transport Calculations

The technical constraints that affect this study arise from two basic areas. First, the study is constrained by the data provided to the calculations. For example, sufficient data to support conceptual models must be obtained from geochemical and hydrologic characterization studies. Second, the numerical methods used require significant computational resources. This constraint requires that the code be formulated in a computationally efficient manner in order to allow sufficient resolution for three-dimensional representation of the retardation processes.

This activity will produce no adverse impacts on the site. It will not collect data at the site but rather will rely on other studies for data collection. The study will not need to directly simulate repository conditions; however, validation exercises (Section 3.2.3.3) must provide a sufficient basis for demonstrating that transport models may be used to predict long-term performance. This study is partially concerned with quantitatively determining the accuracy with which parameters must be known and the limits to which transport modeling techniques may use the data to predict effects of site geochemistry on transport of radionuclides.

The time required for this activity is consistent with that provided by the current program schedule, provided that the level of effort required is sustained throughout that period and that the other characterization activities supplying hydrologic (SCP Investigation 8.3.1.3.2) and transport properties proceed on schedule. Because characterization data will not be collected by this study, the analyses described below will require data from other studies as input to the conceptual models used for this study. These data are the coefficients of the flow and transport equations (Section 3.2.1), which will be used to evaluate initial conditions, boundary conditions, constitutive relationships, and other coefficients in the transport equations for radionuclide transport. These data include those hydrologic parameters and conditions required to assess groundwater velocities at a resolution sufficient to determine transport of radionuclides in the units between the repository and the accessible environment. They also include the diffusion, dispersion, effective retardation coefficients, and decay constants found in the transport equation. These constants and coefficients are supplied by the studies on site hydrology (SCP Section 8.3.1.2) and site characterization activities for measurement of transport parameters (SCP Sections 8.3.1.2 and 8.3.1.3.7.2). Information from the undisturbed and disturbed case performance-assessment scenario classes (SCP Section 8.3.5.13) will be used to estimate boundary conditions. Source terms for radionuclides will be taken to be the engineered barrier releases as predicted by the studies described under SCP Section 8.3.5.10. Retardation models and parameters will be supplied by studies described in SCP Section 8.3.1.3.4. A means by which the spatial distribution of sorption parameters may be obtained will also be supplied by the studies described in SCP Section 8.3.1.3.4. Availability of these data serves as a constraint on this study.

2.2.2 Analysis of Physical/Chemical Processes

In addition to the constraints presented in Section 2.2.1, other constraints will be applicable to this activity. For colloid transport, fracture velocities and information concerning birth, death, and growth rates of colloids are required. Data concerning colloid formation are supplied by SCP Studies 8.3.1.3.4.1.4 and 8.3.1.3.5.2.1. For the geochemical studies, sorption coefficients as functions of pH and water chemistry may be required from the sorption (SCP Section 8.3.1.3.4) and groundwater geochemistry (SCP Section 8.3.1.3.1) tasks. To study transport through fractures in the unsaturated zone, information is needed concerning the partitioning of both moisture and radionuclides between the fractures and matrix material. This information is supplied by the geohydrology (SCP Section 8.3.1.2) and the dynamic transport (SCP Section 8.3.1.3.6.1) tasks. To study dispersive behavior, the dependence of the dispersion tensor on such factors as saturation, length scales, and time must be determined from dynamic transport studies (SCP Section 8.3.1.3.6.1) and field testing (SCP Section 8.3.1.3.7.2). The dependence of diffusion on saturation, tortuosity, and scale will be determined from information gathered under SCP studies 8.3.1.2.2.5 and 8.3.1.3.6.2. For the coupled stress task, intact rock strength properties and regional stress data are required. For the coupled heat/flow task, thermal conductivities and fluid properties as functions of temperature are required (SCP Section 8.3.1.15).

2.2.3 Transport Models and Related Support

This activity has few constraints because it is basically a support activity for the activities described in Sections 2.2.1 and 2.2.2. However, validation activities will require a project-wide consensus on a validation approach and a program of experimental studies to produce data for model validation. In addition, an independent peer review mechanism must be established as part of validation activities.

With regard to the specific factors to be considered as constraints, the only factor that would appear to constrain this activity is the time available for model validation. Validation exercises must begin as early in the project schedules as possible in order to gather the required data.

3.0 DESCRIPTION OF ANALYSES

3.1 General Approach and Purpose

The purpose of this study is to provide analyses of the effects of physical and chemical processes on the transport of radionuclides between the repository and the accessible environment. Much of this work will be performed numerically using Sun work stations and Cray computers (Section 3.3). The codes used for this study run in one-, two-, and three-dimensions. Some three-dimensional simulations will be performed for this study, but we will also rely on one-dimensional and especially two-dimensional simulations. For example, two-dimensional simulations can perform extensive parameter studies for sensitivity analyses. The results of these simulations can be used to intelligently plan a more limited sensitivity analysis of three-dimensional geometries. We estimate that a typical two-dimensional calculation will run in a few hours on the Sun-4 work stations, while a very large two-dimensional problem would take on the order of a day. A moderately sized three-dimensional simulation will take one to two days on the Sun-4 work stations, and a very large three-dimensional simulation will require a few hours of Cray time. These requirements are not extraordinary; necessary results will be obtainable in a reasonable time frame.

3.1.1 Sensitivity Analyses Using a Geochemical Transport Model of Yucca Mountain and Integrated Geochemical Transport Calculations

The purpose of this activity is to construct a model capable of providing quantitative estimates of the retardation effectiveness of the geologic units between the repository and the accessible environment (Section 2.1.1). Model development will proceed in phases as data on geochemical effects on radionuclide transport are obtained and as validation exercises are analyzed. As model phases are completed, the model will be used to indicate where characterization efforts should be concentrated in order to assess the effectiveness of the barrier. Site characterization, model development, and model validation tasks will work hand-in-hand to develop the conceptual model of the site's geochemical barriers and to limit the scope of the characterization effort. Calculations to support conclusions on the effectiveness of the geochemical barrier will be performed by modeling the transport of radionuclides released from the engineered barrier system through the geologic units between the emplacement horizon and the accessible environment and by application of sensitivity analysis techniques.

Model calculations will integrate the effects of retardation processes, such as those described in Section 3.2.2.2, with the geologic and geochemical data developed in studies necessary to summarize geochemical retardation, as described in SCP Sections 8.3.1.3.1.2, 8.3.1.3.1.4, 8.3.1.3.1.5, 8.3.1.3.1.6, 8.3.1.3.1.7.2, and 8.3.1.3.1.8. The geochemical/geophysical model will be made as realistic as is practical; for example, lateral flow, tipped beds, and discrete faults will be included in the geologic description. Groundwater chemistry activities (SCP Section 8.3.1.3.1) will supply a description of changes in background groundwater chemistry for scenarios to be analyzed in total system performance assessments. Mineralogic and petrologic characterization activities (SCP Section 8.3.1.3.2) will provide spatial distributions of mineralogy that provide the basis for distributing transport and sorption parameters throughout the solution domain of the model.

Geochemical interaction between the host rock and the transported materials will be represented principally through effective or scenario-dependent sorption relationships. These relationships may be in the form of linear or nonlinear isotherms. Provision in the computational model will be made for solubility-limited sorption and reversible processes. The parameters and models representing the sorption processes will be supplied by the characterization activities described in SCP Section 8.3.1.3.4. The sorption characterization activities (SCP Section 8.3.1.3.4) will also provide a method by which the sorption parameters may be distributed in space. Such a method may, for example, be based on the mineral distributions obtained from the activities of SCP Section 8.3.1.3.2. The transport mechanism may also affect the sorption parameters. For example, radionuclides moving through fractures are likely to encounter different minerals and therefore different sorption properties than if they were transported through the matrix. Solubility limits on radionuclides in solution will be obtained from the studies described in SCP Section 8.3.1.3.5. Experimental evidence of the effects of geochemical processes on transport will be incorporated in the transport model. These results will be obtained from the studies described in SCP Section 8.3.1.3.6

Some transport properties for the saturated zones will be obtained from the studies of SCP Section 8.3.1.3.7.3. Data will also be gathered from the geohydrologic and transport activities described in SCP Section 8.3.1.2. Source term data for radionuclide releases from the engineered barrier system will be collected from activities described in SCP Sections 8.3.5.9 and 8.3.5.10. Data from rock characteristic studies described in SCP Sections 8.3.1.4 and 8.3.1.15, as well as data from studies on the potential effects of erosion (SCP Section 8.3.1.6), future climate changes (SCP Section 8.3.1.5), and tectonic activities (SCP Section 8.3.1.8), will be used.

3.1.2 Analysis of Physical/Chemical Processes Affecting Transport

There are currently four classes of physical/chemical processes being studied as part of this activity:

- transport of radionuclides in the form of colloids;
- effects of geochemical processes on transport;
- effects of physical processes on transport; and
- effects of coupled mechanical/hydraulic/thermal processes on transport and retardation.

The studies in these areas will be discussed in detail below. The overall approach for these studies is to assess the importance of the above-mentioned process to radionuclide transport. If the calculated effects are found to be significant, then the process will be incorporated into the conceptual geochemical model of Yucca Mountain developed under this study. The mechanism by which the results will be incorporated in an overall evaluation of the effectiveness of the geochemical barrier will vary.

For colloid transport, it appears likely that a separate calculation for colloid transport can be made. The population balance model described below relies (Section 3.2.2.1) on velocity calculations for the liquid phase. These velocities, for both fractures and matrix, are generated by the TRACRN code as part of the dissolved species transport calculations. Therefore, it may be possible to couple colloid transport with the calculations of the TRACRN model by performing a colloid transport calculation based on water flow velocities predicted by the TRACRN model. If significant, these results would become a component of our overall conceptual geochemical model.

The effects of geochemistry on transport measurements will couple with either TRACRN or FEHMSN calculations through the retardation coefficients of the transport equation. Examination of Equation 3 (Section 3.2.1.1) shows that the primary geochemical interaction with transport is through sorption constants. It may be expected that simple linear isotherm approaches will not suffice for all conditions to be modeled. Rather, some form of effective sorption coefficients that integrate effects of varying conditions and transport on sorption will be required for accurate results. The work in this area will aid in developing effective sorption coefficients or alternate submodels that may be incorporated directly in TRACRN or FEHMSN.

Studies concerning the effects of fracture flow in the unsaturated zone on transport are likely to show that under certain scenarios, a composite porosity approach (see Section 3.2.2.3) is sufficient, and under other scenarios, discrete fracture modeling or a dual-porosity model is required. TRACRN can be used to model the composite porosity approach and to study a small number of discrete fractures. FEHMSN has a dual-porosity capability.

Components of the dispersion tensor may depend on saturation, length scale, and time. Likewise, the effective diffusion coefficient will depend on saturation and tortuosity. Dependencies in these terms can be directly incorporated into the TRACRN code.

In the cases of coupled phenomena, if the coupling with mechanical stress changes or heat effects in the mountain is found to be important, the effects will be quantified with the FEHMSN code, and the results will become a component of our study results. If the coupling is unimportant, then the issue of the effects of coupled mechanical/hydraulic processes on radionuclide transport may be quantitatively resolved as unimportant.

Work under this activity will require input from geochemical characterization activities described in SCP Sections 8.3.1.3.1, 8.3.1.3.2, 8.3.1.3.4, 8.3.1.3.5, and 8.3.1.3.6. Again, groundwater chemistry from SCP Section 8.3.1.3.1 will provide baseline water compositions for transport modeling activities. The mineralogic and petrologic distributions developed in the studies of SCP Section 8.3.1.3.2 are expected to provide an indication of the spatial distribution of sorption and transport properties. Sorption data from the studies of SCP Investigation 8.3.1.3.4 are required input to the assessment of transport effects on geochemical parameters. This investigation (8.3.1.3.4) will also provide data to be used to assess the importance of microbes on colloidal transport mechanisms. Solubility measurements from the studies of SCP Section 8.3.1.3.5 will form part of the input to the geochemical/transport modeling. Finally, the dynamic transport studies (SCP Section 8.3.1.3.6) will provide experimental transport measurements.

Additional data needs from studies external to SCP Section 8.3.1.3 parallel those described in Section 3.1.1.

3.2 Method

3.2.1 Sensitivity Analysis Using a Geochemical Transport Model of Yucca Mountain and Integrated Geochemical Transport Calculations

3.2.1.1 Geochemical Transport Model of Yucca Mountain

A model of the transport system at Yucca Mountain is needed to perform the sensitivity analyses described below. This model will integrate the site geochemical and physical data with a three-dimensional porous media transport code that will provide a computational representation of the conceptual model for transport and the effects of site geochemistry. Initially, the transport code to be used for this work will be TRACRN, a version of TRACR3D (Travis, 1984), currently under development for YMP applications. TRACRN is essentially TRACR3D with documentation sufficient for YMP QA requirements. Previously, TRACR3D has been applied to Yucca Mountain for preliminary calculations of flow and transport (Travis et al., 1984; Cederberg et al., 1987; Travis and Nuttall, 1987; and Greenwade and Cederberg, 1987). These simulations were performed in two dimensions, using predominantly estimated values for many of the flow, transport, and geochemical parameters. More recently, repository-scale transport calculations in three dimensions using spatially distributed sorptions coefficients were run with TRACRN (Birdsell et al., 1989, 1990). Fully developed three-dimensional flow fields were calculated for these sets of simulations. These simulations demonstrate the feasibility of transport modeling in several dimensions at Yucca Mountain.

TRACRN is being constructed from TRACR3D to deterministically represent most of the physical and geochemical processes currently thought to have the most direct effect on transport at Yucca Mountain. A description of the TRACRN code, based on the description of the TRACR3D code by Travis (1984), is provided below. The TRACR3D code was developed to model mass flow and chemical species transport in a three-dimensional, deformable, heterogeneous, reactive porous medium. Problems ranging from steady, single-phase, one-dimensional flow, to transient, three-dimensional, multiphase flow and transport in fractured porous media are simulated by the code. The equations that the model comprises are the mass and chemical species conservation equations, a reduced form of the momenta equations, an equation of state, and several constitutive relationships. These equations may be found in fundamental texts on flow and transport in porous media (e.g., Bear, 1972, and de Marsily, 1986) and are adapted for this problem.

Conservation of mass for the gas phase is

$$\frac{\partial(\phi \rho_g S_g)}{\partial t} + \nabla \cdot (\rho_g \vec{u}_g) = \dot{S}_g \quad , \tag{1}$$

and, for the liquid phase,

$$\frac{\partial(\phi \rho_\ell S_\ell)}{\partial t} + \nabla \cdot (\rho_\ell \vec{u}_\ell) = \dot{S}_\ell \quad , \tag{2}$$

where

$\dot{S}$ = phase source rate $[M/L^3T]$,
t = time [T],
$\vec{u}$ = phase velocity vector [L/T],
ϕ = medium porosity,
ρ = phase density $[M/L^3]$,
S = degree of phase saturation of pore space,

and subscripts g and ℓ refer to the gas and liquid phases.

Equations 1 and 2 are written for isothermal systems in which water vapor is neglected and no diffusion or dispersion of water occurs. Dispersion of air has also been neglected. Porosity is assumed to vary dynamically only with pressure. Dynamic changes in porosity can have a dramatic effect on flow because storage capacity and permeability are generally quite sensitive to changes in porosity. Equations 1 and 2 cover conditions of flow ranging from fully water-saturated to fully air-saturated porous media.

TRACRN does not model speciation and complexation processes, only a variety of equilibrium and nonequilibrium, linear and nonlinear sorption dynamics. Other models, such as EQ3/EQ6, have the capability of capturing complexation processes. Such models can be used to determine the accuracy of equilibrium sorption models and whether more sophisticated dynamics should be included.

For most studies, TRACRN uses a simple sorption model for transport,

$$\frac{\partial(\phi\, S_i\, \rho_i\, C_\alpha)}{\partial t} + \nabla \cdot (\rho_i\, \vec{u}_i\, C_\alpha) = \nabla \cdot (\phi\, S_i\, \tau_e\, D_\alpha\, \rho_i\, \nabla C_\alpha) + \phi\, C_\alpha\, \dot{S}_i$$

$$+ \nabla \cdot [\phi\, S_i\, \bar{D}_\alpha\, \nabla(\rho_i\, C_\alpha)] - \phi\, \lambda_\alpha\, S_i\, \rho_i\, C_\alpha + \phi\, \lambda_{\alpha-1}\, S_i\, \rho_i\, \frac{C_{\alpha-1}}{M_{\alpha-1}}\, M_\alpha$$

$$- \rho_i\, \rho_m\, (K_{d\alpha}\, (\frac{\partial C_\alpha}{\partial t} + \lambda_\alpha\, C_\alpha) - \lambda_{\alpha-1}\, K_{d(\alpha-1)}\, C_{\alpha-1}\, \frac{M_\alpha}{M_{\alpha-1}}) \quad , \qquad (3)$$

which allows for advection, dispersion, diffusion, radioactive decay, sources/sinks, and equilibrium sorption of an arbitrary number of tracers in a single phase. The terms in this equation are

C = solute concentration in transporting fluid [M solute/M fluid],
D = molecular diffusivity of a species in the transporting phase [L^2/T],
$\bar{D}$ = mechanical dispersion coefficient of a species in the transporting phase [L^2/T],
K_d = equilibrium sorption coefficient [L^3/M]
M = molecular weight [M/mole],
ρ_m = density of rock matrix [M/L^3],
λ = ln 2/half-life of solute, and
τ_e = constrictivity,

and subscript i refers to ith phase (i.e., g or ℓ), α refers to αth species of radionuclide, and α-1 refers to the parent of the αth species).

The tracer concentrations are assumed to be small, and the traditional velocity-dependent dispersion tensor is used. Transport under unsaturated conditions is also handled through the appearance of saturation (S_i in Equation 3). The solution of Equation 3 can be performed by either explicit or implicit means. An option is available which envokes Henry's Law for transport of volatile tracers in both the liquid and gas phases. If sufficient data are available, which is usually only true for laboratory experiments, a more complex kinetic sorption model can also be used. This model accounts for sorption kinetics that are limited by the fraction of available sorption sites and by the solubility limits of the solute in water.

The conservation equations, Equations 1 through 3, involve quantities that represent local volume averages. The averages are obtained by integrating the continuum conservation equations over small "representative" volumes (small compared with the scale of the problems at hand but large compared with the individual flow paths between the matrix grains). This averaging is necessary because our present mathematics cannot provide a practical means of solving the continuum equations at arbitrary points in such a complex system as a porous rock.

The momenta conservation equations are solved in a reduced form known as Forchheimer's equation (McWhorter and Sunada, 1977):

$$\vec{u}_i \left[1 + \frac{1}{(1-\phi)} \frac{L\rho_i \,|\,\vec{u}_i\,|}{85.7\,\mu_i} \right] = -\frac{kR_i}{\mu_i} \left(\nabla P_i + \rho_i \vec{g} \right) \quad , \tag{4}$$

where

$\vec{g}$ = acceleration caused by gravity [L/T^2],
k = permeability [L^2],
L = a typical-length scale [L],
P = fluid pressure [M/LT^2]
R = relative permeability
μ = dynamic viscosity of fluid [M/LT],

and the subscript i refers to a gas or liquid phase. This form neglects the acceleration term and uses a phenomenological treatment of inertial terms and viscous drag. At low Reynolds numbers ($L\rho\vec{u}/\mu < 10$), this expression reduces to the well-known Darcy equation; at higher Reynolds numbers, the nonlinear term in Equation 4 becomes important.

In Equation 4, R_i is a function of the degree of saturation of the pore space. The term kR_i (the effective permeability) represents the exchange of momentum between the fluids and the drag on the fluids by the matrix. The current formulation of the code provides for an anisotropic representation of permeability when the computational grid is aligned with the ellipsoid of permeability. The relationships of both the relative permeability and the pressure of the liquid phase to the degree of saturation are user inputs. Under the current conceptual model of Yucca Mountain, these relationships attempt to represent both fracture and matrix hydraulic characteristics in a composite porosity approach. The consequence of using this approach for transport calculations will be determined under the study of fracture/matrix interactions (Section 3.2.2.3).

Heterogeneities in hydrologic and transport properties can create preferential flow paths for water and radionculide migration. As information concerning such heterogeneities becomes available, it will be included as input to transport calculations run with TRACRN to determine the effect of heterogeneities in various properties on the calculated results.

A difficult problem facing the task of modeling radionuclide transport is the quantification of members of the dispersion tensor in the unsaturated zone. Dispersivities in unsaturated regions may be expected to be functions of the degree of saturation (Nielson et al., 1986) in addition to scale (Dugan, 1986) and time (Gelhar, 1986), as discussed for the saturated zone. These factors will be studied in more detail (Section 3.2.2.3), and the results will be incorporated into the calculations done under this activity.

Much of the discussion above has centered on the unsaturated zone underlying the repository. This emphasis is appropriate because the travel times for radionuclides through the unsaturated zone are currently thought to be long (DOE, 1986). However, paths to the accessible environment pass through long segments of saturated rock. The formulation of the TRACRN code provides for simulation of flow and transport in variably saturated porous media. Yucca Mountain will be simulated as a continuum from the unsaturated to the saturated zone. Initially, this analysis will concentrate on the unsaturated transport and retardation problem. Under some scenarios, saturated conditions may be encountered in a zone that is currently unsaturated. Examples of such scenarios include disturbed case performance-assessment scenarios (SCP Section 8.3.5.13) that result in increased recharge through the unsaturated zone or increased elevation of the water table. Analyses for the currently saturated zone will be added to the unsaturated work after completion and interpretation of the C-wells experiments.

A study plan on reactive tracer experiments for the C-wells has been presented (YMP-LANL-SP-8.3.1.2.3.1.7). The C-wells study plan outlines plans for simulation of transport and radionuclide retardation through saturated regions beneath Yucca Mountain using TRACRN and FEHM (Zyvoloski et al., 1988). The results of the reactive tracer study will be incorporated in the geochemical transport model for simulation of the saturated portions of radionuclide flow paths. Data to be incorporated include dispersion coefficients and behavior of sorbing tracers in the saturated zone.

The discussion above briefly summarizes the current status of the TRACRN transport code. As the studies of the next activity proceed, modifications to TRACRN may be necessary to incorporate those results in the analyses. However, at this time, it appears that the effects of the processes described below may be incorporated into TRACRN calculations either through modification of input variables or through off-line calculations. Therefore, the basic approach for modeling the effects of retardation on transport is as described above.

3.2.1.2 Sensitivity Analysis

Several authors have demonstrated the desirability of quantitative sensitivity analysis for improving the understanding of waste isolation processes in geologic media (Jacobson et al., 1985; McWilliams, 1985; Oblow et al., 1986). Sensitivity analyses for the purpose of guiding geochemical characterization will be performed by constructing an adjoint version of the TRACRN code.

A code using the adjoint method may be used to map the spatial sensitivity of concentration to variables of interest, such as permeability or sorption ratios (Morris, 1982). For example, a response function can be defined as

$$F(\bar{x}) = \int_{t_1}^{t_2} C(\bar{x}, t)\, dt \quad . \tag{5}$$

In this example, the functional F depends indirectly on permeability, porosity, and the sorption ratio because the concentration C at location x and time t depends on those variables through the tracer transport equation (Equation 3, p 23). The adjoint technique provides a method for finding the derivative of F with respect to the sorption ratio and other quantities. Once determined, contour maps can be generated to determine the sensitivity of F to sorption ratio. This information may then be used to determine the spatial locations most affecting concentrations and where, for example, additional sampling is required. This is the method to be used to perform sensitivity analyses for the geochemical characterization program. As posed, the example discusses only linear isotherms as a sorption model. The transport and inverse codes are written in sufficient generality to accept a variety of sorption functions. The procedure for determining sensitivity to parameters is basically as described above. Because of the interactions between transport and retardation, a systematic approach for the sensitivity analysis will be needed. Delineation of this approach will be the first component of this work.

The adjoint equations will be derived and implemented in parallel with development of geochemical models of Yucca Mountain. The adjoint sensitivity method will be verified by direct manipulation of key parameters, such as permeability, for a number of scenarios. Monte Carlo methods can be used to study the effect of correlation structure on flow and transport. Fortunately, our TRACRN code can be linked easily with routines to determine realizations of correlated (spatially correlated) fields, such as permeability or retardation coefficients. The adjoint method can also be used to reduce the effort required in Monte Carlo simulations by considering the Fokker-Planck equations as a model for stochastic variable dynamics.

Laboratory validation of flow and transport codes requires only a forward solution capability. Field validation, however, is not so clear-cut. Usually, in a field situation, porosity, permeability and other material properties are known only at a few locations; it is assumed that these properties are essentially continuous between observation wells, but this may not be the case. A comparison between field measurements and model calculations will likely show differences, even significant differences. It cannot be assumed that the model is wrong or incorrect in principle; it may be the case that the actual spatial distribution of material properties is significantly different in some regions than what the modeler is led to believe from sparse field measurements. An inverse modeling capability can be very useful in resolving this fairly common situation. With an inverse capability, field measurements can be used to determine what the spatial distribution of properties must be to allow the particular flow and transport model in question to match the field data. In this way, one will have guidance as to where in the field to take more measurements, which will resolve the differences between the model and measurements. This is as valid a means of testing a model as is a forward calculation.

Adjoint methods have frequently been used to solve inverse problems in flow and transport in geologic media (Thomas et al., 1972; Seinfeld and Kravaris, 1982; Travis, 1985b; Wasserman et al., 1975; and Wilson and Metcalfe, 1985). Inverse problems are calculations to determine parameters of a solution on the basis of observations of flow (usually inferred from hydraulic head) and transport at specific points. Most simulation models are run in a predictive or "forward" mode; that is, a model result is predicted from knowledge of the model inputs, initial conditions, boundary conditions, and model parameters. Depending on its formulation, an inverse problem allows calculation of model parameters, initial conditions, or boundary conditions from knowledge or specification of model results.

Using transport calculations as an example, the inverse methods begin with a history of concentration measurements taken at specified locations, as well as a set of estimates of the model parameters. An inverse version of a model is then used in a forward calculation to compute a concentration history resulting from the assumed set of model parameters. The difference between observed and calculated concentrations is then used to modify the model parameters, and another forward calculation is made. The results are again compared with the original observations in order to estimate a new set of model parameters. This iterative process continues until the observed and calculated results agree within some specified tolerance. At each iteration, the adjoint equation, derived from the transport equation, is also solved to provide new parameter estimates.

Nonuniqueness is a fundamental issue for inverse problems. Generally, without any *a priori* information or constraints, there are no unique solutions. There is, however, an infinite number of possible solutions. The approach to overcoming this difficulty is to choose one solution out of the possibilities that has the simplest or smoothest structure. This is an application of the philosophical principle known as "Occam's razor," or choosing the model with the least structure possible that matches or explains the observations.

There are several ways to impose uniqueness in the problem by restraining solution structure. This method— regularization— was developed by Tikhonov (1963). It provides uniqueness and stability by requiring a solution whose derivative of a specified order (usually 0th plus 1st or 2nd derivative) has the smallest norm:

$$\text{norm } f = \int_a^b f^2 + (f')^2 \, dx \quad .$$

Additional constraints, such as positivity, can also be imposed, thereby improving resolution. Regularization can be derived within the more general framework of Bayesian estimation theory based on rules for consistent inferential reasoning.

The governing equations may be nonlinear, depending on the level of realism used. However, the adjoint equations are linear and are, consequently, easy to solve. The calculation of sensitivity coefficients requires one forward solution of the governing equations and then calculation of the adjoint equation, followed by evaluation of an integral involving the forward and adjoint functions. This is very efficient when the number of nodes is large.

Solution of an inverse problem for flow and/or transport is very similar to evaluating sensitivity coefficients. The same steps are taken. The sensitivity coefficients are based on a different definition of the functional, relating observation to desired spatially distributed property. An interative process is required for the inverse problem because the end product of each pass is an updated estimate of the sought-for field. Usually, convergence is reached in 4-7 iterations.

For sensitivity coefficients, the computer time required is roughly 2.5 times that required for a single forward equation set solution. An inversion requires about 10-12 times the time necessary for a single forward solution. With current computer technology, only inversion for moderate to large three-dimensional scenarios would be very time-consuming; all other combinations pose no particular difficulty in regard to computing resources.

3.2.2 Analysis of Physical/Chemical Processes Affecting Transport

3.2.2.1 Colloid Transport

The purpose of the colloid transport effort is to quantitatively determine the role that colloids play in the transport of radionuclides. Considerable interest has been focused on the extent to which colloid transport may be important in radionuclide migration (Kelmers et al., 1987). There is evidence that a small fraction of colloidal material breaks through in saturated fracture experiments much earlier than conservative tracer species (Harvey and George, 1987; Rundberg et al., 1989). Currently, it is thought that this phenomenon may be due to selective transport along relatively higher velocity flow paths in fractures. For this reason, the relative importance of colloidal transport mechanisms must be assessed.

It is expected that some radionuclides (e.g., plutonium and americium species) may form true colloids (Olofsson et al., 1981, 1982a, and 1982b) and that other radionuclides are likely to be sorbed to clay (Buddemeier, 1987) and possibly to microbial material (Hersman, 1986a and 1986b), forming so-called natural colloids. The definition of true or natural colloids is somewhat arbitrary, and, in general, we will simply note that the type and character of the colloids may be defined.

The analysis of colloidal transport of radionuclides will be conducted for both the saturated and unsaturated zones. Because flow in fractures is of particular interest, analyses will be conducted stressing scenarios that produce flow in unsaturated-zone fractures. Currently these scenarios are other than what is termed the nominal case in the total system performance assessment for flow in the unsaturated zone. However, fracture flow is expected to dominate flow through the saturated regions leading to the accessible environment. Scenario classes that include flow in unsaturated fractures are discussed in SCP Section 8.3.5.13. These classes define the conditions and environments for which analysis will be conducted in the unsaturated zone. All scenarios are expected to produce flow in the fractures of the saturated zone.

As stated above, colloids represent a potential vector for relatively early release of radionuclides from the repository. Colloids (clays and perhaps container particles) may be expected to be present at the Yucca Mountain site, and they have been shown to migrate both in saturated and unsaturated geological formations (Harvey and George, 1987; Germann et al., 1987; Torok et al., 1990). Because relatively little is known about the role of colloids in the transport of radioactive waste (Parker et al., 1984), both mathematical and experimental programs will be conducted to obtain an understanding of the role of colloids in waste transport. The experimental programs are described in the study plans for reactive tracer testing (Activity 8.3.1.2.3.1.7) and for dynamic transport (Study 8.3.1.3.6.1). The modeling program described below will support these experimental programs and is based on a population balance approach for colloid transport.

The population balance approach is well established (Nuttall, 1986), although it has only recently been applied to modeling of colloid transport. Randolph (1962), and later Hulburt and Katz (1964), derived the general form of the population balance equation. These very formal and complete derivations of the population balance equation set the foundation for the subsequent mathematical analysis of many particulate system studies in fields ranging from engineering to biology. The population balance is a transport equation that is commonly used to model systems of countable entities. The equation is similar to the mass balance equation, except, rather than conserving mass, it conserves the number of particles or colloids. The resulting dependent variable of the population balance is number density. Randolph and Larson (1971) provide references to numerous applications of the population balance equation including processes such as crystallization, grinding, air pollution, and biological systems.

The population balance equation permits a full treatment of the colloid problem, from the birth of colloids to their capture on the surrounding media. It also allows modeling the gradual processes of colloid growth or dissolution. Radioactive decay of specific nuclides in the colloids is treated by assigning a concentration property axis in the population balance to each species of interest. The addition of these property axes allows proper treatment of the decay chain problem with full accounting of the daughter product concentrations. Also, the adsorption of multiple nuclides on the same colloid (heterogeneous colloids) can be modeled using the population balance equation.

Randolph and Larson (1971) discuss in detail an example of using the concentration property axis in the population balance equation. For each nuclide, there is a separate concentration property axis that defines the number of colloids at a point in time/space/size that have a particular concentration. Integrating over the concentration property axis and the size axis gives the amount of colloidal material at a point in time and space. The population balance approach provides a proper accounting and quantitative assessment of the nuclear colloid problem.

Modeling colloidal migration requires coupling of the hydrology equations and the dissolved species' mass balance to the population balance. The hydrology equations could be included and solved by CTCN though it may be more practical to simply transfer the steady state velocity profiles from TRACRN into CTCN. Fracture and matrix velocities can be backed out of composite porosity simulations (Peters and Klavetter, 1988) run with TRACRN, or velocities calculated under the study of fracture flow in the unsaturated zone (Section 3.2.2.3) can be used. Since the mass transport equations and colloid population balance equations are likely coupled, we will include both in the description presented here.

To describe dissolved species migration, one equation is needed for each species, using Equation 3, without chaining daughters for this example and ignoring sorption, the equation is written for the αth species:

$$\frac{\partial(\phi S_i \rho_i C_\alpha)}{\partial t} + \nabla \cdot (\rho_i \vec{u}_i C_\alpha) = \nabla \cdot (\phi S_i \tau_\alpha D_{\alpha_i} \rho_i \nabla C_\alpha) + \phi C_\alpha \dot{S}_i$$
$$+ \nabla \cdot [\phi\, S_i \bar{D}_{\alpha i} \nabla (\rho_i C_\alpha)] \quad . \qquad (6)$$

In this case, the sink term, $\phi C_\alpha \dot{S}_i$, is required in the mass balance to represent the dynamic transfer of dissolved species to colloids.

Additional population balance equations are required to model the particulates, i.e., the formation and migration of radioactive colloids. Some assumptions are required in order to specify the number and type of population balance equations needed. These assumptions may be changed as needed. It is necessary to assume the number of types of colloids such as clay particles, container degradation products, or plutonium precipitates to suggest a few. A separate population balance equation is required for each unique type of colloid that one chooses to model. Hence it is necessary to assume the number and character of colloids.

Within the population balance equation there is a term to account for the number of colloids containing a specific concentration of a radionuclide. In the case where we follow several radionuclides, a concentration level property axis is required for each nuclide adsorbed or appearing as a reactive constituent on a particular type of colloid. The general form of the population balance allows for an arbitrary number of these continuous property axes. Note that in addition to concentration, particle size is also treated as a property with a size axis (Randolph, 1962; Randolph and Larson, 1971). In this way, the population balance can track the adsorption and decay of each nuclide of interest. The population balance equation for the transport of an arbitrary type "k" colloid in a saturated porous media is given below. The development of the population balance equation for colloid transport in unsaturated porous media is an active area of research. Therefore, only the saturated model is presented here.

For the kth type colloid, the population balance equation is (Randolph, 1962)

$$\frac{\phi\partial\psi_k}{\partial t} + \nabla \cdot (\overline{u}_i\psi_k) - \phi D_k \nabla^2 \psi_k + \phi\sum_{j=1}^{m} \frac{\partial(\nu_{kj}\psi_k)}{\partial\xi_j} + \phi E_k - \phi B_k = 0 \ , \tag{7}$$

where

ψ_k	is the colloid number concentration for a type k colloid,
D_k	is the colloid dispersivity, is generally size dependent, and is a combination of diffusion and dispersivity, and
ξ_j	is the property axis, such as particle size or concentration.

The mass and population balance equations together describe mathematically the near-field process where physical and chemical processes are occurring simultaneously. To complete the above model, the system geometry, boundary conditions, and specific terms in the equations must be specified. Note that the velocity profiles are obtained from TRACRN. Submodels or kinetic expressions are required to represent the terms needed in the balance equation. The exact form of the terms required for these equations must be determined for the Yucca Mountain application. Key terms in Equation 7 that require special consideration are listed below.

E_k	This term represents the rate of particle number disappearance from a particular particle size category per unit solution volume. Death is caused by colloidal capture on the rock matrix, agglomeration, and dissolution. Death term submodels are described by Nuttall (1989). These models describe both reversible and irreversible capture of colloids onto the rock matrix.
B_k	In a similar fashion, this term represents the rate of appearance of particles in a size category per unit solution volume. Births result from nucleation, agglomeration, and release of captured or new colloids from the rock matrix. Experimental work is ongoing to develop proper models that will describe the birth of colloids from tuff.
ν_{kj}	If the property is particle size, this variable is the growth or dissolution rate on a molecular scale of colloids. This terms accounts for the gradual increase or decrease of particle size because of mass addition or subtraction from colloids. If the property is concentration, this term is the rate of a radionuclide addition or removal from colloids.
$\sum_{j=1}^{m} \frac{\partial(\nu_{kj}\psi_k)}{\partial\xi_j}$	This term represents the rate of population density change along a property axis, for example, colloid growth along the particle size axis. Also, it represents and accounts for the concentration of radionuclides on the colloids.

The population balance, coupled with the dissolved species transport equations, represents a complex set of partial differential equations that must be solved numerically in the CTCN code. A general solution to the population balance is particularly difficult because of the high dimensionality of the problem. In general, one may be required to solve for up to three spatial dimensions and several additional property axes dimensions. Common property axes include particle size and radionuclide concentration. Hyman (1976 and 1979) and Hyman and Larrouturou (1982) have developed a numerical method of lines approach for solving parabolic partial differential equation. An extended version of this method will be used to solve the coupled population balance and dissolved species transport problem.

Parameters in the submodels can, in many cases, be assigned conservative values or may require estimates from experimental data. Mathematical submodels must be developed in order to solve the transport equations discussed above. For example, it is necessary to mechanistically understand how colloids are captured by the surrounding rock and whether the colloidal suspensions are free from agglomeration. In general, small colloids (1 μm) are most affected by their electrostatic charge (Israelachvili, 1985) and that of the surrounding rock. Representative charge measurements of both the expected colloids and the rock will be required to develop the appropriate submodel for capture and agglomeration needed by the population balance.

In addition to understanding capture mechanisms, some information and measurements are needed to define the appearance rate of clay or other types of colloids that can enter the groundwater system. It is expected that clay colloids will be released from the surrounding rock and that container and waste form materials will form certain types of radiocolloids. Information on the nature and formation rates of these colloids will be required.

In addition, submodels will be developed for the following subprocesses:

- birth rate (includes heterogeneous and homogeneous nucleation, also release of colloids from the rock matrix),
- death rate (Nuttall, 1989),
- growth rate, and
- decay of nuclei in or on a colloid.

These submodels are generally site specific, incorporating the appropriate geochemistry, reaction kinetics, and transport processes for a potential repository. Studies to determine the exact form of these submodels for YMP will also be conducted under this activity. Phenomena relevant to these submodels are being studied by the activities described in SCP Section 8.3.1.3.5.

Because colloids have a large radionuclide carrying capacity, it may be expected that they will be an important factor, primarily in the transport of radionuclides through fractures in the rock matrix. Therefore, the velocities in Equations 6 and 7 that are likely to be of interest are the fracture velocities. Further, scenarios and processes that are likely to produce fracture flow are of particular interest to the analysis of colloid transport.

3.2.2.2 Effects of Geochemical Processes on Transport

The effectiveness of natural barriers to inhibit the movement of radionuclides may be dependent on the groundwater geochemistry. Considerable evidence exits that points to the need to investigate this relationship. The K_d of americium and neptunium can change by orders of magnitude over a pH change of 0.5 unit (8-8.5). Plutonium can change valence states three times (affecting adsorption characteristics) with a 0.5 unit change in Eh (the oxidation potential). The absorption characteristics of technetium and strontium are also affected by pH. Geochemical effects can strongly influence adsorption coefficients in the saturated and unsaturated zones. The

Groundwater Geochemistry task (SCP Section 8.3.1.3.1) plans to perform experimental work in both the saturated and unsaturated zones.

Several authors have discussed the coupling of transport and geochemical processes, and it is clear that a signicant coupling occurs and can be modeled. Cunningham (1981), Cederberg et al. (1985), Lichtner (1985), Miller and Benson (1983), and Nguyen et al. (1982) report successful applications of combined chemical and transport models to a variety of systems, using different theoretical approaches to their specific problems.

The most general approach to modeling coupled geochemistry and flow is to combine the transport codes TRACRN and FEHMN with a geochemistry equilibrium code such as EQ3/6. This formulation would lead to a large computer memory overhead and excessive execution times, severely impairing the ability to model the geometric distribution of the rock types and hence mineral distribution in Yucca Mountain. A simpler approach will be used by this study.

A model will be developed that is both computationally efficient and contains the necessary chemistry to assess the effect of groundwater chemistry on the retardation of actinides at Yucca Mountain. The tentative plan is to solve simultaneously for the concentrations of Ca^{2+}, Mg^{2+}, Na^+, K^+, SO_4^{2-}, Cl^-. HCO_3^- and several actinide species. Simplified expressions for ion exchange terms for appropriate species will be developed by working with the Groundwater Chemistry task (SCP Section 8.3.1.3.1.1). This work will also interact significantly with the Radionuclide Sorption task (SCP Section 8.3.1.3.4) where the ion exchange or sorption terms will be developed for the actinides. The pH is a potentially important variable as discussed above and will be considered as a constant to make the calculations simpler. The constant value will be varied on different runs between 6.5-8.5 or as directed by the Geochemistry task. If in the course of investigations it is necessary to have a variable pH, the H^+ and OH^- concentrations or mineral water interactions affecting pH will be incorporated in a manner similar to that discussed by Miller and Benson (1983). The effect of redox on the adsorption process and water composition also will be investigated.

The numerical model will be similar to those presented by Miller and Benson (1983) and Jennings et al. (1982) in that the geochemistry will be implemented within the transport code. The following equations give an outline of the approach used and follow the discussion of Cederberg (1985). The formation of species c_e in the aqueous phase or species s_e on the solid phase can be described by the following equilibrium expressions.

$$c_e = \frac{K_{c,e}}{\gamma_{c,e}} \prod_{j=1}^{N_c} (\gamma_{x,j} X_j)^{a_{e,j}} \tag{8}$$

and

$$s_e = \frac{K_{s,e}}{\gamma_{s,e}} \prod_{j=1}^{N_s} (\gamma_{x,j} X_j)^{b_{e,j}} \tag{9}$$

where

$a_{\alpha j}$ = stoichiometric coefficient of component j in species c_α,
$b_{\alpha j}$ = stoichiometric coefficient of component j in species s_α,
c_α = concentration of species α in the aqueous phase [M/L^3],
K_{c_α} = equilibrium formation constant for species c_α,
K_{s_α} = equilibrium formation constant for species s_α,
n_{aq} = number of species in aqueous phase,
n_s = number of species in solid phase,
N_c = total number of components,
s_α = concentration of species α in the solid phase [M/L^3 fluid],
X_j = concentration of component j [M/L^3],
γ_{c_α} = activity coefficient for species c_α,
γ_{s_α} = activity coefficient for sorbed species s_α,
γ_{xj} = activity coefficient for complex x_j.

The material balance equations may be written as

$$T_j = \sum_{\alpha=1}^{n_{aq}} a_{\alpha j} c_\alpha + \sum_{\alpha=1}^{n_s} b_{\alpha j} s_\alpha \quad \cdot \quad j = 1, 2, \ldots N_c \quad . \tag{10}$$

Activity coefficients can in many cases be expressed functionally in terms of ionic strength (Stumm and Morgan, 1981) such as

$$\log_{10} \gamma_{x\alpha} = -\frac{1}{2} V_\alpha^2 \left[\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3\, I \right] \quad , \tag{11}$$

where the ionic strength is defined as

$$I = \sum_{\alpha=1}^{n_{aq}} c_\alpha V_\alpha^2 \quad , \tag{12}$$

where V_α is the valence and the sum taken over all complexes in the aqueous phase.

Equilibrium constants of the form shown in Equations 8 and 9 will describe processes for speciation of radionuclides in groundwater (such as complexation) and sorptive interactions with the solid phase. The data describing the speciation information and interaction of radionuclides with the solid phase will be obtained from YMP Studies on Batch Sorption (SCP Section 8.3.1.3.4.1), Biological Sorption and Transport (SCP Section 8.3.1.3.4.2), Development of Sorption Models (SCP Section 8.3.1.3.4.3), Dissolved Species Concentration Limits (SCP Section 8.3.1.3.5.1), Colloid Behavior (SCP Section 8.3.1.3.5.2), Application of Results (SCP Section 8.3.1.3.5.3), Dynamic Transport Column Experiments (SCP Section 8.3.1.3.6.1), and Diffusion Studies (SCP Section 8.3.1.3.6.2). Thus the final values for the activity coefficients will most likely be different from those given in Equation 11. The best values will be incorporated as they are developed by the above mentioned tasks.

The general transport equation for computing the concentration of a single dissolved chemical species in a saturated aquifer system can be expressed as

$$\frac{\partial \phi c_\alpha}{\partial t} + \frac{\partial \phi s_\alpha}{\partial t} = \nabla \cdot [\phi(\bar{D} + D) \cdot \nabla c_\alpha] - \nabla \cdot [\phi \bar{u}\, c_\alpha] + \dot{S}_{c_\alpha}$$

$$\alpha = 1, 2, \ldots, n_{aq} \quad , \tag{13}$$

where $\dot{S}_{c_\alpha}$ is a source/sink term $[M/L^3T]$ for species α attributable to aqueous phase complexation. Equation 13 assumes no radioactive decay and is applicable to the saturated zone only.

In a multispecies solution where the sorbed phase concentration of species α, s_α is a function of the aqueous species concentration, a nonlinear system of coupled solute transport equations arises such as those of Jennings et al. (1982). By making use of the definitions in Equations 8, 9, and 10, for c_j, s_j, and Tj, the set of n_{aq} equations described in Equations 13 can be reduced to a set of N_c mass transport equations given by

$$\frac{\partial}{\partial_t}(\phi c_j) + \frac{\partial}{\partial_t}(\phi s_j) = L(c_j) \qquad j = 1, 2, \ldots, N_c \quad ,$$

where

$$c_j = \sum_{\alpha=1}^{n_{aq}} a_{\alpha j}\, c_\alpha \quad \text{and} \quad s_j = \sum_{\alpha=1}^{n_s} b_{\alpha j}\, s_\alpha \quad . \tag{14}$$

If $T_j = c_j + s_j$, and the operator $L(c_j)$ is defined to be

$$L(c_j) = (\nabla \cdot \phi \bar{D} \cdot \nabla c_j - \nabla \cdot \phi \vec{u} c_j) \quad ,$$

then

$$\frac{\partial}{\partial_t}(\phi T_j) = L(c_j) \qquad j = 1, 2, \ldots, N_c \quad . \tag{15}$$

The coupled species equations will be incorporated into TRACRN or FEHMN by a modular subroutine structure. They currently have capability for multiple uncoupled tracers. The codes will employ a Newton-Raphson iteration to solve the coupled geochemical transport equations. Some simplifications will occur because of the differing strengths of the reactions.

The results of the radionuclide transport calculations with the sorption coefficients based on the spacially distributed pH field can be compared with previous transport calculations to determine if further sophistication in the geochemical transport model is warranted.

3.2.2.3 Effects of Physical Processes on Transport

This activity will focus primarily on three physical processes that may affect transport in the unsaturated zone. The first of these processes is transport through fractures in the unsaturated zone. This activity will be used to determine the conditions under which various models (i.e., composite porosity, dual-porosity, or discrete fracture models) are appropriate for modeling transport through unsaturated or partially saturated tuffs. The second and third processes are dispersion and diffusion. Under this activity, we hope to establish an appropriate form for the dispersion tensor and for the diffusion coefficient in unsaturated, fractured tuff.

The composite porosity approach has been used recently for calculations of transport at Yucca Mountain (Birdsell et al., 1989, 1990). Under some recharge scenarios (e.g., slow, uniform infiltration), this approach may be appropriate for modeling transport through the fractured tuffs. This approach, suggested by Montazer and Wilson (1984) and quantified by Peters and Klavetter (1988), assumes that the characteristic curves for matrix and fractures may be combined in a single function by assuming equivalent capillary pressures and parallel flow in the two media. Characteristic curves for matrix materials have been measured (Peters et al., 1984); however, water retention and relative permeability curves are estimated for fractures. These significant assumptions provide a single-porosity representation of the media that is computationally simpler than dual-porosity approaches. The composite porosity assumption of equal pressures in the matrix and fracture fluids does not necessarily imply equal solute concentrations in the matrix and in the fractures. Time constants for local solute redistribution may be longer than for local pressure equilibration. Therefore, the effects of this assumption on transport calculations must be assessed in order to understand its implications on the effectiveness of the geochemical barrier.

A discrete fracture model or a dual-porosity model may be required to model transport under higher recharge scenarios (e.g., increased infiltration or episodic recharge). By comparing flow results for the composite porosity approach and a discrete fracture model, Buscheck and Nitao (Buscheck and Nitao, 1991; Nitao, 1990; Nitao and Buscheck, 1989) have recently shown that the composite porosity approach may be adequate to model flow under a limited domain during episodic infiltration events. They have developed a set of criteria, which describe the flow mechanism as being fracture or matrix dominated, that can be used to determine when the different models are appropriate. This study will determine whether an analogous criteria for transport can be established. A dual-porosity formulation may also be considered in the model comparison.

A difficult problem facing the task of modeling radionuclide transport is the qualification of members of the dispersion tensor in the unsaturated zone. The problem is also complicated by the fractures in the units comprising Yucca Mountain. Hydrodynamic dispersion in the unsaturated zone has been the subject of considerable research in the past few years (Bond, 1986; Dagan, 1986; Sposito and Barry, 1987; Sposito et al., 1986; Tompson et al., 1987). Several approaches to the problem of dispersion in the saturated zone have been presented (Dagan, 1987; Gelhar et al., 1985; Schwartz et al., 1983; Smith and Schwartz, 1984; Springer, 1988). Some of these methods may hold promise for application to the unsaturated zone. However, dispersivities in unsaturated regions may be expected to be functions of the degree of saturation (Nielsen et al., 1986) in addition to scale (Dagan, 1986) and time (Gelhar, 1986), as discussed for the saturated zone.

Currently, it is unclear which approach for determining dispersivities is best suited to the unsaturated regions underlying Yucca Mountain. Methods that show promise include a method presented by Tompson et al. (1987) and stochastic approaches, such as those suggested by Gelhar (1986). These methods are based on knowledge of the statistics of heterogeneous fields of hydraulic and transport properties. Mean, variance, and autocorrelation length are required input data for the generation of random fields of properties. Although these methods do not provide direct input for a model such as TRACRN, they may allow a basis for estimation of dispersion parameters to be used in the model. Tests of this approach to dispersive modeling will be conducted as part of validation exercises under SCP Study 8.3.1.3.7.2.

At low flow rates, molecular diffusion can be a predominate mechanism contributing to hydrodynamic dispersion (Bear, 1972). The molecular diffusivity in the diffusive term (Equation 3) is effectively decreased by the tortuosity of the medium, $1/\tau_e$. Under unsaturated conditions, a decreased number of pores are available for transport which effectively causes an increase in the tortuosity. This increase will be modeled by assuming that the diffusion coefficient is a function of saturation. The goals of this activity are to determine the applicability of laboratory measured diffusion coefficients and tortuosity values to field conditions, and to determine the dependence of the diffusion coefficient on saturation. If the dependence significantly affects calculated transport results, it will become a part of the geochemical conceptual model of the site (Section 3.2.1.1).

3.2.2.4 Coupled Processes

There has been considerable discussion regarding the coupled effects of heat and stress on mass transport from a repository. Tsang (1987) provides a good summary of this discussion. Coupled processes may be important to far-field transport. Heat driven convection has been demonstrated in wells UZ-6 and UZ-6S (Weeks, 1987). Magmatic intrusion, verified to have occurred within 5,000 yr, can produce high gas flow rates from the thermal source. This could cause releases of ^{14}C and ^{129}I to the atmosphere. Also, changing regional stress fields in the Basin and Range province could lower porosity in the saturated zone at Yucca Mountain and, thereby, significantly raise the water table. To determine the effects that changes in the state of stress or thermal gradient would make on radionuclide transport, a modeling activity that integrates these effects is proposed as described below.

The transport of radionuclides depends on the chemical and physical characteristics of the host rock and the state of the rock. Chemical characteristics that may be important include zeolite and clinoptilolite concentrations (Daniels et al., 1982). State variables that may change as a result of repository activities or long-term environmental trends include temperature and state of regional lithologic stress. An important rock property affecting transport is the permeability of the rock mass. Fracture permeability may be particularly important because fractures present a potentially rapid path for migration of radionuclides. Montazer and Wilson (1984) report that the tuffs in the vicinity of the repository may have fracture densities in the range of tens of fractures per cubic meter. Because it is well established that fracture aperture is a function of stress (Tsang and Witherspoon, 1981; Witherspoon et al., 1980), and therefore of temperature (Cook, 1987), this activity will attempt to quantify the effects of processes affecting permeability on transport calculations for Yucca Mountain. At present no capability exists for modeling the clogging of pores due to precipitation. We plan to investigate this phenomena under the guidelines set forth in the geochemistry section (3.2.2.2). If it turns out that precipitation (or dissolution) is important, the permeability changes will at first be modified by a Karmen-Keozeny relation.

The FEHM (Zyvoloski et al., 1988) code is currently used to calculate the effects of heat on flow and transport. Work has begun to modify the existing code FEHM to simulate conditions at Yucca Mountain. FEHM was developed for assessing the effects of processes associated with geothermal reservoirs (Heiken and Goff, 1983). FEHM was modified to the FEHMS code (Zyvoloski and Kelkar, 1987) by coupling the equations of rock mass deformation in order to predict changes in permeability resulting from temperature or stress changes. The YMP version of the FEHMS code, which will be further modified to represent the Yucca Mountain environment, is known as FEHMSN. The current mathematical formulation of FEHMSN is summarized below.

The flow and solute transport equations in FEHMSN are essentially the same as Equations 1-4. The exceptions are that, in FEHMSN, Darcy flow is assumed, the contaminant transport equation does not contain radioactive decay terms and various absorption models are included. Current plans call for adding the radioactive decay terms used in TRACRN to FEHMSN. Temperature-dependent sorption characteristics can be added if such data become available. The primary difference between the mathematical formulations of these codes is that the energy transport and stress/strain equations are also solved simultaneously in FEHMSN. The value of FEHMSN will be to change the flow field in response to stress or heat changes. At present the chemical transport will be no more sophisticated than currently available in TRACRN. Another code, WAFE (Travis, 1985a), has been used in preliminary calculations; however, because of FEHMSN's greater generality, current plans call for the replacement of WAFE by FEHMSN for YMP purposes.

The following discussion is simplified from Zyvoloski and Kelkar (1987). Considerably greater detail on the FEHMS model is available in that reference. In summary, the energy transport equation results from the combination of the conservation of energy equation and Darcy's Law. This equation basically has the following form:

$$\frac{\partial \bar{A}}{\partial t} - \nabla \cdot \left[d_{e\ell} \left(\nabla P_\ell - \rho_\ell \mathbf{g} \right) + d_{eg} \left(\nabla P_g - \rho_g \mathbf{g} \right) \right]$$

$$- \nabla \cdot (\kappa \nabla T) - q_e = 0 \ , \qquad (16)$$

where

$\bar{A}$ = energy per unit volume $[E/L^3]$,
P_ℓ = liquid pressure $[F/L^2]$,
P_g = gas pressure $[F/L^2]$,
q_e = energy source term $[E/L^3 T]$,
T = temperature $[\theta]$,
κ = effective bulk thermal conductivity $[E/TL\,\theta]$, and
ρ = fluid density $[M/L^3]$.

The transmissibilities d are defined as

$d_{e\ell} = h_\ell\,(kR_\ell\,\rho_\ell)/\mu_\ell$; and
$d_{eg} = h_g\,(kR_g\,\rho_g)/\mu_g$.

Here,

h_ℓ = specific enthalpy of liquid $[E/M]$,
h_g = specific enthalpy of vapor $[E/M]$,
k = permeability $[L^2]$, and
R = relative permeability.

The model can describe both flow in porous media and in discrete fractures. Discrete fractures can be described by using very small finite elements of appropriate size. For Yucca Mountain applications, it is likely that larger grid blocks will be used, and, in this case, fracture flow will be addressed using either the equivalent porous medium or a dual porosity/dual permeability model. In the first case, the permeability, k, is a volume averaged quantity representing both fracture and matrix permeability. In the second case, the permeability of the fracture and matrix are distinct. We anticipate significant differences between the models since the relative permeability functions are very nonlinear and very different between the matrix and fracture materials.

The coupling between the stress solution and the permeabilities is, at present, taken to be a power law relationship

$$k = f\,w^n,$$

where

f = function factor,
w = fracture aperture $[L]$, and
n = exponent (at present, $n = 2$).

An exponent of 2 gives the cubic law relationship because the flow area is also proportional to w. Those general laws are envisioned, with the ultimate goal of utilizing a dual porosity and damage model simultaneously. It is further anticipated that shear stress-aperture models will be incorporated using relationships obtained from experimental studies (Barton et al., 1985).

To incorporate the effects that change in the state of stress have on transport, the following equations are also added to FEHMSN. In contrast to the transport and flow equations, the stress equations are formulated at steady state. The approach is based on the general theory of elasticity and consolidation of porous solids developed by Biot (1941 and 1955) and the theory of linear thermoelasticity (Lubinski, 1955; Timoshenko and Goodier, 1951). The current formulation assumes an isotropic matrix material but provides for discrete fractures. This approach has been used by others in the field (Hart, 1981; Noorishad et al., 1982).

The strain/displacement relationships in Cartesian coordinates are given by

$$\epsilon_{xx} = \frac{\partial u}{\partial x}, \; \epsilon_{yy} = \frac{\partial v}{\partial y}, \; \epsilon_{zz} = \frac{\partial w}{\partial z} \; ,$$

$$\epsilon_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \; ,$$

$$\epsilon_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \; ,$$

$$\epsilon_{zx} = \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \; , \tag{17}$$

where

u = x-displacement [L],
v = y-displacement [L],
w = z-displacement [L], and
ϵ = strain tensor.

The constitutive relationships for the porous solid are given by

$$\epsilon_{xx} = \frac{\sigma_{xx}}{E} - \frac{\nu}{E}(\sigma_{yy} + \sigma_{zz}) - \frac{\Delta P}{3H} + \alpha\Delta T \quad ,$$

$$\epsilon_{yy} = \frac{\sigma_{yy}}{E} - \frac{\nu}{E}(\sigma_{xx} + \sigma_{zz}) - \frac{\Delta P}{3H} + \alpha\Delta T \quad ,$$

$$\epsilon_{zz} = \frac{\sigma_{zz}}{E} - \frac{\nu}{E}(\sigma_{yy} + \sigma_{xx}) - \frac{\Delta P}{3H} + \alpha\Delta T \quad ,$$

$$\epsilon_{xy} = \frac{2(1+\nu)}{E}\sigma_{xy} \quad ,$$

$$\epsilon_{yz} = \frac{2(1+\nu)}{E}\sigma_{yz} \quad , \qquad \text{and}$$

$$\epsilon_{xz} = \frac{2(1+\nu)}{E}\sigma_{xz} \quad . \tag{18}$$

Here,

σ = stress tensor [M/LT^2],
α = coefficient of thermal expansion [θ^{-1}],
E = Young's modulus [M/LT^2]
ν = Poisson's ratio, and
H = Biot's physical constant [M/LT^2].

The first subscript on σ indicates the direction in which the stress acts, and the second indicates the plane on which the stress acts. The first subscript on ϵ indicates the direction in which the strain occurs, and the second refers to the direction in which the gradient is taken. The quantity 1/(3H) is the compressibility of the material with respect to fluid pressure (Biot, 1941).

For simplicity, the following discussion is limited to two dimensions to describe the coupled equations being solved. For plane strain,

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{Bmatrix} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & \frac{\nu}{1-\nu} & 0 \\ \frac{\nu}{1-\nu} & 1 & 0 \\ 0 & 0 & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix} \cdot \begin{Bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{xy} \end{Bmatrix}$$

$$- (\delta \Delta T - \gamma \Delta P) \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} \quad , \tag{19}$$

where

$$\gamma \equiv \frac{E}{3(1-2\nu)H} \quad ,$$

$$\delta \equiv \frac{E\alpha}{1-2\nu} \; [M/LT^2/\theta] \quad ,$$

ΔP = change in pore pressure $[M/LT^2]$, and
ΔT = change in temperature $[\theta]$.

Combining the equations above with the static equilibrium equations for the material provides the following equations:

$$E_1 \frac{\partial^2 u}{\partial x^2} + E_2 \frac{\partial^2 v}{\partial x \partial y} + E_3 \left[\frac{\partial^2 v}{\partial x \partial y} + \frac{\partial^2 u}{\partial x^2} \right] - \beta \frac{\partial}{\partial x} (T - T_0)$$

$$+ \frac{(3E_2 + 2E_3)}{3H} \frac{\partial P}{\partial x} = 0 \quad , \tag{20}$$

and

$$E_1 \frac{\partial^2 v}{\partial y^2} + E_2 \frac{\partial^2 u}{\partial x \partial y} + E_3 \left[\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial y^2} \right] - \beta \frac{\partial}{\partial y} (T - T_0)$$

$$+ \frac{(3E_2 + 2E_3)}{3H} \frac{\partial P}{\partial y} \rho g = 0 \ , \tag{21}$$

where the notation is

$$E_1 = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \ ,$$

$$E_2 = \frac{E_1 \nu}{(1 - \nu)} \ ,$$

$$E_3 = \frac{E_1 (1 - 2\nu)}{2(1 - \nu)} \ ,$$

and

$$\beta = (3E_2 + 2E_3)\alpha \ .$$

Equations 20 and 21 provide the coupling of the stress solution to the pressure and temperature terms of Equations 4 and 16 and form the basic mathematical model used in FEHMSN. A Galerkin finite element approach is used for the simultaneous numerical solution of Equations 1, 2, 4, 16, 20, and 21. The technique used is discussed by Zyvoloski and Kelkar (1987) and will not be further discussed here.

The approach for analysis of the coupled thermal stress flow and transport model will be to use FEHMSN to quantify potential effects of changes in temperature gradient and state of stress. These calculations will proceed by examining the effects of scenarios that affect stress and temperature gradients on radionuclide transport. If the effects of changes in temperature gradients or state of stress are significant, then a means for representing those changes in TRACRN will be found, or TRACRN will be replaced by FEHMSN, whichever approach seems most efficient. If the effects are found not to be important, then a quantitative basis for resolving the question will have been achieved, and the work will be concluded.

3.2.3 Transport Models and Related Support

3.2.3.1 Description of Transport Models Currently in Use

The following are short descriptions of existing flow and transport codes being modified for use in retardation sensitivity analysis. All further development, modifications, and qualification of these codes will follow the guidance found in the LANL Software Quality Assurance Plan for the YMP (see Appendix A).

TRACRN

TRACRN, the YMP version of TRACR3D (Travis, 1984), was described in detail in Section 3.2.1.1. It is a finite difference code that models single- or two-phase flow (currently air and water) and transport in porous, deformable heterogeneous media. It operates in Cartesian or cylindrical coordinates in 1, 2, or 3 dimensions and time. Several transport mechanisms are included: advection, molecular diffusion, dispersion, adsorption, radioactive decay, and chaining to daughter products. Adsorption models accommodate a range of possibilities from linear/reversible to nonequilibrium/saturable/irreversible processes. A very efficient sparse matrix solver is used in conjunction with a modified Newton-Raphson iteration scheme for nonlinear flow and transport terms. The resulting rapid execution time allows examination of problems of considerable complexity at high resolution.

CTCN

The CTCN code (Section 3.2.2.1) is designed to solve the unsteady population balance equations along with mass, energy, and momentum equations in up to four axes. The code allows the user to input, in addition to the model equations, a wide range of boundary conditions and submodels. The package uses the Method of Lines technique with a special section that automatically processes the equations to form the finite difference discretizations. To model colloid transport processes in porous and fractured media, the CTCN code solves the population balance equations along with the usual dissolved species transport equations and with the user provided boundary conditions.

TRACRIN

TRACRIN (Section 3.2.1.2) is a version of TRACRN that is capable of three additional computations, selected by the user through an input variable. For the first option, the model will perform a sensitivity simulation through solution of an auxiliary equation set, i.e., the adjoint equations for TRACRN. For the second option, the model will perform a Monte Carlo series of simulations, given distributions for permeability, porosity, and sorption coefficients. For the third option, TRACRIN will compute an inverse solution for permeability/flow path distribution when given a set of flow and transport measurements and an estimate of measurement errors.

FEHMN

FEHMN is the YMP version of FEHM which can simulate non-isothermal multiphase multicomponent flow in porous media. The equations of heat and mass transfer for multiphase flow in porous and permeable media are solved using the finite element method. The permeability and porosity may vary with pressure and temperature. The code also has provisions for movable air and water phases and noncoupled tracers; that is, tracer solutions that do not affect the heat and mass transfer solutions. The tracers can be passive or reactive. The code can simulate two-dimensional, two-dimensional radial, or three-dimensional geometries. This code also is being applied in the reactive tracer experiment supporting the C-wells task (SCP Activity 8.3.1.2.3.1.7).

FEHMSN

FEHMSN is the YMP version of FEHMS (Zyvoloski and Kelkar, 1987). FEHMS is a three-dimensional finite-element code that couples single- or two-phase flow with heat transport in porous media to stress fields in the media. Both *in situ* stresses and stresses induced by thermal and hydraulic gradients are modeled. In particular, the code computes the effect on fracture flow resulting from hydromechanical coupling. The code also has the capability of dual porosity simulation.

3.2.3.2 Verification

In most cases, the codes used for transport calculations are finite-difference, finite-element, or adaptive-mesh algorithms that are written with sufficient generality to allow solution of problems that cannot be addressed with analytical solutions. Therefore, only partial verification of these codes is possible using analytical solutions to the approximated partial differential equations. Analytical solutions under restricted boundary conditions or highly simplified problem geometries will be used for partial verification. However, to verify the codes in their full generality as they are applied to the Yucca Mountain transport problem, it is necessary to compare numerical solutions between independently developed codes applied to a set of common problems that exercise the full capabilities of the codes. These activities are usually referred to as benchmarking, and they will serve as the primary verification method for complex transport codes.

A formal code verification (COVE) activity has been established by the YMP Repository Performance Assessments Division at Sandia National Laboratories. YMP participants will compare the flow and transport codes being applied to radionuclide transport at Yucca Mountain. The participants will run a series of problems designed to test the flow and transport solutions obtained by these codes. Currently, two verification activities are under way: COVE 2 and COVE 3. COVE 2 is designed to compare flow solutions under isothermal conditions. Both steady and unsteady flow cases are examined in an unsaturated, fractured, heterogeneous porous medium. COVE 2 activities include the following calculations:

- one-dimensional flow through a vertical column with five material layers (COVE 2a),
- two-dimensional flow through a vertical section with two or more material layers (COVE 2b), and
- two-dimensional flow through a vertical section with two material layers and an explicitly modeled fault (COVE 2c).

The COVE 2a calculations were made with TRACR3D (Birdsell and Travis, 1987 and 1988) and will be rerun as part of the verification of TRACRN. Calculations will be run with TRACRN. COVE 3 is a benchmarking activity for hydrothermal multiphase flow codes. This problem is an analysis of two-phase flow of water, water vapor, air, and heat through a fractured porous medium. FEHMSN may be used for this effort as the modifications necessary to apply FEHMSN are completed. More benchmarking problems will be necessary in the future to test the capabilities of FEHMSN and CTCN. Benchmarking between TRACRN and FEHMSN will also be done.

3.2.3.3 Validation

A central question for the resolution of characterization and performance issues concerns the methods by which data collected over a relatively short term can be used to assess the long-term performance of the repository. The method that must be used to predict long-term performance is to incorporate significant processes in validated computer models that are capable of modeling the response of the repository under expected and unexpected conditions. Characterization issues must supply the information and understanding of the site required to complete and support performance calculations. This information for geochemistry is to be summarized in validated computer models and a supporting data base. The process of model validation is clearly a key problem in demonstrating that model predictions accurately represent future conditions and repository performance.

Validation of the conceptual models used to predict long-term geochemical processes is a much more difficult problem than code verification. An idealized approach to validation requires that the models be shown to accurately predict the processes that they model over the performance period of the repository. To accomplish such a validation, model input and output data must span the set of expected conditions and scenarios and must be available for periods of time at least of the order of those for which the model is to be applied. Model outputs for the modeled systems would then be compared with observed data from the system for scenarios and periods commensurate with performance periods. Obviously, experimental data will not be available for durations approaching required performance periods of 10,000 years or more, or for many of the scenarios and conditions that may develop during those periods. Because of this, partial validation of conceptual models is all that is possible for most of the performance-assessment models used for the YMP. The methodology discussed below will be used to lend credibility to the models used in this study.

The validation oversight group (VOG) has developed a draft version of "A Validation Methodology for Performance-Assessment Models" for the Office of Civilian Radioactive Waste Management (VOG, 1990). The validation methodology consists of three components: (1) a record of model development; (2) a comparison of experimental results with model predictions; and (3) a technical review. The methodology emphasizes thorough documentation of model development including the identification of, the technical basis for, and the significance of each assumption in the conceptual model. Laboratory and field investigations will be used for hypothesis testing and to provide data to compare with model output. Experiments and their analysis will be thoroughly documented. A formal technical review committee (FTRC) will then review the supporting information to determine the model's validity. The committee will identify problems that they perceive in the model, and the modelers and experimentalists will then resolve the issues. The process is iterative until the FTRC is satisfied that the development record is adequate to demonstrate the model's validity. Because true validation of performance-assessment models is not possible, the purpose of this process is "to establish that a model is appropriate and adequate for the problem being addressed, that it was logically developed using the best available technology, that it can be supported by experimental and observational data, that the quality of the data is high, and that the limitations of the model are well understood (VOG, 1990)." As new data become available, the model will be reexamined to identify and make modifications for any inconsistencies. Validation activities for this study will be conducted in a manner consistent with this methodology, upon its approval, and with project and LANL software QA requirements.

Validation of transport models will be performed using data generated from sources both within and outside the YMP. Sources within the Project include laboratory measurements using columns of fractured and crushed tuff performed as parts of the dynamic transport and sorption tasks (SCP Investigations 8.3.1.3.6 and 8.3.1.3.4, respectively). These laboratory experiments include measurements of diffusive, dispersive, and colloid transport through fractured core experiments (SCP Section 8.3.1.3.6). Tracer experiments, both in the exploratory shaft (SCP Study 8.3.1.2.2.2.3 and Birdsell et al., 1988) and in the C-wells area (SCP Activities 8.3.1.2.3.1.7 and 8.3.1.2.3.1.8), will be used for larger-scale validation. Caisson and field studies will be conducted as part of large-scale laboratory and field-scale experiments to be conducted under SCP Study 8.3.1.3.7.2. Details of these experiments may be found in the respective study plans. Validation activities will correlate results from experimental activities of various scales to modeling results to help determine the applicability of laboratory data to the field. Pre-experimental modeling will be used to design experiments that yield optimum results for model validation.

The principal outside source of model validation data is the experiments being conducted under the INTRAVAL Project. INTRAVAL is an international activity for the validation of mathematical models used in performance assessment of waste repositories. The project is conducted by the Organization for Economic Cooperation and Development/Nuclear Energy Agency. As part of this project, modelers work with experimentalists to design field and laboratory tracer experiments.

Experiments for the first phase of INTRAVAL have been completed. The data from three unsaturated zone experiments and several saturated zone experiments are available from this phase. The unsaturated zone experiments include (1) infiltration along a trench face near Las Cruces, NM, (2) infiltration from inclined boreholes into the fractured Apache Leap Tuffs in Arizona, and (3) drilling and imbibition experiments in welded and nonwelded tuffs at G-tunnel. The data from these three field experiments are accompanied by the data from laboratory-scale measurements of porosity, permeability, and characteristic curves on cores from the respective sites. Planning for the second phase of INTRAVAL is underway. Follow-up experiments are being planned for the Las Cruces trench site and the Apache Leap site. Such follow-up experiments will provide a broader data base for the sites so that independent calibration and model validation exercises can be performed. The experiments can also be designed to look at additional processes or to help resolve issues that led to ambiguous results in the first set of experiments.

Experiments used for validation of models used for this study can be separated into two broad classes. The first class consists of experiments that provide insights into modeling flow and transport through porous media systems in general. These experiments will be used to support model development by testing the basic assumptions concerning the physics of flow and transport through saturated and unsaturated systems. Questions concerning scale-up of parameters will also be addressed by using this class of experiments. These experiments include the INTRAVAL experiments and some of the proposed laboratory-, large-, or caisson-scale experiments (Study 8.3.1.3.7.2). Much can be learned about the mechanistic assumptions and modeling approaches used in flow and transport models through simulation of results of these general experiments. However, these experiments are not directly applicable to the Yucca Mountain environment.

The second class consists of experiments that provide insights into modeling flow and transport at Yucca Mountain. These experiments will help demonstrate the applicability of flow and transport models to the geologic units at Yucca Mountain and will help to define a conceptual model of the mountain that can be used for subsequent transport calculations. Experiments proposed under SCP Section 8.3.1.2 and those listed under the investigations of SCP Section 8.3.1.3 are included in this class. In particular, the experiments proposed under SCP Study 8.3.1.3.7.2 and SCP Investigations 8.3.1.3.6 and 8.3.1.3.4 will be required for site-specific transport model calibration and partial validation. Pre-experimental modeling will be used to design some of these experiments and to predict results that will be compared to actual experimental results. Results from experiments of various scales will be used to study site-specific scale-up problems.

Both classes of experiments will be used for model validation. Successfully modeling experiments run at various sites, at different scales, and under a variety of conditions will lend confidence to the models. What constitutes successful modeling has yet to be determined but will evolve as guidelines are established by the VOG and as validation exercises and technical reviews are performed.

Another technique that is being considered as part of model validation is the use of numerical simulations to investigate processes that are not explicitly described in the transport equations. Unfortunately, not every possible long-term process that can act to modify transport from the repository can be foreseen. However, quantitative analysis of such processes can be made by performing a "hidden variable" analyses. Generic studies of "two-timing" analysis can be carried out. For these analyses an unknown process is assumed to be in a particular category [e.g., diffusion, oscillatory (wave), first-order kinetics (chemical reactions), relaxation (strain relief), and episodic (weather)] and to operate on a very different time scale from the known processes. (The unknown process may or may not be of small amplitude.) Each of these kinds of processes can be described mathematically in a generic way. This is quite reasonable since the expression of any hidden variable process will be controlled by physical laws, and these fall into a few general classes. Well-established mathematical methods (Cole, 1968; Kreiss, 1979) can then be used to investigate the conditions under which the unknown process will have a first-order impact on transport, and even to determine what the nature of the effect will be. Decisions can then be based on how likely these conditions are, or will be.

Proper scaling of the governing equations will reveal nondimensional parameters. This should allow for experimental verification of this approach to studying the effect of processes operating on different time scales. For example, a test can be devised in which the primary processes operate on a fairly short time scale (e.g., minutes or hours), and a known process characterized by one of the categories mentioned above and operating on a considerably longer time scale (e.g., days or weeks) can be imposed. Successful validation of this approach would then give confidence that it can be applied to Yucca Mountain through appropriate values of the nondimensional parameters.

3.3 Equipment List

Equipment requirements for this study consist primarily of computer hardware to perform sensitivity analyses and transport calculations. The Central Computing Facility (CCF) and the Advanced Computing Laboratory at LANL, especially the Cray computers available on the CCF, as well as a local area network of SUN work stations will be used for the calculations performed for this study.

3.4 Accuracy and Precision

This study is affected by the numerical accuracy of the computer codes used and by the accuracy of data gathered during site characterization. Numerical accuracy is affected by factors such as grid refinement, time-step size, solution technique, and solution and machine tolerances. This topic will be handled for the individual codes as they undergo code verification (Section 3.2.3.2).

Both the accuracy and quantity of data supplied to this study by site characterization activities will affect the accuracy of the transport calculations produced to a certain extent. Sensitivity studies and parametric analyses can help establish how performance measures are impacted by data accuracy.

Accurate experimental data may be crucial to model validation activities as well as for discriminating between alternative conceptual models. Nonlinear processes such as unsaturated flow, which generally shows a strong power law relationship between effective permeability and degree of saturation, and transport in fractures need to be understood. Experimentalists will need to be meticulous in providing reliable error bars on measurements used to validate these types of highly nonlinear phenomena. Required accuracy limits for input data cannot be established *a priori*, as this is a topic of research within this study. However, through parametric studies, sensitivity analyses and pre-experimental modeling, this study can help define accuracy limits required by various tests to achieve a desired level of reliability in site characterization.

3.5 Representativeness of Analysis

This study will attempt to describe radionuclide retardation by all processes along flow paths to the accessible environment. Conceptual models of these processes will be developed based on data collected during site characterization and from other related studies. Sensitivity analyses will be used to determine the appropriate level of detail required to describe the various processes examined. For example, to study transport in unsaturated, fractured media, a single fracture may first be modeled to determine tracer responses under various flow scenarios. Such responses may then be correlated to the flow scenarios to be used in larger-scale modeling studies where modeling of single fractures is not practical. The correlations would be validated by comparing calculated results with results from experiments of various scales. This same method can be used to determine the relative effects of various processes or parameter heterogeneities under different flow scenarios on transport calculations. The assumption is that by studying the sensitivity of transport processes to different factors and at different scales that models will be developed that adequately represent the processes.

The uncertainties related to this study are difficult to predict. Flow and transport through unsaturated, fractured porous media are currently not well understood. Although studies conducted during the site characterization phase and the confirmation period will greatly increase the understanding of these processes, the time and length scales of the tests will be small compared to those required for predicting repository performance. Processes that are not observed or appear insignificant over shorter time periods or smaller length scales than those associated with repository performance may become more significant as time and length scales increase. This problem is probably the central scientific issue associated with the YMP and, unfortunately, is unresolvable. The method that will be used to decrease uncertainties related to the modeling activities performed under these studies is as follows:

- thoroughly study and attempt to explain data collected during site characterization;
- incorporate this information into conceptual models of the transport processes thought to occur at the site;
- study the sensitivity of the transport processes to various factors;
- validate these models to the extent possible; and
- test and modify, when appropriate, the model assumptions during the repository confirmation period.

Although this method will not resolve the issue of inappropriate scales, it is the most reasonable method that can be used and emphasizes continued study throughout the conformation period.

4.0 APPLICATION OF RESULTS

4.1 Resolution of Performance Issues

The results of this study will be used to satisfy SCP Investigation 8.3.1.3.7 (DOE, 1988) and to partially guide the geochemical characterization needs described in SCP Section 8.3.1.3. The results will also be used to test assumptions for the total system performance assessments used to resolve Issue 1.1.

4.2 Interfaces with Other Site Characterization Studies

4.2.1 Sensitivity Analyses Using a Geochemical Transport Model of Yucca Mountain and Integrated Geochemical Transport Calculations

This activity serves to guide the characterization activities concerned with gathering geochemical data for the Yucca Mountain site. The approach is to interact in an iterative fashion with the geochemical program through sensitivity analyses based on transport modeling. As data are incorporated, sensitivity analysis techniques will be used to provide quantitative direction to the geochemical characterization activities (SCP Section 8.3.1.3) by identifying areas where further work is required and by indicating where characterization is sufficient for the purposes of transport modeling. Models will also be used to design and interpret geochemical characterization experiments.

Further, the transport models developed as the basis of sensitivity analysis will also allow quantitative assessment of the effects of assumptions made in higher-level total system performance assessments (SCP Section 8.3.5.13). Finally, as data collection is completed and the baseline set of model parameters are established, the model may be used to summarize the effect of geochemical retardation on releases from the repository. These summary calculations will also aid in demonstrating knowledge of the effectiveness of the geochemical barrier to radionuclide migration for the purpose of resolving issues related to SCP Section 8.3.1.3.

4.2.2 Analysis of Physical/Chemical Processes Affecting Transport

This activity serves to partially guide geochemical characterization activities by investigating processes that may have a significant effect on transport and thereby provides information that may be used to restrict the scope of geochemical characterization to those processes and parameters that most affect radionuclide transport. The activity will determine the most appropriate computational representations for processes and will use them to assess the importance of these processes to radionuclide transport by calculating the relative contributions of each process to radionuclide transport to the accessible environment. The process models developed under this activity will be used to improve the geochemical transport model of Yucca Mountain. These models will be incorporated in the study described in Section 3.2.1.1.

Currently four broad categories of processes are being studied. These include (1) transport of radionuclides in the form of colloids, (2) effects of geochemical processes on transport, (3) effects of physical processes on transport, and (4) effects of coupled processes, in particular, the effects of regional stress and heat on transport and geochemistry. Once a process has been shown to have a significant effect on transport, the sensitivity of radionuclide transport calculations to parameter changes in the process model will be assessed.

4.2.3 Transport Models and Related Support

This activity will ensure that the codes applied in this study are compatible with the standards put forth in NUREG-0856 (Silling, 1983) and the LANL Software Quality Assurance Plan for the YMP (see Appendix A). Principal among these requirements are documentation, verification, validation, and support of the YMP versions of the codes used in this study. The results of this activity will be used in the two activities described above in Sections 3.2.1 and 3.2.2.

5.0 SCHEDULE AND MILESTONES

The milestones for the study are listed in Table 3. A diagram of the schedule is presented in Figure 2.

This schedule also includes timing relative to the geochemistry program data collection activities, the most crucial to the success of this study. Data from many other SCP activities are required by this study, in particular, hydrologic and geologic data. Section 2.2 of this study plan lists the rest of the data gathering activities that constrain this study.

TABLE 3

MILESTONES FOR RETARDATION SENSITIVITY ANALYSIS

Milestone	Description
R746	Interim report: Sensitivity analysis of integrated radionuclide transport based on a three-dimensional geochemical/geophysical model
R344	Interim report: Sensitivity analyses of integrated radionuclide transport using an updated geochemical/geophysical model
P381	Revised integrated transport calculations
R537	Final report on significance of physical processes affecting transport
R565	Final report on particulate transport
R538	Final report on significance of geochemical processes affecting transport
R366	Final report on sensitivity analysis of integrated radionuclide transport
R536	Final report on coupled phenomena
M390	Issue final geochemical/geophysical model

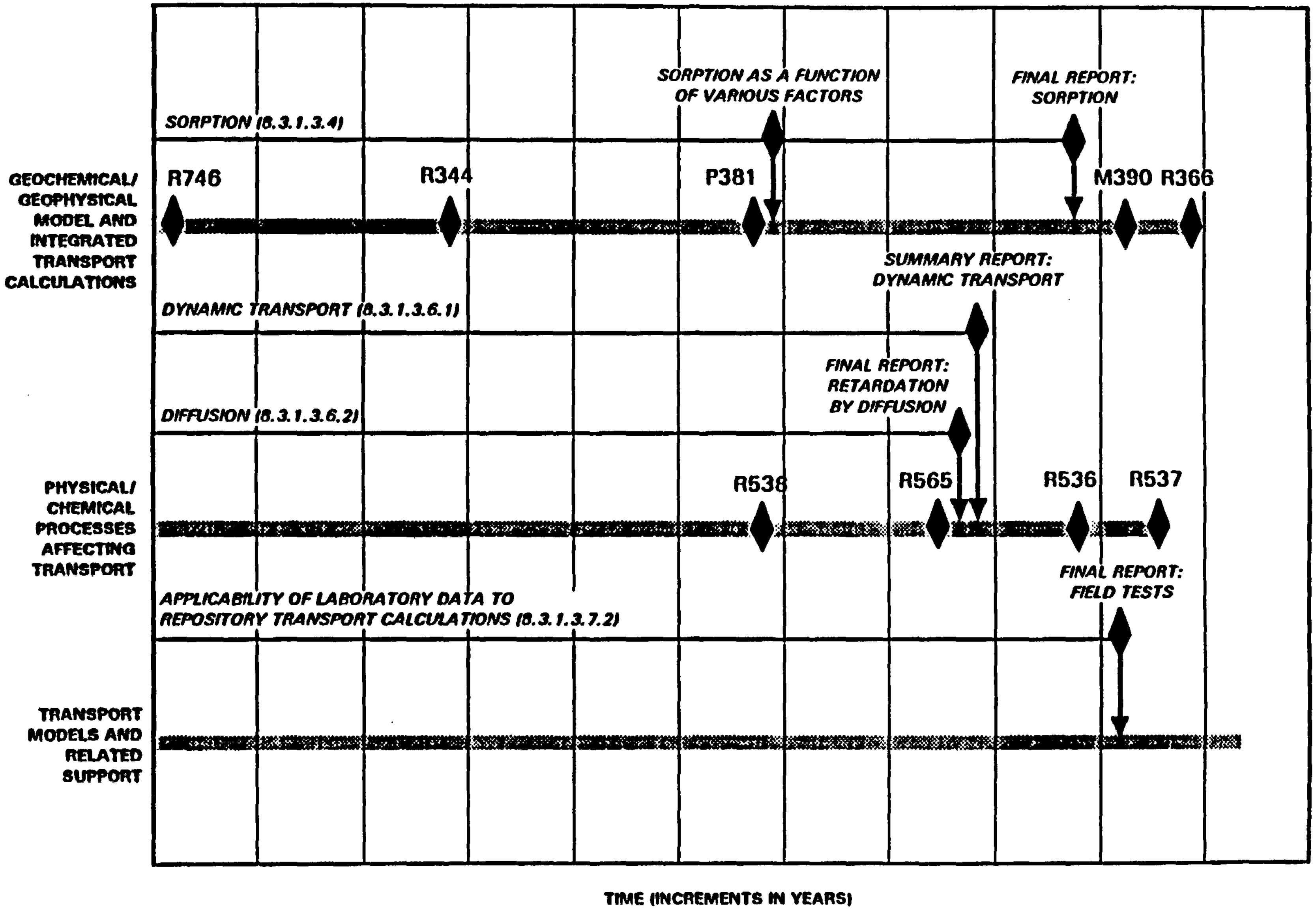

Figure 2. Milestones and Schedule for Retardation Sensitivity Analysis

6.0 REFERENCES

Barton, N., Bardis, S., Bakhtar, K., 1985. "Strength, Deformations, and Conductivity. Coupling of Rock Joints," Int. J. Mech. Min. Sci. and Geomech Abstr., Vol. 22, No. 3, 121-140.

Bear, J., 1972. Dynamics of Fluids in Porous Media, American Elsevier Publishing Co., New York, NY.

Biot, M. A., 1941. "General Theory of Three-dimensional Consolidation," Journal of Applied Physics, Vol. 12, 543-561.

Biot, M. A., 1955. "Theory of Elasticity and Consolidation for a Porous Anisotropic Solid," Journal of Applied Physics, Vol. 26, No. 2, 182-185.

Birdsell, K. H., and B. J. Travis, 1987. "Progress on the COVE 2 and COVE 3 Benchmarking Activities," Los Alamos National Laboratory Report No. LA-UR-87-3031, Los Alamos, NM.

Birdsell, K. H., and B. J. Travis, 1988. "Results of the COVE 2a Benchmarking Calculations Run with TRACR3D," Los Alamos National Laboratory Report No. LA-UR-88-2094, Los Alamos, NM.

Birdsell, K. H., P. G. Stringer, L. F. Brown, G. A. Cederberg, B. J. Travis, and A. E. Norris, 1988. "Modeling Tracer Diffusion in Unsaturated Porous Media, Both Fractured and Unfractured," Journal of Contaminant Hydrology, Vol. 3, No. 2-4, 145-170.

Birdsell, K. H., K. Cambell, K. G. Eggert, and B. J. Travis, 1989. "Preliminary Integrated Calculation of Radionuclide Cation and Anion Transport at Yucca Mountain Using a Geochemical Model," Los Alamos National Laboratory Report No. LA-UR-89-3503, Los Alamos, NM.

Birdsell, K. H., K. Campbell, K. G. Eggert, and B. J. Travis, 1990. "Simulation of Radionuclide Retardation at Yucca Mountain Using a Stochastic Mineralogical/Geochemical Model," Proceedings of the International Topical Meeting on High Level Radioactive Waste Management, Las Vegas, NV, Vol. 1, 153-162.

Bond, W. J., 1986. "Velocity-Dependent Hydrodynamic Dispersion During Unsteady, Unsaturated Soil Water Flow: Experiments," Water Resources Research, Vol. 22, No. 13, 1881-1889.

Buddemeier, R. W., and J. R. Hunt, 1987. "Radionuclides in Nevada Test Site Groundwater," published abstract, American Chemical Society, Division of Environmental Chemistry, Vol. 27, No. 1, 534-536.

Buscheck, T. A. and J. J. Nitao, 1991. "Nonequilibrium Fracture-Matrix Flow During Episodic Infiltration Events in Yucca Mountain," Draft Report, Lawerence Livermore National Laboratory, Livermore, CA.

Cederberg, G. A., 1985. "TRANQL, A Groundwater Mass-transport and Equilibrium Chemistry Model for Multicomponent Systems," Ph.D. dissertation, Department of Civil Engineering, Stanford University, Palo Alto, CA.

Cederberg, G. A., 1986. "Scientific Investigation Plan for NNWSI WBS Element 1.2.3.4.1.7.A: Retardation Sensitivity Analysis," SIP No. 86/4.1.7, Los Alamos National Laboratory, Los Alamos, NM.

Cederberg, G. A., L. E. Greenwade, and B. J. Travis, 1987. "Geochemical Simulation of Yucca Mountain: Modeling the Transport of Uranium and Technetium Through the Unsaturated Tuffs," TWS-ESS-5/6-86-01, Los Alamos National Laboratory, Los Alamos, NM.

Cederberg, G. A., R. L. Street, and J. O. Leckie, 1985. "A Groundwater Mass Transport and Equilibrium Chemistry Model for Multicomponent Systems," Water Resources Research, Vol. 21, No. 8, 1095-1104.

Cole, J. D., 1968. Perturbation Methods in Applied Mathematics, Blaisdell Publishing Co., Waltham, MA.

Cook, N. G. W., 1987. "Coupled Processes in Geomechanics," in Coupled Processes Associated with Nuclear Waste Repositories, C. F. Tsang (ed.), Academic Press, Orlando, FL.

Cunningham, A. B., 1981. "Geologically-constrained Hydrologic and Geochemical Modeling of Supergene Weathering Processes Using Physical Rock Parameters, Geochemical Profiles and Modal Data," Master's thesis, Geology Department, University of California, Berkeley, CA.

Dagan, G., 1986. "Statistical Theory of Groundwater Flow and Transport: Pore to Laboratory, Laboratory to Formation, Formation to Regional Scale," Water Resources Research, Vol. 22, No. 9, 120S-134S.

Dagan, G., 1987. "Theory of Solute Transport by Groundwater," Annual Review of Fluid Mechanics, Vol. 19, 183-215.

Daniels, W. R., K. Wolfsberg, R. S. Rundberg, A. E. Ogard, J. F. Kerrisk, C. J. Duffy, T. W. Newton, J. L. Thompson, B. P. Bayhurst, D. L. Bish, J. D. Blacic, B. M. Crowe, B. R. Erdal, J. F. Griffith, S. D. Knight, F. O. Lawrence, V. L. Rundberg, M. L. Skyes, G. M. Thompson, B. J. Travis, E. N. Treher, R. J. Vidale, G. R. Walter, R. D. Aguilar, M. R. Cisneros, S. Maestas, A. J. Mitchell, P. Q. Oliver, N. A. Raybold, and P. L. Wanek, 1982. "Summary Report on the Geochemistry of Yucca Mountain and Environs," Los Alamos National Laboratory Report No. LA-9328-MS, Los Alamos, NM.

de Marsily, G., 1986. Quantitative Hydrogeology, Academic Press, New York, NY.

DOE (U. S. Department of Energy), 1986. "Environmental Assessment, Yucca Mountain Site, Nevada Research and Development Area, Nevada," DOE/RW-0013, Office of Civilian Radioactive Waste Management, Washington, DC.

DOE (U. S. Department of Energy), 1987. "General Guidelines for the Recommendation of Sites for Nuclear Waste Repositories," Code of Federal Regulations, Energy, Title 10, Part 960, Washington, DC.

DOE (U. S. Department of Energy), 1988. "Site Characterization Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada," DOE/RW-0199, Office of Civilian Radioactive Waste Management, Washington, DC.

EPA (U. S. Environmental Protection Agency), 1986. Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes," Code of Federal Regulations, Protection of Environment, Title 40, Part 191, Washington, DC.

Gelhar, L. W., 1986. "Stochastic Subsurface Hydrology from Theory to Applications," Water Resources Research, Vol. 22, No. 9, 135S-145S.

Gelhar, L. W., A. Mantoglou, C. Welty, and K. R. Rehfeldt, 1985. "A Review of Field-Scale Physical Solute Transport Processes in Saturated and Unsaturated Porous Media," Report No. EA-4190, Electric Power Research Institute, Palo Alto, CA.

Germann, P. F., M. S. Smith, and G. W. Thomas, 1987. "Kinematic Wave Approximation to the Transport of Echerichia coli in the Vadose Zone," Water Resources Research, Vol 23, No. 7, 1281-1288.

Greenwade, L. E., and G. A. Cederberg, 1987. "Preliminary Geochemical/Geophysical Model of Yucca Mountain," Los Alamos National Laboratory Report No. LA-UR-87-3389, Los Alamos, NM.

Hart, R. A., 1981. "A Fully Coupled Thermal-Mechanical-Fluid Flow Model for Non-linear Geologic Systems," Ph.D. dissertation, University of Minnesota, Minneapolis, MN.

Harvey, R. W., and L. H. George, 1987. "Transport of Bacteria Through a Contaminated Freshwater Aquifer," published abstract, American Society of Chemical Engineers, Division of Environmental Chemistry, Vol. 27, No. 1, 498-501.

Heiken, G., and F. Goff, eds., 1983. "Geothermal Energy of Hot Dry Rock," Journal of Volcanology and Geothermal Research, Vol. 15, No. 1-3.

Hersman, L, 1986a. "Sorption of ^{239}Pu by a Pseudomonas," presented at American Society for Microbiology annual meeting, Washington, DC, March 23-28, abstract, Los Alamos National Laboratory Report No. LA-UR-85-3780, Los Alamos, NM.

Hersman, L, 1986b. "Biodegradation of Drilling Fluids: Effects on Actinide Sorption," NNWSI Milestone Report M312, Los Alamos National Laboratory, Los Alamos, NM.

Hulburt, H. M., and S. Katz, 1964. "Some Problems in Particle Technology," Chemical Engineering Science, Vol. 19, 555-574.

Hyman, J. M., 1976. "The Method of Lines Solution of Partial Differential Equations," New York University Report, COO-3077-139, New York, NY.

Hyman, J. M., 1979. "MOLID: A General Purpose Subroutine Package for the Numerical Solution of Partial Differential Equations," Los Alamos National Laboratory Report No. LA-7595-M, Los Alamos, NM.

Hyman, J. M., and B. Larrouturou, 1982. "The Numerical Differentiation of Discrete Functions Using Polynomial Interpolation Methods," Los Alamos National Laboratory Report No. LA-UR-81-3282, Los Alamos, NM.

Isrealachvili, J. N., 1985. Intermolecular and Surface Forces, Academic Press, Inc., Orlando, FL.

Jacobson, E. A., M. D. Freshley, F. Harvey Dove, 1985. "Investigations of Sensitivity in Some Hydrologic Models of Yucca Mountain and Vicinity," Sandia National Laboratories Report No. SAND84-7212, Albuquerque, NM.

Jennings, A. A., D. J. Kirkner, and T. L. Theis, 1982. "Multicomponent Equilibrium Chemistry in Groundwater Models," Water Resources Research, Vol. 18, No. 4, 1089-1096.

Kelmers, A. D., R. E. Meyer, J. G. Blencoe, and G. K. Jacobs, 1987. "Radionuclide Sorption Methodologies for Performance Assessment of High Level Nuclear Waste Repositories: A Perspective Gained from a NRC Workshop," Nuclear Safety, Vol. 28, No. 4, 515-522.

Kreiss, H. O., 1979. "Problems with Different Time Scales for Ordinary Differential Equations," SIAM Journal of Numerical Analysis, Vol. 16, 980-998.

Lichtner, P. C., 1985. "Continuum Model for Simultaneous Chemical Reactions and Mass Transport in Hydrothermal Systems," Geochimica et Cosmochimica Acta, Vol. 49, 779-800.

Lubinski, A., 1955. "The Theory of Elasticity for Porous Bodies Displaying a Strong Pore Structure," Proceedings of the Second U. S. National Congress of Applied Mechanics of the American Society of Mechanical Engineers, 247-256.

McWhorter, D. B., and D. K. Sunada, 1977. Groundwater Hydrology and Hydraulics, Water Resources Publications, Fort Collins, CO.

McWilliams, T. B., 1985. "Sensitivity of Radionuclide Transport Times to Uncertainties in Chemical Sorption and Molecular Diffusion," TWS-ESS-5/10-85-01, Los Alamos National Laboratory, Los Alamos, NM.

Miller, C. W., and L. V. Benson, 1983. "Simulation of Solute Transport in a Chemically Reactive Heterogeneous System: Model Development and Application," Water Resources Research, Vol. 19, No. 2, 381-391.

Montazer, P., and W. E. Wilson, 1984. "Conceptual Hydrologic Model of Flow in the Unsaturated Zone, Yucca Mountain, Nevada," U. S. Geological Survey Water-Resources Investigations, Report 84-4345, U. S. Geological Survey, Denver, CO.

Morris, W. A., 1982. "Oil Shale Rock Fragmentation Research: Progress Report for October-December, 1982," Los Alamos Oil Shale Working Group, Los Alamos National Laboratory, Los Alamos, NM.

Nguyen, V. V., W. G. Gray, G. F. Pinder, J. F. Botha, and D. A. Crerar, 1982. "A Theoretical Investigation on the Transport of Chemicals in Reactive Porous Media," Water Resources Research, Vol. 18, No. 4, 1149-1156.

Nitao, J. J., 1990. "Theory of Matrix and Fracture Flow Regimes in Unsaturated, Fractured Porous Media," Lawrence Livermore National Laboratory, Report UCRL-JC-104933, Livermore, CA.

Nitao, J. J., and T. A. Buscheck, 1989. "On the Infiltration of a Liquid Front in an Unsaturated, Fractured Porous Medium," Proceeding of American Nuclear Society Topical Meeting on Nuclear Waste Isolation in the Unsaturated Zone (Focus 89), Las Vegas, NV.

Nielsen, D. R., M. Th. van Genuchten, and J. W. Biggar, 1986. "Water Flow and Solute Transport Processes in the Unsaturated Zone," Water Resources Research, Vol. 22, No. 9, 89S-108S.

Noorishad, J., M. S. Ayatollahi, and P. S. Witherspoon, 1982. "A Finite-Element Method for Coupled Stress and Fluid Flow Analysis in Fractured Rock Masses," International Journal of Mechanics and Mineralogical Society, Vol. 19, 185-193.

NRC (U. S. Nuclear Regulatory Commission), 1987. "Disposal of High-Level Radioactive Wastes in Geologic Repositories," Code of Federal Regulations, Energy, Title 10, Part 60, Washington, DC.

Nuttall, H. E., 1986. "Population Balance for Colloid Transport," Los Alamos National Laboratory Report No. LA-UR-5/9-86-02, Los Alamos, NM.

Nuttall, H. E., 1989. "Interim Report on Particulate Transport, Milestone No. T424," Los Alamos National Laboratory Report, Los Alamos, NM.

Oblow, E. M., F. G. Pin, and R. Q. Wright, 1986. "Sensitivity Analysis Using Computer Calculus: A Nuclear Waste Isolation Application," Nuclear Science and Engineering, Vol. 94, 46-65.

Olofsson, U., B. Allard, K. Andersson, and B. Torstenfelt, 1981. "Formation and Properties of Radiocolloids in Aqueous Solution--A Literature Survey," Programradet for Radioaktivt Avfall, National Council for Radioactive Waste, Report Proav 4.25, Department of Nuclear Chemistry, Chalmers University of Technology, Gotenborg, Sweden.

Olofsson, U., B. Allard, K. Andersson, and B. Torstenfelt, 1982a. "Formation and Properties of Americium Colloids in Aqueous Systems," Scientific Basis for Nuclear Waste Management, S. Topp (ed.), Elsevier Scientific Publishing Co., New York, NY.

Olofsson, U., B. Allard, B. Torstenfelt, and K. Andersson, 1982b. "Properties and Mobilities of Actinide Colloids in Geologic Systems," Scientific Basis for Nuclear Waste Management, Vol. 5, Werner Lutze (ed.), North-Holland, NY, 755-764.

Parker. F. L., R. E. Broshears, and J. Pasztor, 1984. "The Disposal of High-Level Radioactive Waste, 1-2," The Beijer Institute of the Royal Swedish Academy of Sciences.

Peters, R. R., E. A. Klavetter, I. J. Hall, S. C. Blair, P. R. Heller, and G. W. Gee, 1984. "Fracture and Matrix Hydrologic Characteristics of Tuffaceous Materials from Yucca Mountain, Nye County, Nevada," Sandia National Laboratories Report No. SAND84-1471, Albuquerque, NM.

Peters, R. R., and E. A. Klavetter, 1988. "A Continuum Model for Water Movement in an Unsaturated Fractured Rock Mass," Water Resources Research, Vol. 24, No. 3, 416-430.

Randolph, A. D., 1962. "A Population Balance for Countable Entities," Canadian Journal of Chemical Engineering, Vol. 42, 280-281.

Randolph, A. D., and M. A. Larson, 1971. Theory of Particulate Processes, Academic Press, New York, NY.

Rundberg, R. S., A. J. Mitchell, M. A. Ott, J. L. Thompson, and I. R. Triay, 1989. "Laboratory Studies of Radionuclide Migration in Tuff," Proceedings of the American Nuclear Society Topical Meeting on Nuclear Waste Isolation in the Unsaturated Zone, Las Vegas, NV, 248-255.

Schwartz, F. W., L. Smith, and A. S. Crowe, 1983. "A Stochastic Analysis of Dispersion in Fractured Media," Water Resources Research, Vol. 19, 1253-1265.

Seinfeld, J. H., and C. Kravaris, 1982. "Distributed Parameter Identification In Geophysics--Petroleum Reservoirs and Aquifers," Distributed Parameter Control Systems--Theory and Application, S. G. Tzafestas (ed.), Pergamon Press, New York, NY, 369-390.

Silling, S. A., 1983. "Final Technical Position on Documentation of Computer Codes for High-Level Waste Management," U. S. Nuclear Regulatory Commission, NUREG-0856, Washington, DC.

Smith, L., and F. W. Schwartz, 1984. "An Analysis of the Influence of Fracture Geometry on Mass Transport in Fractured Media," Water Resources Research, Vol. 20, 1241-1252.

Sposito, G., and D. A. Barry, 1987. "On the Dagan Model of Solute Transport in Groundwater: Foundational Aspects," Water Resources Research, Vol. 23, No. 10, 1867-1875.

Sposito, G., W. A. Jury, and V. K. Gupta, 1986. "Fundamental Problems in the Stochastic Convection-Dispersion Model of Solute Transport in Aquifers and Field Soils," Water Resources Research, Vol. 22, No. 1, 77-88.

Springer, E., 1988. "Reactive Tracer Experiments in the C-Well and Other Wells in the Yucca Mountain Vicinity," Los Alamos National Laboratory Report No. YMP-LANL-SP 8.3.1.2.3.1.7, 8; R0, Los Alamos, NM.

Stumm W., and J. J. Morgan, 1981. Aquatic Chemistry, Second Ed., Wiley Interscience, New York, NY.

Thomas, L. K., L. J. Helliums, and G. M. Reheis, 1972. "A Nonlinear Automatic History Matching Technique for Reservoir Simulation Techniques," Society of Petroleum Engineers Journal, Transactions of American Institute of Mechanical Engineers, Vol. 253, 508-514.

Tikhonov, A. N., 1963a. "Solution of Incorrectly Formulated Problems and the Regularization Method," Soviet Math. Dakl., Vol. 4, 1035-1038.

Tikhonov, A. N., 1963b. "Regularization of Incorrectly Posed Problems," Soviet Math. Dakl., Vol. 4, 1624-1627.

Timoshenko, S., and J. N. Goodier, 1951. Theory of Elasticity, Second Ed., McGraw-Hill, Inc., New York, NY.

Tompson, A. F. B., E. G. Vomvoris, and L. W. Gelhar, 1987. "Numerical Simulation of Solute Transport in Randomly Heterogeneous Porous Media: Motivation, Model Development and Application," draft report, Massachusetts Institute of Technology, Cambridge, MA.

Torok, J., L. P. Buckley, and B. L. Woods, 1990. "The Separation of Radionuclide Migration by Solution and Particle Transport in Soil," Journal of Containment Hydrology, No. 6, 185-203.

Travis, B. J., 1984. "TRACR3D: A Model of Flow and Transport in Porous/Fractured Media," Los Alamos National Laboratory Report No. LA-9667-MS, Los Alamos, NM.

Travis, B. J., 1985a. "WAFE: A Model for Two-phase Multicomponent Mass and Heat Transport in Porous/Fractured Media," Los Alamos National Laboratory Report No. LA-10488-MS, Los Alamos, NM.

Travis B. J., 1985b. "A Regularization Technique for the Solution of Multidimensional Inverse Transport Problems," abstract in EOS, Transactions, American Geophysical Union, Vol. 66, No. 46, Nov. 12, 1985.

Travis, B. J., and L. E. Greenwade, 1985. "A One-dimensional Numerical Model of Two-phase Flow and Transport in Porous Media Using the Dynamics of Contours Methodology," Los Alamos National Laboratory Report No. LA-UR-85-3328, Los Alamos, NM.

Travis, B. J., and H. E. Nuttall, 1987. "Two-dimensional Numerical Simulation of Geochemical Transport in Yucca Mountain," Los Alamos National Laboratory Report No. LA-10532-MS, Los Alamos, NM.

Travis, B. J., S. W. Hodson, H. E. Nuttall, T. L. Cook, and R. S. Rundberg, 1984. "Preliminary Estimates of Water Flow and Radionuclide Transport in Yucca Mountain," Los Alamos National Laboratory Report No. LA-UR-84-40, Los Alamos, NM.

Tsang, C. F. (ed.), 1987. Coupled Processes Associated with Nuclear Waste Repositories, Academic Press, New York, NY.

Tsang, Y. W., and P. A. Witherspoon, 1981. "Hydromechanical Behavior of a Deformable Rock Fracture Subject to Normal Stress," Journal of Geophysical Research, Vol. 86, No. B10, 9287-9298.

Validation Oversite Group, 1990. "A Validation Methodology for Performance-Assessment Models," Draft Version 0.0. Prepared for the Office of Civilian Radioactive Waste Management, Washington, D. C.

Wasserman, M. L., A. S. Emanuel, and J. H. Seinfeld, 1975. "Practical Applications of Optimal-Control Theory to History-Matching Multiphase Simulator Models," Society of Petroleum Engineers, Transactions of American Institute of Mechanical Engineers, 49th Annual Meeting, Houston, TX, 347-355.

Weeks, E. P., 1987. "Effect of Topography on Gas Flow in Unsaturated Fractured Rock: Concepts and Observations," Proceedings of the American Geophysical Union Symposium on Flow and Transport in Unsaturated Fractured Rock, D. Evans, and T. Nicholson, eds., Geophysical Monograph 42.

Wilson, J. L., and D. E. Metcalfe, 1985. "Illustration and Verification of Adjoint Sensitivity Theory for Steady State Groundwater Flow," Water Resources Research, Vol. 21, No. 11, 1602-1610.

Witherspoon, P. A., J. S. Y. Wang, K. Iwai, and J. E. Gale, 1980. "Validity of Cubic Law for Fluid Flow in a Deformable Rock Fracture," Water Resources Research, Vol. 16, No. 6, 1016-1024.

Zyvoloski, G. A., Z. Dash, and S. Kelkar, 1988. "FEHM: Finite Element Heat and Mass Transfer Code," Los Alamos National Laboratory Report No. LA-11224-MS, Los Alamos, NM.

Zyvoloski, G. A., and S. Kelkar, 1987. "FEHMS: Finite Element Heat-Mass-Stress Code for Coupled Geological Processes," NNWSI Milestone Report R346, Los Alamos National Laboratory Report No. LA-UR-87-1323, Los Alamos, NM.

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 8.3.1.3.7.1 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 8.3.1.3.7.1 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 8.3.1.3.7.1 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 QPs also apply:		
	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

The following number is for the Office of Civilian Radioactive Waste Management Records management purposes only and should not be used when ordering this document.

Accession Number: NNA.920729.0002