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Saturated Zone Flow and Transport Abstraction/Testing Workshop Results

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Civilian Radioactive Waste Management System

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EXECUTIVE SUMMARY

This report documents the planning, proceedings, and results of the Saturated Zone (SZ) Flow and Transport Abstraction/Testing Workshop held on April 1-3, 1997 in Denver, Colorado. This workshop was one of a series of abstraction/testing workshops held in support of the Total System Performance Assessment for Viability Assessment (TSPA-VA) of the potential high-level radioactive waste repository at Yucca Mountain, Nevada. These workshops were designed to contribute to a valid, defensible TSPA by integrating current site and design data and models into the TSPA-VA analyses.

The three primary goals of the SZ Flow and Transport Workshop were to 1) develop a comprehensive list of issues related to key uncertainties about SZ flow and transport behavior, 2) prioritize the list of issues based on impact to long-term performance of the potential repository, and 3) develop analysis plans to aid in the resolution of high-priority issues and provide a basis for model abstraction in TSPA-VA. These goals were accomplished by convening a workshop that included researchers from within the Yucca Mountain Project in the areas of site characterization, numerical flow and transport modeling, and TSPA analysts. Follow-up activity to the workshop consists of implementation of the abstraction/testing analysis plans by the workshop participants and integration of the results with other components (e.g., unsaturated zone (UZ) transport and biosphere) into TSPA calculations.

Organization and implementation of the SZ Flow and Transport Workshop was accomplished by the abstraction core team that consisted of Bill Arnold (Sandia National Laboratories - team leader), Jack Gauthier (Sandia National Laboratories, Spectra Research - TSPA representative), Pat Tucci (USGS - flow modeling representative), and Bruce Robinson (Los Alamos National Laboratory - transport modeling representative). Preparation for the workshop included listing the important issues (parameters, processes, conceptualizations) for consideration at the workshop and selection of the participants. Participants were solicited for their opinions prior to the workshop and their comments on the relevant issues were provided in written form to all of the participants before the workshop. The workshop organizers also developed a set of performance criteria. Each of the issues could thus be ranked according to its influence on 1) peak radionuclide concentration in the SZ at 5 km from the repository, 2) peak concentration at 30 km, 3) time to first arrival of radionuclides, 4) the spatial distribution of the contaminant plume, and 5) spatial distribution of groundwater flux. In addition to participants, the workshop was attended by observers from the Department of Energy, Nuclear Regulatory Commission, the Nuclear Waste Technical Review Board, and the TSPA Peer Review Team.

The SZ workshop consisted of 1) introductory TSPA presentations, 2) participant presentations on individual issues, 3) prioritization of issues, and 4) development of abstraction/testing analysis plans by teams of participants. Presentations by TSPA representatives outlined the goals, schedule, and constraints of TSPA calculations to workshop participants, many of whom were not familiar with TSPA methods. Individual participants gave presentations on issues covered by their research in four main categories: 1) conceptual models of SZ flow, 2) conceptual models of SZ geology, 3) transport processes and parameters, and 4) coupling to other components of TSPA. Working groups consisting of six to seven participants quantitatively and independently scored the various issues within each category following the presentations. Scoring of issues for the prioritization process was performed relative to the pre-determined set of five criteria based on anticipated effects on repository performance. Analysis plans for sensitivity studies and abstraction of SZ flow and transport modeling were developed to address the higher priority issues identified in the initial phases of the workshop. TSPA representatives were consulted regarding the applicability of analysis plan products to TSPA analyses.

The primary products of the SZ Flow and Transport Workshop are the prioritized list of relevant issues and the analysis plans. A listing of the higher priority issues for the four categories indicated is given in Table 1 below. The titles of the six abstraction/testing analysis plans are presented in Table 2. The analysis plans address at least some aspect of a majority of the higher priority issues identified by the workshop. Most of the analysis plans represent a modification or focusing of existing workscopes to deliver products that are more directly useful to the TSPA-VA analysis.

Table 1. Higher Priority Issues

Category 1: Conceptual Models of SZ Flow	Category 2: Conceptual Models of SZ Geology	Category 3: Transport Processes and Parameters	Category 4: Coupling to Other Components of TSPA
Regional discharge. Regional recharge. Vertical flow. Alternative conceptual models.	Channelization in vertical features. Properties of faults. Channelization in stratigraphic features. Distribution of zeolites. Fracture network connectivity.	Dispersivity. Matrix diffusion (effective porosity). Matrix sorption. Fracture sorption.	Climate change. UZ and SZ coupling. Thermal and chemical plume. Well withdrawal scenarios.

Table 2. Analysis Plan Titles

Analysis Plan Titles
1. Sensitivity Study on Uncertainties in Site-Scale Saturated-Zone Transport Parameters and Models
2. Coupling UZ and SZ Transport Models
3. The Effects of Large-Scale Channelization on Effective Transport Parameters
4. Determination of Effective Field-Scale Transport Parameters Using C-Wells Testing Results
5. Past, Present, and Future Saturated Zone Fluxes
6. Geologic Structure and Processes Affecting Flow Channelization

1. INTRODUCTION

This report documents the planning, proceedings, results, and products of the Saturated Zone (SZ) Flow and Transport Abstraction/Testing Workshop held on April 1-3 in Denver, CO. The SZ Workshop was one of a series of abstraction/testing workshops held in support of Total System Performance Assessment for Viability Assessment (TSPA-VA). These workshops, which addressed various components of the natural and engineered barrier systems for the potential high-level radioactive waste disposal facility at Yucca Mountain, Nevada, were designed to integrate current process-level modeling and site characterization and design data into TSPA analyses.

1.1 INTRODUCTION TO TSPA-VA

The Viability Assessment for the potential repository system, as defined in the FY 1997 Energy and Water Appropriations Act, includes four major components: three of the components are related to repository and waste package design, plan and cost to complete a license application, and an estimate of costs to construct the repository. The fourth component is "a total-system performance assessment based on the design concept and scientific data and analysis available by September 30, 1998, describing the probable behavior of the repository in the Yucca Mountain geological setting relative to the overall system performance standards." Part of the basis for developing the total-system performance assessment is the subject of this report.

The models used to perform the Total System Performance Assessment-Viability Assessment (TSPA-VA) are generally expected to be formulated as "abstractions" from more detailed process models. In the case of a TSPA, an abstraction is defined as a simplified/idealized model that reproduces or bounds the essential elements of more detailed process models. For an abstraction, the inputs may be those that form a subset of those required for a process model, or they may be a response function derived from intermediate results. However, the abstracted form must capture uncertainty and variability. They must also be tested against process models to assure their validity. The generalized form of abstractions is discussed in more detail in Section 1.7.

Abstractions are used because of the probabilistic/stochastic nature of TSPA analyses. The intent of the abstraction process is to retain key aspects of process models, while producing results usable in multiple realization probabilistic models. Following is a general discussion of the activities currently ongoing to produce abstracted models. Also presented are the specific results generated by the initial phases of one activity specifically directed at the development of models for saturated zone flow and transport.

1.2 CONTEXT FOR USE OF THE SZ FLOW MODEL WITHIN THE PA PROGRAM

The SZ flow and transport models will provide a basis for calculating the radionuclide mass flux, travel times, and radionuclide concentrations in the saturated zone in the region beneath and downgradient of the potential repository. Groundwater flow in the saturated zone is the pathway for movement of radionuclides that have percolated downward through the unsaturated zone to the water table. Horizontal migration and dispersal of radionuclides in the SZ will dictate the temporal and spatial variability in concentration of radionuclides released to the accessible environment by pumping wells or spring discharge. The SZ flow and transport models thus link two other components of TSPA: Unsaturated Zone Transport and Biosphere.

1.3 GOALS OF THE ABSTRACTION/TESTING WORKSHOPS

During FY97-98, a series of abstraction/testing (A/T) activities were initiated to identify and construct appropriate numerical or analytical representations of components of the potential Yucca Mountain repository system to assure the development of a valid, defensible total-system performance assessment for the Viability Assessment. This objective requires that Performance Assessment (PA) incorporate the most complete and current information available from the Yucca Mountain Project. It also requires that the essential behavior of key processes (defined relative to the contribution that process makes to long-term performance of the repository system) be captured in a computationally efficient manner. The important issues, including the alternative hypotheses must be identified, quantified, and evaluated. Due to time and resource constraints, the model development must be focussed on only those issues that are most important to performance. And, to provide traceability and transparency, the bases for assumptions must be well defined, justified, and documented.

The total-system performance assessment performed for the TSPA-VA will be constructed of models developed to represent processes and features of both the natural and the engineered system. Although the responses of the components are strongly interdependent, The PA analysts have broken the processes up into somewhat artificial components to facilitate analysis. These components are: 1) Unsaturated Zone Flow, 2) Thermohydrologic Flow, 3) Near Field Environment, 4) Waste Package Degradation, 5) Waste Form Alteration and Mobilization, 6) Unsaturated Zone Transport, 7) Saturated Zone Flow and Transport, and 8) Biosphere. A separate abstraction/testing activity has been defined for each of the eight components defined above.

In order to meet the goal of constructing a valid, defensible TSPA-VA, the abstraction/testing activities were designed to integrate the work of PIs from site characterization, design, environmental programs, and performance assessment. In order to achieve this integration, analysts from each these areas of the project have been identified to participate in all aspects of the activities. These activities have 3 major elements. The first part includes the planning needed to identify a preliminary list of relevant issues for the subject component and to define the activities to be accomplished in a workshop. This work is accomplished by a team (the Abstraction Core Team, or ACT) that includes at least one subject matter expert in the component of interest, a TSPA expert, and a PA subsystem modeler. The latter person is the task lead for the entire A/T activity. The next step in the A/T activity is to hold a workshop, and to finally perform a set of analyses to develop the parameters, models of processes, and alternate conceptualizations for use in the TSPA-VA.

Because the ultimate goal of these abstraction/testing activities is a single TSPA-VA, there is a need to reintegrate the components for the final analyses. The primary responsibility for the reintegration process lies with an oversight group called the TSPA Core Team (or TCT) and PA management. The TCT members are Michael Wilson, David Sevougian, Jack Gauthier, and Jerry McNeish. The TCT and PA management will attend all of the A/T workshops and a representative from the TCT is part of each ACT to ensure consistency and usefulness of the products generated by all the activities. The actual method for convolving the products of the A/T activities will be developed in Summary Account TR541FB1 (Develop TSPA-VA Methodology).

1.4 SYNOPSIS OF THE WORKSHOP PROCESS

The three primary goals of the abstraction/testing workshops were:

1) Develop a comprehensive list of issues related to key uncertainties about the subject component of the workshop that are relevant to repository performance,

2) Prioritize the list of issues based on impact to long-term repository performance, and

3) Develop analysis plans to aid in the resolution of high-priority issues and provide a basis for model abstraction in TSPA-VA.

A methodology for conducting the abstraction/testing workshops evolved as the various workshops were planned and implemented. By the time that plans were being finalized for the SZ Flow and Transport workshop, an effective methodology had been firmly established by TSPA workshop organizers. This methodology consisted of both careful pre-workshop planning and a fairly rigid workshop structure. The key components of this methodology are summarized below.

Pre-workshop Planning

- Produce a list of important issues that are relevant to the subject of the workshop, defining the scope of the workshop.

- Produce a list of potential workshop participants. Cross check this list of participants with the list of issues. Issue invitations to potential participants in a memo explaining the goals of the workshop and soliciting responses to the listed issues and strawman proposals.

- Collate participant input and analysis proposals. Revise the list of issues based on participant responses and develop a list of speakers to make presentations at the workshop.

- Develop a set of performance criteria to be used by workshop participants in the prioritization of issues. These performance criteria should be directly linked to the regulatory criteria to be addressed in TSPA analyses.

- Divide participants into four working groups for the initial phases of the workshop. Each working group is to be seated at a separate table and should include at least one site-characterization researcher, process-level modeler, sub-system performance assessment modeler, and a TSPA analyst.

Workshop Implementation

- Presentation of background information on TSPA-VA, workshop goals and schedule, and TSPA methodology, including model abstraction options.

- For each category of issues, presentation of previous TSPA approaches and presentations on individual issues by workshop participants.

- Discussion and prioritization of issues based on pre-defined performance criteria, carried out separately by the four working groups.

- Global prioritization of all issues across categories carried out by a voting method including the entire group of participants.

- Discussion of related workscopes to serve as a guide in the development of analysis plans.

- Definition of broad analysis plan subjects and self-selection of analysis plan working groups.

- Develop analysis plans for abstraction/testing based on the prioritized list of issues. The products to TSPA from each analysis plan are defined and these, along with details of the plan, are discussed by the entire group.

Post-Workshop Activities

- Coordination of implementation of analysis plans for abstraction/testing through the establishment of a set of base-case parameters.

- Completion of abstraction/testing activities.

- Documentation of abstraction/testing activities.

- Development of schedule and method to integrate abstractions and other components of the total system into TSPA-VA analyses.

1.5 SUMMARY OF THE WORKSHOP RESULTS

The overriding objective of the SZ Flow and Transport Workshop was to determine how PA would incorporate valid, defensible models into the TSPA-VA analyses. The strategy for accomplishing this objective was to prepare a comprehensive list of issues relevant to SZ flow and transport, to prioritize these issues, and to develop analysis plans to address these issues in the context of abstraction methodology. Development of the analysis plans was guided by the higher priority issues delineated by the workshop. These workshop results are briefly summarized below.

1.5.1 Prioritization of Issues

The higher ranked issues in each of the four categories are listed in Table 1-1 below. Ranking of these issues was accomplished from the combined results of a numerical scoring procedure within four individual working groups, as described in more detail in Section 3.3. These higher priority issues are also more fully described in Table 1-4.

1.5.2 Abstraction/Testing Analysis Plans

Consideration of these higher priority issues resulted in the development of six abstraction/testing analysis plans. The titles of the analysis plans are given in Table 1-2 below. Detailed documentation of the analysis plans is presented in Chapter 4.

1.6 DISCUSSION OF RELEVANT ASSUMPTIONS

The relevant modeling and analysis assumptions are listed in each of the analysis plans (see Chapter 4). These assumptions are summarized in Table 1-3. These assumptions are, for the most part, directly related to the issue(s) being addressed in the particular analysis plan. The listed assumptions are not comprehensive, in that they generally do not include all of the underlying assumptions that are implicit in the process-level models and codes being used in the analyses. However, the basic assumptions in these models and computer codes are explained or referenced in related YMP deliverables that document the relevant process-level models.

Table 1-1. Higher Priority Issues

Category 1: Conceptual Models of SZ Flow	Category 2: Conceptual Models of SZ Geology	Category 3: Transport Processes and Parameters	Category 4: Coupling to Other Components of TSPA
1.6: Regional discharge 1.5: Regional recharge 1.4: Vertical flow 1.1: Alternative conceptual models	2.1: Channelization in vertical features 2.4: Properties of faults 2.2: Channelization in stratigraphic features 2.8: Distribution of zeolites 2.6: Fracture network connectivity	3.1: Dispersivity 3.2: Matrix diffusion (effective porosity) 3.3: Matrix sorption 3.4: Fracture sorption	4.1: Climate change 4.4: UZ and SZ coupling 4.2: Thermal and chemical plume 4.3: Well withdrawal scenarios

Table 1-2. Analysis Plan Titles

Analysis Plan Titles
1. Sensitivity Study on Uncertainties in Site-Scale Saturated-Zone Transport Parameters and Models
2. Coupling UZ and SZ Transport Models
3. The Effects of Large-Scale Channelization on Effective Transport Parameters
4. Determination of Effective Field-Scale Transport Parameters Using C-Wells Testing Results
5. Past, Present, and Future Saturated Zone Fluxes
6. Geologic Structure and Processes Affecting Flow Channelization

In addition to the conceptual assumptions necessary for individual analysis plans, an assumed set of reference or base-case flow and transport parameters will be developed for use in modeling. This is necessary to provide consistency among the analyses and facilitate comparison of abstraction/testing results. The values of these base-case parameters are less important than that they be consistently applied in modeling studies. The base-case parameter values will be established by consensus among principle participants in abstraction/testing tasks. It should be noted that base-case hydrologic parameters may be different for the regional-scale SZ flow model than for the site-scale SZ flow model. This may be necessary because of differences in definition of hydrostratigraphic units in the two models and because of differences in scale.

Table 1-3. Assumptions from Analysis Plans

Analysis Plan	Assumptions
1. Sensitivity to Transport Parameters and Models	(a) the dual porosity model is assumed to adequately represent radionuclide transport in the SZ; (b) colloid-facilitated radionuclide transport in the SZ is not being considered.
2. Coupling of UZ and SZ Transport Models	(a) a generic SZ transport simulation will be used to test hypotheses; (b) solute mass flux from UZ transport simulations is delivered to the SZ directly at the water table.
3. Effects of Large-Scale Channelization	(a) vertical, large-scale channelization features do not significantly alter the distribution of head and groundwater flow immediately downgradient of the repository.
4. Effective Transport Parameters from C-well tests	(a) the dual porosity model is assumed to adequately represent radionuclide transport in the SZ.
5. Past, Present, and Future SZ Fluxes	(a) steady-state solutions of regional groundwater flow are an adequate approximation of the system (i.e., transient effects are not significant); (b) the regional-scale flow model does not capture detailed distribution of flux at the site-scale;
6. Geologic Structure and Processes Affecting Flow Channelization	(a) a single-continuum flow model is used; (b) the upper SZ is modeled as confined flow; (c) faults are assumed to be vertical.

1.7 Approaches to Model Abstraction/Testing

Because TSPA calculations must be performed for hundreds or thousands of probabilistic realizations of the system, it is desirable (and most probably necessary) to abstract the results of individual process-level models for incorporation into the analysis. The abstraction reduces the computational burden from that particular component of the TSPA calculation, while retaining the essential behavior of the underlying process-based model. There are several alternatives available for abstracting modeling results that are described below.

Another possible result of model abstraction/testing is a conclusion regarding the validity of assumptions about alternative conceptual models. If a simplified or less computationally intensive conceptual model produces a result needed for TSPA calculations that is approximately the same as the more complex model, then the simplified conceptual model can be used either directly in the TSPA calculations or as the basis for further abstraction. An example from SZ flow and transport is the question of whether or not a single continuum model is adequate to represent a dual-porosity system through the use of the effective porosity concept. Numerical testing of the more complex dual-porosity model could reveal that the single continuum model may be used for subsequent modeling and provide a value (or range of values) for effective porosity.

There are three basic options for the abstraction of models: (1) use the model to produce a response surface or multidimensional table, (2) reduction in dimensionality (i.e., perform calculations in 1-D or 2-D rather than in 3-D), and (3) develop simplified models that exhibit the expected or observed behavior of the complex model, but do not explicitly simulate the underlying physical processes. These options are described below in relation to their possible implementation for SZ flow and transport simulations.

Response Surface

In the response surface approach to model abstraction, one or more dependent variables are determined as a function of one or more of the independent model parameters. This is accomplished through multiple runs of the process-level model over ranges of values of the relevant independent model parameters. The advantage of this approach is that once the response surface has been established calculation of the dependent variables is extremely rapid. The disadvantage can be that a very large number of model realizations may be necessary to define the response surface.

An example of a high degree of abstraction for SZ flow and transport would be to calculate a dilution factor for radionuclides at given locations as a function of parameters such as dispersivity, effective porosity, hydraulic conductivity, and sorption coefficients. A method related to the response surface approach is to establish a library of transfer functions based on the convolution integral method to calculate radionuclide concentrations downgradient of the repository as a function of transient radionuclide mass flux to the water table from the unsaturated zone (UZ) component of the TSPA analysis.

Dimensionality Reduction

In this abstraction approach, the complete process-level model is employed, but in a geometrically simplified form. If a 1-D abstraction of a flow and transport model is used, the 1-D columns would be defined by stream tubes simulated in a 3-D representation of the system. Multiple 1-D columns may be used to approximate flow along different pathways through the system. The advantage of this approach is that the flow and transport model can retain some complex features of the original process-level model (e.g., matrix diffusion and sorption). The primary disadvantage is that a 1-D model is incapable of simulating some key processes (e.g., transverse dispersion) that may have a significant impact on the simulation results.

Dimensionality reduction is a form of abstraction that has been used in previous TSPA analyses of Yucca Mountain (see Section 1.9). Multiple realizations of the SZ flow and transport system were constructed for a single or a group of 1-D flow tubes. It should be noted that previous TSPA efforts have focused on cumulative release of radionuclides and not on peak dose as the primary measure of repository performance. The 1-D abstraction of flow and transport in the SZ is a more appropriate abstraction method for calculation of cumulative release than for peak dose, which is directly related to peak concentration. Peak concentration is sensitive to transverse dispersion, which can only be implicitly incorporated into 1-D flow and transport simulations.

Simplified Models

Simplified models incorporate some basic aspects of the behavior of the system without modeling the physical processes involved. Simplified models may take a variety of forms depending on the particular behavior of the system that is deemed most significant. The advantages of this abstraction approach include computational efficiency and the ability to simulate behavior that is impossible to explicitly model with a physically-based model. A major disadvantage of this approach is defensibility; support for the behavior of the model depends on the strength of evidence indicating the assumed behavior.

An example of a simplified model for SZ flow and transport would be a "mixed tank" type of model. In this type of model the total mass of a radionuclide is assumed to be mixed with an assumed volume of groundwater. This volume of groundwater could be based on flow rates and an assumption regarding the maximum depth of the plume. Alternatively, the volume of groundwater could be defined by the assumed total volume of pumping from a well or wells.

1.8 PRODUCTS OF THE ABSTRACTION PROCESS

The form of the products of the abstraction process differ for the various abstraction/testing analysis plans and is expected to evolve as the applicability of various results is assessed. There are three basic types of product from the abstraction activities. The product may be a range of values for a particular parameter to be used internally within process-level models (e.g., an improved estimate of fracture sorption from analysis of tracer-test results or a new estimate of average groundwater flux from the regional-scale flow model). The product may be a conclusion regarding the importance of a particular feature or process to modeling results (e.g., the significance of postulated structural features to flow channelization and transport). The third type of product is an abstraction that can be used directly in feeding the radionuclide concentration history to the biosphere component of the TSPA-VA calculation (e.g., a suite of radionuclide breakthrough curves to use as the basis of the convolution integral method for UZ-SZ transport coupling).

1.9 COMPARISON TO PREVIOUS TSPA MODELING

Previous TSPA calculations of flow and transport in the SZ have abstracted flow modeling results by representing the system as a single or series of one-dimensional flow tubes. Dilution by transverse mixing (both lateral and vertical) has been approximated by assuming complete mixing across an area transverse to groundwater flow or using an analytical solution for solute transport in a uniform flow field. TSPA-91 (Barnard et al., 1992) used the results of two-dimensional subregional flow modeling by Czarnecki and Waddel (1984) to derive a distribution of groundwater travel times in the SZ from the repository to the accessible environment. This distribution of velocities was then applied in Monte Carlo simulations to advective-dispersive transport in a single, one-dimensional, homogeneous flow_tube to calculate cumulative release.

TSPA-93 (Wilson et al., 1994) calculations involved development of a three-dimensional, site-scale flow model of the SZ that considered two alternative conceptual models of flow related to the large-hydraulic gradient, a fault-controlled model and a carbonate-aquifer-drain model. Five to eight one-dimensional flow tubes (corresponding to representative UZ flow and transport columns) were used in the abstraction of SZ behavior, with two classes of velocity and dispersivity distributions derived from the three-dimensional flow and transport modeling. Radionuclide concentrations at the downstream end of the flow tubes were calculated by assuming complete mixing across an area defined by the transverse dispersivity and a somewhat arbitrary range of mixing depth (10 to 500 m).

TSPA-95 (M&O, 1995) used a similar representation of the SZ, with multiple one-dimensional, homogeneous flow tubes corresponding to UZ columns. TSPA-95 used the same distribution of groundwater fluxes in the SZ derived in Wilson et al. (1994) and assumed complete mixing to a depth of 50 m in concentration calculations. This assumption of complete mixing is justified as a conservative estimate in the TSPA-95 report by derivation of dilution factors using an analytical solution of solute transport in a three-dimensional, uniform flow field, which are larger than the dilution factors from the mixing model. For calculations of radionuclide concentration at a distance of 30 km, the TSPA-95 calculations also assume additional dilution by mixing with flow from other groundwater sub-basins.

The results from all of these performance assessment calculations agree that the SZ contributes little to the total system as a barrier to cumulative radionuclide release. Even within the range of uncertainty about factors which influence transport times in the SZ, the resulting impact on cumulative release over a 10,000 year period is small. On the other hand, flow and transport processes in the SZ have a large influence on radionuclide concentrations used in dose calculations. Simulated radionuclide concentrations vary directly with highly uncertain assumptions about the extent of natural mixing in the SZ. In addition, concentrations in drinking water from water well withdrawals can vary dramatically depending on assumptions about well construction and discharge rate.

The current plans for TSPA-VA, as reflected in the conclusions and analysis plans from the SZ Flow and Transport Workshop, are to make more direct use of process-level modeling, without the need for dimensionality reduction.

1.10 REVIEW OF PROCESSES TO BE CONSIDERED

The processes, parameters, and issues to be considered prior to the workshop are shown in Figure 1-1. These issues were determined by the ACT and divided into four major categories as indicated. The participants were asked to respond to any of the issues about which they wished to make proposals and to suggest any additional issues they felt were relevant. The final set of issues that was considered at the workshop was expanded somewhat relative to the initial list and is reflected in the list of presentations shown in Section 2.4. The four major categories reflect important uncertainties in the SZ groundwater flow system, in the geometry of the physical features controlling flow, in the transport parameters, and in the coupling to other processes and components of the system. Preliminary responses to these issues were sent to workshop participants in the form of strawman proposals as documented in Section 2.3.

1. Conceptual Models of SZ Flow

    1.1 Alternative conceptual models (e.g., of the large hydraulic gradient)
    1.2 Hydraulic properties of faults
    1.3 Vertical flow
    1.4 Distribution of recharge
    1.5 Regional discharge

2. Conceptual Models of SZ Geology

    2.1 Flow channelization
    2.2 Spatial distribution of hydraulic conductivity
    2.3 Geologic and mineralogic framework

3. Transport Processes and Parameters

    3.1 Dispersivity
    3.2 Matrix diffusion (effective porosity)
    3.3 Sorption
    3.4 Colloid transport

4. Coupling to Other Components of TSPA

    4.1 Climate change
    4.2 Thermal and chemical plume
    4.3 Well withdrawal scenarios
    4.4 Coupling with UZ transport

Figure 1-1. List of issues considered by the workshop participants prior to the workshop. Issues are divided into four major categories.

1.11 KEY ISSUES TO BE ADDRESSED

The key issues considered for the development of analysis plans in the workshop are listed in Table 1-4. These were the issues determined to be those of higher priority within each category using the prioritization process employed in the workshop (see Sections 1.5.1 and 3.3). Note that the issues are ranked according to priority in Table 1-4, with the highest priority issue in each category placed in the uppermost row.

Table 1-4. Key Issues

Category 1: Conceptual Models of SZ Flow	Category 2: Conceptual Models of SZ Geology	Category 3: Transport Processes and Parameters	Category 4: Coupling to Other Components of TSPA
1.6: What is the distribution and magnitude of regional discharge?	2.1: Do vertical, large-scale channelization features impact transport?	3.1: What is the appropriate range of longitudinal and transverse dispersivity to use in transport modeling?	4.1: What are the impacts of climate change on groundwater flux, water table elevation, and discharge locations?
1.5: What is the distribution and magnitude of recharge on a regional scale?	2.4: How do the hydrologic and mineralogic characteristics of faults influence flow and transport?	3.2: What is the impact of matrix diffusion on transport? Can effective porosity be used to approximate matrix diffusion?	4.4: How should SZ transport be coupled to UZ transport?
1.4: To what extent would vertical flow influence the radionuclide plume?	2.2: To what extent does channelization through stratigraphic zones impact transport?	3.3: What range of values should be used for the matrix sorption coefficient?	4.2: What impacts do thermal and chemical alterations have on SZ flow and transport?
1.1: Which alternative conceptual models of the flow system should be considered?	2.8: What is the distribution of zeolites in the SZ?	3.4: What range of values should be used for the fracture sorption coefficient?	4.3: What scenarios and modeling methods should be used to simulate withdrawals from wells?
	2.6: What is the connectivity of the fracture network at intermediate scales (10's to 100's m)?		

1.12 ISSUES NOT ADDRESSED IN THE ABSTRACTION PROCESS

The abstraction/testing analysis plans developed during the workshop do not address all of the issues that were proposed before the workshop and that were revealed during the workshop. The issues that do not appear in the analysis plans (see Chapter 4) are listed in Table 1-5. Many of these issues were ranked lower in the prioritization process and do not appear in the list of key issues (see Table 1-4). Other issues are being addressed in other components of the abstraction/testing work that is being performed in support of TSPA-VA. Some issues are not being addressed because of resource limitations.

Issue 1.1 is not being specifically addressed in any of the analysis plans, but continues to be explored in the development of the USGS site-scale flow model. Alternative representations of the large-hydraulic gradient to the north of the potential repository are being implemented in the site-scale model. If the potential impacts on performance appear to be large from these alternative flow models, the alternative representations can be incorporated into the abstraction process at that time.

Under the category of conceptual models of SZ geology, it was a consensus agreement that issue 2.8 be addressed by incorporating conclusions of the LANL mineralogic framework model into the site-scale SZ transport model. Aspects of issues 2.3, 2.5, 2.7, and 2.8 are implicit in some of the higher priority issues in this category (e.g., issues 2.1, 2.2, and 2.6).

The issue of colloid transport (3.5) was not ranked highly in the prioritization of issues during the workshop. In part this was due to the fact that colloid transport was not thought to be as significant for the longer travel distances in the SZ relative to the UZ. Participants were also aware that an analysis plan had been developed for the effects of colloids in the UZ transport workshop and that a similar implementation for simulation of colloid transport could be exported to SZ transport calculations if necessary. Conclusions regarding issue 3.6 will be forthcoming from proposed field work by researchers at LANL and were not included because of insufficient data at this time.

Although participants recognized the potential importance of issue 4.3, consideration of this issue was deferred to the biosphere abstraction/testing workshop. Definition of the well scenarios to be considered in the interface between SZ flow and transport and the biosphere are primarily dependent upon assumptions that have not yet been fully developed within the biosphere component of the abstraction/testing task. The coupling of thermal, chemical, and mechanical effects with the SZ flow and transport modeling are not addressed in the analysis plans primarily due to resource limitations.

Table 1-5. Issues Not Addressed in the Abstraction Process

Category 1: Conceptual Models of SZ Flow	Category 2: Conceptual Models of SZ Geology	Category 3: Transport Processes and Parameters	Category 4: Coupling to Other Components of TSPA
1.1: Alternative conceptual models	2.8: Distribution of zeolites	3.5: Colloid transport	4.2: Thermal and chemical plume
	2.3: Scale effects of geologic properties	3.6: Radionuclide solubility	4.3: Well withdrawal scenarios
	2.5: Spatial distribution of hydraulic conductivities		4.6: Stress effects on hydraulic properties

Table 1-5. Issues Not Addressed in the Abstraction Process

Category 1: Conceptual Models of SZ Flow	Category 2: Conceptual Models of SZ Geology	Category 3: Transport Processes and Parameters	Category 4: Coupling to Other Components of TSPA
	2.7: Lumping of stratigraphy		
	2.9: Relationship of welding to degree of fracturing		

1.13 SCHEDULE FOR ABSTRACTION/TESTING PROCESS

The schedules for the six abstraction/testing analysis plans are summarized in Tables 1-6 to 1-11. Note that the details of each analysis plan are given in Chapter 4 of this document.

The working schedule for Analysis Plan 1: Sensitivity Study on Uncertainties in Site-Scale Saturated-Zone Transport Parameters and Models,

Table 1-6. Task 1 Schedule

Date	Activity	Responsible Party
5/31/97	- Deliver data and parameter values	LANL (Jake Turin) LANL (Ines Triay)
6/16/97	- Deliver site-scale SZ flow model	USGS (John Czarnecki)
8/31/97	- Complete sensitivity analysis	LANL (Bruce Robinson) LANL (George Zyvoloski) INTERA (Chunhong Li)

The working schedule for Analysis Plan 2: Coupling UZ and SZ Transport Models,

Table 1-7. Task 2 Schedule

Date	Activity	Responsible Party
4/30/97	- Determination of UZ transport base-case model	LANL (Bruce Robinson) LANL (Kay Birdsell)
6/16/97	- Deliver site-scale SZ flow model	USGS (John Czarnecki)

Table 1-7. Task 2 Schedule

Date	Activity	Responsible Party
7/31/97	- Calculation of SZ base-case transport, comparison of convolution method to detailed (transient) model	LANL (Kay Birdsell) LANL (Bruce Robinson)

The working schedule for Analysis Plan 3: The Effects of Large-Scale Channelization on Effective Transport Parameters,

Table 1-8. Task 3 Schedule

Date	Activity	Responsible Party
6/16/97	- Deliver site-scale SZ flow model	USGS (John Czarnecki)
7/31/97	- Complete conceptual model of channelization features	SNL (Sean McKenna) USGS (Art Geldon) USGS (Chris Potter)
8/31/97	- Incorporate channelization features into flow/transport model	SNL (Sean McKenna) SNL (Bill Arnold) LANL (Bruce Robinson)
9/15/97	- Compare transport simulations with and without channelization features, summarize results	SNL (Bill Arnold) SNL (Sean McKenna) LANL (Bruce Robinson) SNL (Mike Wilson)

The working schedule for Analysis Plan 4: Determination of Effective Field-Scale Transport Parameters Using C-Wells Testing Results,

Table 1-9. Task 4 Schedule

Date	Activity	Responsible Party
7/30/97	- Complete interpretations of conservative tracer testing as C-wells	USGS (M.J. Umari) USGS (Art Geldon)
10/1/97	- Complete analysis of tracer test results using analytical solution	USGS (M.J. Umari)
10/1/97	- Complete analysis of tracer test results using FEHM model	LANL (Jake Turin)

The working schedule for Analysis Plan 5: Past, Present, and Future Saturated Zone Fluxes,

Table 1-10. Task 5 Schedule

Date	Activity	Responsible Party
4/30/97	- Complete climate simulations with existing regional-scale flow model	USGS (Frank D'Agnese) USGS (Pat Tucci)
5/31/97	- Incorporate evapotranspiration data into regional-scale flow model	USGS (Frank D'Agnese) USGS (Pat Tucci)
6/30/97	- Complete regional-scale flow model recalibration	USGS (Frank D'Agnese) USGS (Pat Tucci)
8/1/97	- Deliver synthesis report to YMP on future climate scenarios	USGS (Frank D'Agnese)
7/1/97	- Complete model consistency evaluation between regional-scale model and site-scale model	USGS (John Czarnecki) SNL (George Barr)
9/8/97	- Complete evaluation of hydrochemical and isotopic data with regard to regional-scale flow model	LANL (Arend Meijer) LBNL (Ardyth Simmons)
9/8/97	- Deliver flux estimates under altered climatic conditions to PA	USGS (Frank D'Agnese) USGS (Pat Tucci)

The working schedule for Analysis Plan 6: Geologic Structure and Processes Affecting Flow Channelization,

Table 1-11. Task 6 Schedule

Date	Activity	Responsible Party
8/31/97	- Deliver conclusions using the sub-site-scale flow model	LBNL (Andrew Cohen) LBNL (Ardyth Simmons) LBNL (Curtis Oldenburg)

1.14 INTERFACES TO OTHER COMPONENTS OF TSPA-VA AND OTHER AREAS OF THE PROGRAM

Interfaces between SZ flow and transport and other components of the TSPA-VA analyses are relatively straightforward and generally without the complexities of feedback inherent among some other system components (e.g., UZ flow and UZ thermohydrology). UZ transport calculations provide the input boundary conditions for SZ transport simulations in the form of a time-dependent mass flux term. One potentially important feedback to the UZ transport simulations is the water table elevation, which forms the lower boundary of the UZ, as influenced by climate change. At the "downstream" end of the SZ flow and transport system, the concentration history of radionuclides serves as the link to the biosphere model. Assumptions in the biosphere model may also influence flow and transport in the SZ through the types and locations of wells specified.

In addition to these links with other parts of TSPA-VA, there are direct interfaces between the SZ flow and transport calculations and other elements of the Yucca Mountain Project. These interfaces include the obvious feeds from process-level models and information from site-characterization activities. These interfaces are summarized in Table 1-12.

Table 1-12. Interfaces with Other Areas of the Program

WBS Element	Input to SZ Flow and Transport	Output from SZ Flow and Transport
WBS 1.2.5.4.4: UZ Transport	- transient radionuclide mass flux at the water table	- Water table elevation under alternative climate scenarios
WBS 1.2.5.4.1: Biosphere	- well withdrawal scenarios	- Radionuclide concentration history
WBS 1.2.3.3.1: Site-scale SZ Flow Model	- groundwater fluxes, groundwater flow field, geologic framework	
WBS 1.2.3.3.1: Regional-scale SZ Flow Model	- groundwater fluxes (via site-scale model), groundwater fluxes, water table elevation, and discharge locations under climatic changes,	
WBS 1.2.3.3.1: Well Hydraulic Testing	- conclusions regarding variability and magnitude of hydraulic properties	
WBS 1.2.3.4.1: SZ Transport Model	- process-level model of transport	
WBS 1.2.3.3.1: Well Tracer Testing	- conclusions regarding field-scale effective transport properties	

Table 1-12. Interfaces with Other Areas of the Program

WBS Element	Input to SZ Flow and Transport	Output from SZ Flow and Transport
WBS 1.2.3.4.1: Laboratory Sorption and Diffusion Studies	- sorption and diffusion parameters for specific radionuclides	
WBS 1.2.3.4.1: Studies of Redox Potential in the SZ	- conclusions regarding solubility limits for radionuclides	
WBS 1.2.3.2.1: Mineralogic Framework Model	- spatial distribution of potentially sorptive minerals	

2. WORKSHOP PREPARATION

2.1 INTRODUCTION

Preparation for the SZ Flow and Transport Abstraction/Testing workshop included planning of workshop activities in coordination with other participating organizations, issuance of an invitation memo which included background information on the purpose of the workshop, collection of proposals on relevant issues from workshop participants, and instructions to participants on workshop preparation. This preparation effort focused on establishing a workshop structure that would be conducive to reaching the goals of the workshop described in Section 1.3.

2.2 WORKSHOP PLANNING

Planning for the SZ workshop was accomplished by the abstraction core team (ACT) for this task. The ACT consisted of Bill Arnold (SNL - team leader), Jack Gauthier (SNL, Spectra Research - TSPA representative), Pat Tucci (USGS - flow modeling representative), Bruce Robinson (LANL - transport modeling representative), and Susan Altman (SNL - workshop facilitator). Consultation with Ardyth Simmons (LBNL) also provided coordination with other abstraction/testing workshops. A series of meetings and teleconferences, along with e-mail exchanges of draft documents were used in the planning process. Formal workshop planning meetings were held on 11/21/96 and 2/26/97.

Important steps in the workshop planning process included defining the goals of the workshop, listing the important issues to be considered at the workshop, choosing the participants, establishing the structure and agenda for the workshop, soliciting comments from participants on the issues, and making assignments for presentations on specific issues for the workshop. The planning process was aided greatly by experience gained from previous abstraction/testing workshops. The SZ workshop shared similar goals and followed the general structure of the UZ Thermohydrology and UZ Transport workshops.

The intent of listing important issues and choosing participants was to match issues with individual participants in a matrix to insure that all issues were represented by knowledgeable participants and that all participants could contribute to at least one important issue. An additional consideration in choice of participants was that participants should more-or-less equally represent the three areas of TSPA modeling, process-level modeling, and site characterization. The initial list of issues used in the participant screening process is shown in the workshop invitation memo (see Appendix A and Figure 1-1). The list of participants remained somewhat in flux until shortly before the workshop due to uncertainty in the ability of some people to attend.

Once a list of potential participants was established, an invitation memo (see Appendix A) was drafted outlining the objectives of the workshop and soliciting comments on a set of strawman proposals about the listed issues. The responses from workshop participants were used to refine and add to the list of important issues to be considered during the SZ workshop. In addition, these responses aided in the development of the finalized agenda and were used to assign presentations for the workshop.

2.3 WORKSHOP INVITATION MEMO

The SZ Flow and Transport Abstraction/Testing Workshop invitation memo was intended to invite potential participants to the workshop, inform them of the goals of the workshop, educate participants concerning TSPA analyses, provide a set of strawman proposals addressing key issues, and provide logistical information on the workshop itself. The original invitation memo is reproduced in its entirety in Appendix A.

An effort was made in the invitation memo to communicate to potential participants several important philosophical points concerning the SZ workshop. The first point was that the workshop was intended as an integration activity among data collectors, process-level modelers, and TSPA analysts and as such was an opportunity for researchers to insure that their work is adequately represented in TSPA calculations. A second key point was that the focus of the workshop was on the variability and uncertainty in our knowledge of the SZ system as reflected in the list of issues to be discussed. The focus was to be on how to incorporate this uncertainty into TSPA calculations, *not* on attempting to resolve these issues. This focus was adopted to avoid lengthy and often fruitless discussions of issues that may not be specifically resolvable with presently available information. The third point was that the workshop was expected to be explicitly productive, producing a set of proposals for abstraction/testing analysis plans that would be directly useful in TSPA-VA analyses.

The workshop invitation memo in Appendix A also contained extensive background information on the representation of process-level modeling in TSPA calculations. This information was provided in attachments to the memo on an introduction to TSPA and a discussion of the meaning of abstraction. The ACT felt that it was important to communicate to participants the rather extreme degree of simplification that may be required in the abstraction process, especially in the absence of additional testing and sensitivity analysis of process-level models.

The memo also contained a set of strawman proposals on the issues identified by the ACT and assignments to workshop participants to make additional comments on specific issues. The strawman proposals were intended to serve as a basis for further discussion and as a target for criticism. Participants were asked to provide written comments/counter-proposals on specific issues (see Attachment I in Appendix A) and on any other issues on which they had information or opinions.

2.4 PARTICIPANT PROPOSALS AND ISSUE WRITE-UPS

A second memo sent to workshop participants included updated logistical information, instructions for preparing uniformly formatted presentation viewgraphs, a list of assigned presentation, a revised agenda for the workshop, and participant write-ups on issues. This final memo to workshop participants is reproduced in Appendix B of this report.

The intent of this follow-up memo to participants in the workshop was twofold, to distribute the written comments made by the participants and to provide logistical information. Participants were encouraged to familiarize themselves with the implications of the comments/proposals of other participants in preparation for the workshop. This memo also communicated a format for participant presentations, in an attempt to facilitate the functioning and documentation of the workshop.

3. WORKSHOP PROCEEDINGS AND RESULTS

3.1 INTRODUCTION

This chapter describes in greater detail the organization of the workshop, processes of conducting the workshop, and the results of the SZ Flow and Transport Abstraction/Testing Workshop. A relatively structured approach was taken in the implementation of the workshop. This structure was designed by the ACT to keep the workshop focused, while still allowing participants to influence the direction of the proceedings and maintaining flexibility. As discovered in previous abstraction/testing workshops, the use of a knowledgeable, but somewhat neutral facilitator significantly enhanced the productivity of the workshop.

3.1.1 Workshop Format

The format of the workshop included three major activities. The first was the development of a list of significant issues, which was accomplished through oral presentations and discussion. The second was the prioritization of issues, accomplished in four working groups and through open discussion among all participants. The third activity involved the reorganization of participants into another set of working groups for the development of abstraction/testing analysis plans.

Each category of issues was introduced by a presentation from a TSPA representative outlining the ways in which these issues had or had not been addressed in previous TSPA analyses. Oral presentations were made by participants regarding each issue. Some of these presentations were assigned to specific participants and others were volunteered; many were advocatory in nature, presented to persuade the participants concerning the significance of that issue.

Prioritization of issues within each category was undertaken at the end of the presentations within that category. Issues were prioritized in individual working groups by consensus or voting using the methodology described in Section 3.3. The compositions of the working groups are given in Table 3-1. An attempt was made to balance each working group with members representing TSPA, site characterization, and process-level modeling. Scores were tallied for each of the issues within a category and one member of each working group explained the group's thoughts on the prioritization of each issue to the entire workshop.

The final activity consisted of the global prioritization of all issues, presentations on existing workscopes and analysis plans from other workshops, regrouping of participants, and the development of analysis plans. Global prioritization was accomplished through a voting procedure in which participants were each allotted three votes from each of the five performance criteria (see Section 3.3) and were allowed to cast those votes for any of the issues ranked among the highest four or five issues from each category. The resulting pattern of votes was helpful in defining how groups would be organized for the purpose of developing analysis plans. Participants were allowed to nominate themselves to the new groups for analysis plan development. Preliminary analysis plan development and brainstorming was followed by brief presentations to the entire group concerning the nature of the proposed analysis plan and potential products to TSPA. The analysis plans were written to address the key issues and provide abstraction methods for TSPA-VA (see Chapter 4).

Table 3-1. Working Groups for Issue Prioritization

Table 1	Table 2	Table 3	Table 4
Jack Gauthier David Vaniman Frank D'Agnese George Zyvoloski Sean McKenna Art Geldon	Bill Arnold David Sevougian Ardyth Simmons Chunhong Li John Czarnecki Jake Turin Chris Potter	Bruce Robinson Jerry McNeish Ed Kwicklis George Barr Vinod Vallikat Arend Meijer	Pat Tucci Mike Wilson Jim Duguid M. J. Umari Ines Triay Andrew Cohen

3.1.2 Workshop Agenda

The agenda of the workshop, as provided to the workshop participants in the workshop notebook, is reproduced Appendix C of this report. Note that the actual agenda of the workshop deviated from this agenda due to illness of one of the speakers on the first day of the workshop. The first major category of issues was postponed until the morning of the second day and presentation and prioritization of categories 2, 3, and 4 was accomplished on the first day.

3.1.3 List of Participant Presentations

The presentations and their subjects for each of the issue categories are presented in Figure 3-1. Viewgraphs from these and introductory presentations are reproduced in Appendix E.

3.1.4 List of Attendees

The list of attendees at the SZ Flow and Transport Abstraction/Testing Workshop is presented in Appendix D. Please note that attendees included not only participants, but observers from a variety of organizations, including the Department of Energy (DOE), Nuclear Regulatory Commission (NRC), members of the Nuclear Waste Technology Review Board (NWTRB), and the PA Peer Review Team.

3.2 ORGANIZATION OF PRESENTATIONS

Introductory presentations included an overview of the TSPA-VA task, an introduction to the SZ Flow and Transport Workshop, a general introduction to TSPA, and a review of the important SZ flow and transport issues. Viewgraphs from these presentations are included at the beginning of Appendix E. The TSPA-VA overview presentation discussed the goals, constraints, and schedule of the TSPA-VA analysis and the role of the abstraction/testing tasks within the analysis. The workshop introduction presentation laid out the specific goals of the SZ workshop and summarized the agenda. The introduction-to-TSPA presentation described the various components of the system, examples of SZ modeling from previous TSPA calculations, and explained TSPA needs with regard to SZ modeling. The presentation reviewing the important SZ issues summarized the straw-

Major Issue Category 1: Conceptual Models of SZ Flow

John Czarnecki	1.1	Alternative conceptual models
Bill Dudley	1.1	Alternative conceptual models
George Barr	1.2	Hydraulic properties of faults
Andrew Cohen	1.3	Vertical flow
Frank D'Agnese	1.4	Distribution of recharge
Pat Tucci	1.4	Distribution of recharge
John Czarnecki	1.5	Regional discharge
Frank D'Agnese	1.5	Regional discharge
George Zyvoloski	1.6	Grid sensitivity
Ed Kwicklis	1.7	Implications of isotopic and hydrochemical data

Major Issue Category 2: Conceptual Models of SZ Geology

Chris Potter	2.1	Flow channelization
Bill Arnold	2.1	Flow channelization
Dave Vaniman	2.1	Flow channelization
Sean McKenna	2.2	Spatial distribution of hydraulic conductivity
Art Geldon	2.2	Spatial distribution of hydraulic conductivity
Dave Vaniman	2.3	Geologic and mineralogic framework

Major Issue Category 3: Transport Processes and Parameters

Bruce Robinson	3.1	Dispersivity
Chunhong Li	3.1	Dispersivity
Mike Wilson	3.1	Dispersivity
Jake Turin	3.2	Matrix diffusion (effective porosity)
Bruce Robinson	3.2	Matrix diffusion (effective porosity)
Ines Triay	3.3	Sorption
Jake Turin	3.3	Sorption
Jake Turin	3.4	Colloid transport
Arend Meijer	3.5	Radionuclide solubility

Major Issue Category 4: Coupling to Other Components of TSPA

Frank D'Agnese	4.1	Climate change
George Barr	4.2	Thermal and chemical plume
Bill Arnold	4.2	Thermal and chemical plume
Bill Arnold	4.3	Well withdrawal scenarios
Jerry McNeish	4.3	Well withdrawal scenarios
Bruce Robinson	4.4	Coupling with UZ transport

Figure 3-1. List of presentations for the SZ workshop.

man proposals and participant comments on each of the issues and clarified the meaning of each issue statement.

Within each of the four issue categories, an introductory overview of the issues from the TSPA perspective was given, followed by a series of presentations by workshop participants. Viewgraphs from these presentations are reproduced in Appendix E. There was a break in these presentations between each of the four main categories, during which individual issues were ranked within a category using the prioritization methodology explained in the following section of the report.

3.3 ISSUE PRIORITIZATION METHODOLOGY

The issue prioritization process in the workshop was guided by a set of five criteria that were designated as performance measures by the ACT. These criteria were chosen because they were judged to be significant to the long-term performance of the potential repository at Yucca Mountain. The importance of each issue within a category of issues was evaluated by the four participant working groups relative to these criteria. These criteria, as formulated in the context of the guidance question, were:

Does the process/issue affect the:

A) peak radionuclide concentration at 5 km from the repository?
B) peak radionuclide concentration at 30 km from the repository?
C) time to first arrival (1% of peak)?
D) spatial distribution of the plume (both horizontal and vertical)?
E) spatial distribution of groundwater flux (e.g., dilution at the UZ-SZ interface)?

A quantitative evaluation scale was established that consisted of a scoring method in which issues/processes judged to have a significant effect received a score of 5, those with a medium effect received a score of 3, and those with a negligible effect were give a score of 1. Each of the five criteria were given equal weight in calculating a total score for a particular issue. It should be noted that each issue was ranked according to the participants' opinions regarding the importance of that issue, regardless of the ability of existing site data or models to evaluate that issue.

3.4 ISSUE PRIORITIZATION RESULTS

The results of ranking SZ flow and transport issues have been summarized in Section 1.5 of this report. More complete quantitative documentation of the issue prioritization results are presented in this section. Numerical results of the issue prioritization procedure are presented for the four categories of issues in Tables 3-2 to 3-5. Note that some issues were added or redefined during the course of the workshop and some have been renumbered relative to the original numbering of the issues in the list of presentations shown in Figure 3-1. Also note that the issue of the hydraulic properties of faults seemed to straddle the categories of conceptual models of SZ flow and conceptual models of SZ geology and was consolidated under a single issue (issue 2.4) under the category of conceptual models of SZ geology. Although the issue of hydraulic properties of faults still appears in Table 3-2, it is not ranked relative to the other issues. It is interesting to note that when this issue was scored under two different categories and on two different days of the workshop, the total scores and standard deviations were approximately the same (compare Table 3-2 to Table 3-3).

The results of the prioritization issues are fairly straightforward for Categories 2, 3, and 4, but perhaps somewhat more difficult to interpret for Category 1. The two or three higher ranked issues in Category 2 are within the overlapping ranges of the indicated standard deviations. All of the higher ranked issues within this category are concerned with features that potentially act as conduits or barriers to groundwater flow. The issues that are clearly ranked the highest within Categories 3 and 4 are dispersivity and climate change, respectively. Many of the issues in Category 1 have relatively high standard deviations with respect to the variability in scoring among the four working groups. For the two highest ranked issues, two of the groups scored the issues consistently lower than the other two. It is not apparent whether this variability was a function of differing interpretations of the meanings of the issues or if it reflected basic differences in opinion regarding the significance of these issues with regard to repository performance.

Table 3-2. Ranked Issues, Conceptual Models of SZ Flow

Issue #	Issue	Group 1	Group 2	Group 3	Group 4	Total	Std. Dev.
1.6	Regional discharge	25	11	21	9	66	7.72
1.5	Regional recharge	21	7	21	15	64	6.63
1.4	Vertical flow	21	11	15	15	62	4.12
1.1	Alternative conceptual models (large hydraulic gradient)	19	17	13	11	60	3.65
1.7	Grid sensitivity	19	21	5	13	58	7.19
1.8	Implications of isotopic and hydrochemical data	15	11	11	13	50	1.91
1.2	Alternative conceptual models (flow paths and discharge points)	15	9	11	9	44	2.83
1.9	Implications of geothermal flux	15	5	11	13	44	4.32
1.3	Hydraulic properties of faults	25	21	19	23	88	2.58

Table 3-3. Ranked Issues, Conceptual Models of SZ Geology

Issue #	Issue	Group 1	Group 2	Group 3	Group 4	Total	Std. Dev.
2.1	Channelization in large-scale vertical features	23	21	21	21	86	1.00
2.4	Hydrologic and mineralogic properties of faults	25	21	19	19	84	2.83
2.2	Channelization in stratigraphic features	25	17	19	19	80	3.46
2.8	Distribution of zeolites	21	17	19	19	76	1.63
2.6	Fracture network connectivity	17	19	15	15	66	1.91
2.3	Scale effects of geologic properties	21	11	13	13	58	4.43
2.5	Spatial distribution of hydraulic conductivity	15	17	13	13	58	1.91
2.7	Lumping of stratigraphy	15	17	9	9	50	4.12
2.9	Relationship of welding to degree of fracturing	13	5	5	5	28	4.00

Table 3-4. Ranked Issues, Transport Processes and Parameters

Issue #	Issue	Group 1	Group 2	Group 3	Group 4	Total	Std. Dev.
3.1	Dispersivity	25	21	19	17	82	3.42
3.2	Matrix diffusion (effective porosity)	25	17	11	19	72	5.77
3.3	Matrix sorption	17	19	11	17	64	3.46
3.4	Fracture sorption	19	17	15	11	62	3.42
3.5	Colloid transport	15	11	17	11	54	3.00
3.7	Redox potential	13	13	17	5	48	5.03
3.6	Radionuclide solubility	15	5	9	5	34	4.73

Table 3-5. Ranked Issues, Coupling to Other Components of TSPA

Issue #	Issue	Group 1	Group 2	Group 3	Group 4	Total	Std. Dev.
4.1	Climate change	25	25	23	17	90	3.79
4.4	Coupling with UZ flow and transport	21	15	15	7	58	5.74
4.2	Thermal and chemical plume	15	11	13	11	50	1.91
4.3	Well withdrawal scenarios	11	13	13	9	46	1.91
4.5	Natural discharge	13	11	7	7	38	3.00
4.6	Stress effects on hydraulic properties	5	9	5	5	24	2.00

3.5 PROPOSAL CATEGORY DEVELOPMENT

Following the global prioritization of issues (described in Section 3.1.1), four general categories were established as a framework for the development of analysis plans. These categories were 1) transport parameters, 2) coupling to UZ transport, 3) channelization, and 4) groundwater fluxes. Participants were allowed to choose the group in which they wanted to work. The resulting distribution of participants was approximately even with respect to numbers and expertise.

Once the participants were divided into the four groups, development of the abstraction/testing plans was initiated. Participants were given an outline (as reflected in the organization of the analysis plans presented in Chapter 4) to serve as a guide to producing a written analysis plan. At the end of the second day of the workshop, each group reported on the major issues and approaches covered by their analysis plan(s). First the TCT, then the group at large, provided feedback to each working group on the applicability of the proposed product to TSPA analyses. The groups were allowed more time to work on the analysis plans during the morning of the third day, and then a second "call-out" was made to receive feedback from the entire group and the TCT. The draft abstraction/testing analysis plans were finalized in discussions and communication between participants in the time following the workshop. The final analysis plans are presented in Chapter 4.

3.6 COMMENTS FROM OBSERVERS

Following the development of the analysis plans, comments were taken from the workshop observers. The majority of these comments came from NWTRB members, the NRC and their associates, and from DOE staff. From a technical and strategic perspective, several observers advocated the use of simple models whenever possible. Although they recognized the complexities of some of the issues involved, they stressed that models should be clear and understandable to be defensible.

The most significant comments from observers at the SZ Flow and Transport Abstraction/Testing Workshop are paraphrased below:

Richard Parizek (NWTRB member):

- It is important to make use of available hydrochemical and isotopic data.
- Explicit comparisons among physical models (at different scales and in both the UZ and SZ) should be made.
- Validity of SZ flow and transport modeling rests on the regional-scale flow model, which is tied to estimates of groundwater flux through the system.
- Dilution in the SZ is key to site performance if calculations go beyond 10,000 years.
- Large groundwater withdrawals from extraction wells in the future are possible/likely.
- There is an inconsistency between the pneumatic data in the UZ and modeling faults as low hydraulic conductivity features in the SZ.
- There is a need to identify potential fast paths in the SZ.
- Mineralogic data should be examined for implications to SZ flow.

Victor Palciauskas (NWTRB member):

- It is important to determine if effective properties are appropriate for use in SZ modeling.
- Abstractions are planned from complex models with little supporting data and ambiguity in the underlying conceptual models.
- The use of simple models that incorporate more certain aspects of the system is preferable.

Neil Coleman (NRC):

- The longer travel distances now being considered (30 km) have the advantage that continuum behavior is a more defensible assumption.
- The sorptive characteristics of alluvium (e.g., sorption of Np on iron oxides) should be considered in transport calculations to 30 km.

Robert Baca (Southwest Research Institute):

- The list of issues developed at the SZ workshop is consistent with those of researchers at the Center for Nuclear Waste Regulatory Analyses, but their prioritization would probably be different.
- He expressed concern that time constraints will not allow planned analyses to be completed.
- It is wise to keep the analyses as simple as possible.
- It is important to make comparisons with previous TSPA analyses.
- Clarity in TSPA analyses and documentation is important.

Eric Smistad (DOE):

- Flexibility in current workscopes is necessary to accomplish the analysis plans.
- TSPA-VA is not the ultimate goal; planning for the license application should be integral to current TSPA work.

Abe Van Luik (DOE):

- There is a significant amount of additional scientific work before the project can make a licensing case.
- The SZ is taking on significantly greater importance in the context of current regulatory trends.

4. ABSTRACTION/TESTING PLANS

4.1 SENSITIVITY STUDY ON UNCERTAINTIES IN SITE-SCALE SATURATED-ZONE TRANSPORT PARAMETERS AND MODELS

4.1.1 Participants:

Bruce Robinson, Inez Triay, George Zyvoloski, Jake Turin

4.1.2 Objectives:

(a) To determine if an equivalent continuum model can adequately represent matrix diffusion and fracture/matrix sorption at the site-scale for both non-sorbing and sorbing radionuclides, and if so, what are the appropriate parameter values for the single-porosity model;
(b) to assess the sensitivity of radionuclide releases to the uncertainty in longitudinal and transverse dispersivity at both 5 km and 30 km;
(c) to assess the sensitivity of radionuclide releases to the uncertainty in fracture sorption at both 5 km and 30 km;
(d) to assess the sensitivity of radionuclide releases to the uncertainty in sorption and solubility as a function of redox potential in the saturated zone, and
(e) to assess the role of the alluvium strata in the saturated zone in the retardation of radionuclides.

4.1.3 Hypotheses:

(a) The single porosity model can adequately represent transport in the saturated zone.
(b) Reducing conditions in the SZ can significantly increase radionuclide sorption and decrease solubility, therefore significantly changing the time and amount of radionuclide releases to the accessible environment.

4.1.4 Products to TSPA-VA:

(a) Provide appropriate transport parameters to be used in TSPA.
(b) Study assessing whether the equivalent continuum transport model can adequately describe radionuclide transport through the SZ.

4.1.5 Issues to be Covered:

This proposal will address issues:
3.1 - Dispersivity
3.2 - Matrix diffusion
3.3 - Matrix sorption
3.4 - Fracture sorption
3.7 - Redox potential

4.1.6 Abstraction/Testing Plan

Approach

We will perform a set of calculations to determine release of radionuclides to the accessible environment using a dual porosity model. The uncertainty in the following transport parameters will be studied: dispersivity, effective porosity for matrix diffusion, and fracture/matrix sorption as a function of redox potential. The combined effects of these transport parameters on radionuclide transport will be investigated. We will assume that the results of the dual porosity model are correct and we will determine the transport parameters that need to be invoked in order to get the same results using a single-porosity model. The potentially reactive radionuclides to be studied are Np and Tc. Large-scale hydrologic features such as faults will not be varied in this study.

Metrics:

(1) Integrated breakthrough curves over time (from 0 to 100,000 years)-- The difference must be over a factor of 5 to be significant.
(2) Peak concentrations during the 0 to 100,000 years time frame--The difference must be over a factor of 5 to be significant. (spatially integrated peak concentrations will be compared if more than one-D).
(3) Time of first arrival (1% or 5% of peak). The difference must be a large fraction of 10,000 yrs (e.g., 1,000 yr) to be significant.

For dispersivity sensitivity analysis metrics no. 2 and 3 are the most important.
All three metrics are important for:
(a) sorption onto the fractures vs. no sorption onto the fractures.
(b) sorption under oxidizing conditions vs. sorption under reducing conditions.
(c) sorption onto minerals in the alluvium vs. no sorption onto the alluvium minerals.

Work Covered in Existing Workscopes:

LANL funded to study sorption under oxidizing conditions.
LANL funded to provide a site scale flow and transport model.

Sources of Information:

Sorption values under reducing conditions and dispersivity values will be obtained from the literature.
Sorption under oxidizing conditions will be provided by LANL experimental program.
Ambient redox conditions can be obtained from existing data and ongoing workscope in water chemistry activities

Computer Codes to be Utilized:

FEHM for sensitivity analysis calculation

Roles and Responsibilities:

Zyvoloski (LANL): Provide range for dispersivity values.
Turin (LANL): Provide range of dispersivity values from C-wells data.
Triay (LANL): Provide sorption data using experimental and/or literature values.
Robinson, Zyvoloski (LANL) and Li (Intera): Perform sensitivity analysis study.

Schedule:
Data and Parameters (described above) delivered to Bruce Robinson, George Zyvoloski (LANL) and Li by 5/31/97.
Sensitivity Analysis completed by 8/31/97.

4.1.7 Model Assumptions and Uncertainties

(a) the dual porosity model is assumed to adequately represent radionuclide transport through the SZ;
(b) colloid-facilitated radionuclide transport through the saturated zone has not being considered in this study. If time permits, the effect of colloids in the saturated zone will be taken into account.

4.1.8 Potential Follow-up Work

FY 98 workscope will take into account the results of this analysis

4.1.9 Inputs/Feedbacks to Other WBS Elements

Data to be input from 1.2.3 (Triay) to 1.2.3 (Robinson and Zyvoloski)
Sensitivity Analysis Results to be input from 1.2.3 (Robinson and Zyvoloski) to 1.2.5 (Sevougian)

4.1.10 Potential Problems:

(a) The scarcity of sorption data under reducing conditions.
(b) The uncertainty in the site scale flow model.
(c) Resources are limited and some parts of this effort are outside the currently planned workscope of the investigators listed.

4.2 COUPLING OF UZ AND SZ TRANSPORT MODELS

4.2.1 Participants:

Bruce Robinson

4.2.2 Objectives:

(a) to determine the nature of the coupling of the UZ and SZ radionuclide transport models necessary to capture the details of the UZ transport plume as it enters the saturated zone;
(b) to demonstrate the applicability of a convolution approach to coupling the two models;
(c) to provide PA with a numerical tool that could be used to couple the two models.

4.2.3 Hypotheses:

(a) The details of spatial distribution of radionuclide flux at the water table are relatively unimportant to performance predictions (peak concentration at the accessible environment).
(b) The convolution approach is a streamlined, useful method for coupling the two models to compute integrated transport results (time variation of concentration at the accessible environment).

4.2.4 Products to TSPA-VA:

(a) a sensitivity analysis showing the impact of spatial variability of radionuclide flux at the water table on predictions of peak concentration of radionuclides at the accessible environment. A concrete conclusion will be reached as to whether spatial variability of radionuclide flux matters.
(b) a computer code to perform numerical convolution of the numerical results of the UZ and SZ models that could be used in TSPA-VA Monte Carlo calculations.

4.2.5 Issues to be Covered:

This proposal will address issue 4.4 (Coupling with UZ flow and transport). This was selected because the mechanics of coupling two distinct transport models is necessary in a TSPA exercise. Doing the coupling incorrectly could result in certain processes being left out, having either a negative or positive influence on predicted performance.

4.2.6 Abstraction/Testing Plan

Approach
In this study we will couple a detailed transport simulation or an abstracted transport simulation of UZ radionuclide transport to the site scale SZ flow and transport model. The input to the SZ model is the computed or hypothesized breakthrough at the water table of a conservative radionuclide (Tc). The spatial and temporal variability of the radionuclide mass flux will be mapped directly onto the top of the SZ flow and transport model, and concentration versus time at various locations (5 km and 30 km downgradient) will be computed. This computation will be compared to the results assuming that the entire mass flux of radionuclide is input as a single mass flux directly beneath the repository footprint. If the differences are slight (see Metrics), then the simpler, spatially

smeared input to the SZ model will be shown to be an appropriate abstraction for TSPA.

A corollary to this study is that the method for coupling the models must be simple and versatile. If the same code and the same people construct both models, problems should be minimal. However, what if a detailed UZ transport model is to be coupled to an analytical solution for SZ transport? Alternatively, what if a different number of SZ runs are required to capture the range of uncertainty in the model than for the UZ, or what if two conceptual models of SZ transport (one continuum, and one large-scale feature-based) are carried through the TSPA? What if models of different dimensionality are used? These are examples of the need for a flexible technique for coupling the models that doesn't require that the models be calculated in sequence (UZ, followed by SZ). The convolution integral is the proposed method for performing this coupling. For details on the method, see LANL Milestone SP342HM4. In essence, the convolution approach uses results from the following two sources: 1) a detailed, time-dependent mass flux source term from a UZ model; 2) a generic SZ transport simulation in which a constant source mass flux is assumed. Assuming linear processes, the convolution integral is a straightforward numerical integration procedure to determine the time-varying SZ concentration at the downstream location.

For the convolution approach, another product for TSPA will be a demonstration of the validity of the convolution procedure (validity referring to a proof of correctness of the numerical procedure), and a computer code that can be used for coupling UZ and SZ transport models in TSPA-VA simulations.

Metrics:

(1) For determining if spatial variability in UZ mass flux matters, a criterion of peak concentration and location is appropriate. If the peak concentration differs by no more than a factor of two, the simpler smeared source term is a reasonable approximation. Also, the location of the peak concentration should differ by no more than 1/10th the transport distance (500 m for the 5 km distance and 2 km for the 20 km distance) for the two cases.

(2) For the test of the convolution integral, the peak concentration should differ by no more than 10% for convolution versus direct computation of the concentration (i.e. the numerical method should be more or less exact if linear processes are assumed).

Work Covered in Existing Workscopes:

LANL flow and transport models are being developed for both the UZ and SZ (collaboration on the UZ is with LBNL and with USGS for SZ). LANL Retardation Sensitivity Analysis activities are already computing integrated transport results through the UZ and SZ transport barriers.

Sources of Information:

UZ model: LANL site scale model

Computer Codes to be Utilized:

FEHM

sz_convolute (convolution code)

Roles and Responsibilities:

Determination of base case model geometry and parameter values: UZ - LANL and LBNL: SZ - USGS and LANL.

Calculation of UZ breakthrough curves: LANL (Bruce Robinson and Kay Birdsell)

Calculation of SZ breakthrough curves and convolution: LANL (Kay Birdsell and Robinson).

Reporting of results: LANL

Schedule:
Determination of base case model: UZ - April 30, 1997
Determination of base case model: SZ - May 31, 1997
Calculation of UZ/SZ transport, comparison of convolution method to more detailed model: July 31, 1997
Final report of results: August 31, 1997

4.2.7 Model Assumptions and Uncertainties

(a) Conclusions regarding the use of a smeared solute source and the acceptability of the convolution method will be based on simulations using a conservative solute. It is assumed that these conclusions also apply for sorbing radionuclides.

4.2.8 Potential Follow-up Work

(a) Potential follow-up work includes repeating calculations for sorbing solutes.

4.2.9 Inputs/Feedbacks to Other WBS Elements

(a) The USGS site-scale SZ flow model will be used as the basis for flow and transport simulations.
(b) The time history and spatial variability of the radionuclide source term will be taken from UZ transport simulations
(c) Products will be supplied to TSPA.

4.2.10 Potential Problems:

(a) If the response of the SZ transport model is not approximately linear, the convolution method will not produce acceptable results.

4.3 THE EFFECTS OF LARGE-SCALE CHANNELIZATION ON EFFECTIVE TRANSPORT PARAMETERS

4.3.1 Participants:

Bill Arnold, Sean McKenna, Chris Potter, Art Geldon, Dave Vanniman, Jake Turin, Bruce Robinson, John Czarnecki, Mike Wilson

4.3.2 Objective:

To test whether or not the inclusion of potential large-scale hydraulic features has a significant effect on transport behavior in the site-scale model.

4.3.3 Hypothesis:

Faults and fracture zones control the channelization of radionuclide transport out to the 5km boundary but do not have a significant effect on transport results at the 30km boundary.

4.3.4 Products to TSPA-VA:

Recommendations for effective parameters for TSPA-VA (dispersivity, effective porosity). Conclusion as to whether or not the inclusion of faults and fracture zones is more or less conservative than current baseline site-scale model.

4.3.5 Issues to be Covered:

1.4 Vertical Flow
2.1 Large-scale vertical channelization features
2.2 Horizontal flow channelization
2.4 Hydrologic and mineralogic properties of faults
2.6 Fracture network connectivity
3.1 Dispersivity
4.4 Coupling with UZ flow and transport
3.2 Matrix Diffusion

4.3.6 Abstraction/Testing Plan

Approach

(a) Develop bounding conceptual models of geometry of large-scale channelization features:
- Spatial distribution
- Orientation
- Size (vertical and horizontal extent)
- Channels/Barriers
- Work with new and upcoming maps of faults and fractures being reproduced by the USGS

(b) Develop geostatistical descriptions of channelization features and use geostatistical simulation to produce multiple realizations of the SZ system.

(c) Incorporate features into site-scale flow model

We plan to include these features as affecting transport only in the model. The "calibrated" flow field results of the base-case site-scale flow model will be used without modification. The initial plan is to just adjust the effective porosity in the areas of the features to have faster or slower flow in those areas.

(d) Run site-scale model with features.

(e) Examine transport results of different bounding conceptual models of channeliztion with base case site-scale model (no-channelization).

(f) Summarize results and deliver to PA

Metrics:

(1) The effects of channelization will be considered significant if they affect simulated peak concentration by greater than a factor of two.

(2) The effects of channelization will be considered significant if they affect simulated dispersion in the concentration breakthrough curve by greater than a factor of 50%.

Work Covered in Existing Workscopes:

(a) Site-scale flow model already underway at USGS

(b) Site-scale transport model already underway at LANL

(c) 1:6000 scale mapping by USGS, finished product (Day et al, in press)

(d) 1:24000 scale mapping underway at USGS

(e) Ongoing analysis of C-well tracer tests (deliverable 7/31/97)

(f) Geologic framework model (Clayton and Zelinski) is ongoing

(g) 2-D fault modeling by Andrew Cohen at LBL

Sources of Information:

(a) USGS site-scale flow model

(b) Structural interpretations of fault and fracture zones

(c) Site-scale geologic framework model

Computer Codes to be Utilized:

FEHM

STAFF3D

GSLIB

Roles and Responsibilities:

Bill Arnold: primary responsible party

Sean McKenna: in charge of getting conceptual model put together

Contributors: Chris Potter, Art Geldon, Dave Vaniman, and Jake Turin

Getting features into the transport model (Sean, Bill, Bruce Robinson and John Czarnecki)

Mineralogic and sorption studies of fault-related C-well samples (Dave Vaniman and Jake Turin)

Running transport model (Bill, Sean, Bruce)

Summarizing results for PA (Bill, Sean, Mike Wilson)

Schedule:
Conceptual model complete - 7/31/97
Features into flow/transport model - 8/31/97
Running model - 9/15/97
Examine results and Summarize - 9/15/97)
Documentation of results - 12/97

4.3.7 Model Assumptions and Uncertainties

A large assumption is that the features we are adding to the model do not significantly affect flow, only transport.

4.3.8 Potential Follow-up Work

Investigate role of the large-scale features that we add to the model on fluid flow (i.e., do these features alter the calibration of the baseline site-scale model?)

4.3.9 Inputs/Feedbacks to Other WBS Elements

Recommendations to site characterization:

better understanding of the transmissive properties of faults.

better understanding of the 3-D distribution of structural features that may be significant to transport channelization.

4.3.10 Potential Problems:

(a) Sufficient grid resolution in the site-scale flow model to capture the influence of these channelization features.
(b) Acceptance of the conceptual model of the geometry of channelization features. Is it supportable with available site data?
(c) Because channelization features only affect transport in the simulations, there may be a significant inconsistency between the modeled flow and transport.

(c) Incorporate features into site-scale flow model
We plan to include these features as affecting transport only in the model. The "calibrated" flow field results of the base-case site-scale flow model will be used without modification. The initial plan is to just adjust the effective porosity in the areas of the features to have faster or slower flow in those areas.
(d) Run site-scale model with features.
(e) Examine transport results of different bounding conceptual models of channeliztion with base case site-scale model (no-channelization).
(f) Summarize results and deliver to PA

Metrics:
(1) The effects of channelization will be considered significant if they affect simulated peak concentration by greater than a factor of two.
(2) The effects of channelization will be considered significant if they affect simulated dispersion in the concentration breakthrough curve by greater than a factor of 50%.

Work Covered in Existing Workscopes:
(a) Site-scale flow model already underway at USGS
(b) Site-scale transport model already underway at LANL
(c) 1:6000 scale mapping by USGS, finished product (Day et al, in press)
(d) 1:24000 scale mapping underway at USGS
(e) Ongoing analysis of C-well tracer tests (deliverable 7/31/97)
(f) Geologic framework model (Clayton and Zelinski) is ongoing
(g) 2-D fault modeling by Andrew Cohen at LBL

Sources of Information:
(a) USGS site-scale flow model
(b) Structural interpretations of fault and fracture zones
(c) Site-scale geologic framework model

Computer Codes to be Utilized:
FEHM
STAFF3D
GSLIB

Roles and Responsibilities:
Bill Arnold: primary responsible party
Sean McKenna: in charge of getting conceptual model put together
Contributors: Chris Potter, Art Geldon, Dave Vaniman, and Jake Turin
Getting features into the transport model (Sean, Bill, Bruce Robinson and John Czarnecki)
Mineralogic and sorption studies of fault-related C-well samples (Dave Vaniman and Jake Turin)
Running transport model (Bill, Sean, Bruce)
Summarizing results for PA (Bill, Sean, Mike Wilson)

The numeric and analytic models will then be rerun in an effort to obtain effective transport parameters that would adequately represent the actual dual-porosity medium, and quantify the error involved in this simplification that we know *a priori* does not accurately describe the true transport behavior. Values of "Effective porosity", "effective dispersivity", and "effective retardation factor" for sorbing tracers, will be the only parameters available to match the single-porosity model results to the observed data. These parameters are "fitted" parameters" and will not have 100% correspondence to physical reality, but will enable simplified abstractions for TSPA calculations.

Metrics:
(a) Estimates of field-scale transport parameters, and uncertainty estimates are complete.
(b) Comparison of dual porosity and single-porosity models of C-Wells tracer test results is satisfactory.
(c) Methodology of deriving appropriate single-porosity model parameters from full set of dual porosity model parameters, is robust.
(d) Error calculations are complete.

Work Covered in Existing Workscopes:
Item (a) is the only portion of the work covered in existing workscope.

Sources of Information:
USGS conservative tracer test results and LANL reactive tracer test results.

Computer Codes to be Utilized:
LANL FEHM, and analytical codes; the USGS Moench (1995) analytic solution and its Windows-based implementation.

Roles and Responsibilities:
Turin: Implement, or arrange for implementation, of proposal elements involving the LANL FEHM and analytic codes.
Umari: implement proposal elements involving the USGS Moench (1995) analytic code.

Schedule:
Products proposed above will be delivered to TSPA members by 10/1/97.

4.4.7 Model Assumptions and Uncertainties

The main assumption of the proposed work is that a single-continuum (single-porosity) representation of a truly dual-porosity system is feasible.

4.4.8 Potential Follow-up Work

This work can be refined for future TSPA calculations based on input from TSPA.

4.4.9 Inputs/Feedbacks to Other WBS Elements

Products will be handed from Turin and Umari in WBS 1.2.3. to Dave Sevougian in WBS 1.2.5.

4.4 DETERMINATION OF EFFECTIVE FIELD-SCALE TRANSPORT PARAMETERS USING C-WELLS TESTING RESULTS

4.4.1 Participants:

Jake Turin and M.J. Umari

4.4.2 Objectives:

(a) To determine appropriate values for field-scale transport parameters (matrix/fracture porosity, dispersivity, matrix/fracture sorption, matrix diffusion) consistent with existing hydraulic and tracer-testing results from the C-Wells;
(b) Quantify uncertainties associated with parameters estimates derived in (a);
(c) Determine if an equivalent continuum model can adequately represent transport at the scale of the C-Wells tests for both non-sorbing and sorbing tracers, and if so, what are the appropriate parameter values for the single-porosity model;
(d) Quantify errors associated with the equivalent continuum approach for both C-hole scale, and larger.

4.4.3 Hypotheses:

Although the aquifer medium is believed to be truly a dual-porosity medium, it is possible that it's transport behavior can be adequately represented as a simple single-porosity medium by selecting appropriate effective transport parameters.

4.4.4 Products to TSPA-VA:

(a) Estimates of field-scale transport parameters, complete with uncertainty estimates.
(b) Comparison of dual porosity and single-porosity models of C-Wells tracer test results.
(c) Recommendations for deriving appropriate single-porosity model parameters from full set of dual porosity model parameters.
(d) Estimates of error associated with the single continuum (single-porosity) approach for both C-holes and larger scales.

4.4.5 Issues to be Covered:

This plan involves issues 3.1 Dispersivity, 3.2 Matrix Diffusion, 3.3 Matrix Sorption, and 3.4 Fracture Sorption. The scale of this study is limited to the C-Wells field scale (100 m - 1 km) and will not consider site- or regional-scale features/issues.

4.4.6 Abstraction/Testing Plan

Approach
We will first start with a series of calculations to simulate the results of USGS and LANL tracer tests at the C-hole Complex using numeric and analytic solutions of transport through a dual-porosity medium. The simulations will be constrained by existing stratigraphic and hydraulic data from previous USGS studies. Sensitivity analysis will be conducted on dual-porosity parameter estimates obtained from these calculations in order to quantify associated uncertainty.

4.5 PAST, PRESENT, AND FUTURE SATURATED ZONE FLUXES

4.5.1 Participants:

Frank D'Agnese, George Barr, Arend Meijer Jack Gauthier, Pat Tucci, Ardyth Simmons

4.5.2 Objectives:

(a) To reduce uncertainty in the existing regional ground-water flow model for Yucca Mountain under present-day climate conditions. This includes providing confidence intervals for hydraulic head, hydraulic conductivity, and recharge.
(b) To evaluate changes in the regional ground-water flow occurring under two different climate scenarios, global warming and pluvial climates. This includes changes in simulated water-table elevation, fluxes, and flow paths from present-day conditions, as well as matching paleodischarge locations with present-day discharge locations and those predicted under a pluvial climate.
(c) To provide consistency between a site-scale model and the regional model by matching fluxes and heads between the two models for present-day climate and for future climates, if possible.
(d) To gain confidence in simulated, present-day heads and flow paths by comparison with predictions made using appropriate hydrochemical and isotopic data.

4.5.3 Hypotheses:

The defining information to determine the performance criteria are hydraulic head and flux. All five critical criteria, identified in the SZ Flow and Transport Abstraction/Testing Workshop rely on these parameters: (a) peak concentration of radionuclides at 5 km from the repository,(b) peak concentration of radionuclides at 30 km from the repository, (c) time to first arrival of 1% of the peak, (d) spatial distribution of the plume, and (e) spatial distribution of groundwater flux.

4.5.4 Products to TSPA-VA:

(a) Further calibration of the existing, steady-state, regional model using newly available data (e.g., evapotranspiration data from Ash Meadows and Franklin Lake playa) to produce head distributions and fluxes as inputs for the site-scale flow and transport models. This refined calibration will include an estimate of the uncertainty of results.
(b) Prediction of discharge areas and flux at 30 km for two climate scenarios, global warming and glacial climate. These predictions will include changes in water-table elevations, flow paths, and fluxes from present-day conditions.
(c) An evaluation of what is needed to achieve adequate consistency between the regional and a site-scale model
(d) An evaluation of natural isotopic and geochemical tracers to provide constraint on present-day flow paths and possibly flux and dilution at Yucca Mountain.

4.5.5 Issues to be Covered:

4.1 - Climate change
4.5 - Natural discharge
1.6 - Regional discharge

1.5 - Distribution of recharge
1.2 - Alternative conceptual models for YM flow paths (i.e. divergence of flow paths)
1.8 - Implications of hydrochemical and isotopic data

4.5.6 Abstraction/Testing Plan

Approach
(a) The existing, steady-state, regional flow model will be refined and further calibrated using evapotranspiration data at Ash Meadows and Franklin Lake Playa as observations in the parameter-estimation model to produce an improved estimate of hydraulic heads and fluxes for input into the site-scale flow and transport models.
(b) Two climate-change scenarios will be simulated using the existing regional flow model.
(c) Regional isotopic and geochemical data will be compiled, evaluated, and compared to regional model results.
(d) Model consistency evaluation.

Metrics:
Refined calibration will be considered completed when residuals of observations of head and flux are minimized, and, hopefully, reduced from those of the existing regional model.

Work Covered in Existing Workscopes:
Approximately 50% is covered by existing workscopes. Current regional modeling workscope includes addressing: discharge areas, water-level changes, water-table configuration, regional, large hydraulic gradients, and water-budget components, for two different climate scenarios.

Sources of Information:
Existing regional ground-water flow and hydrogeologic framework models; published and recently available evapotranspiration data for Franklin Lake Playa and the Ash Meadows area; unpublished data concerning paleodischarge area; published and unpublished hydrochemistry and isotope data.

Computer Codes to be Utilized:
MODFLOWP, MODPATH, possibly FEHM

Roles and Responsibilities:
F. D'Agnese and Pat Tucci - regional modeling
J. Czarnecki and G. Barr - site modeling
A. Meijer and A. Simmons - isotopic and hydrochemical data

Schedule:
Climate simulations with existing regional model complete: 4/30/97
Incorporate ET data into model: 5/31/97
Complete model recalibration: 6/30/97
Model consistency evaluation 9/30/97
Complete geochemical evaluation: 9/8/97
All products will be provided to PA by September 8, 1997

Other Significant Components of Plan
Informal report on hydrochemistry and flow paths by USGS that was sent to DOE-NTS for HRMP

program needs to be revised, reviewed, and released to DOE-YMP. This is needed as a starting point for geochemical evaluation of regional model results.

4.5.7 Model Assumptions and Uncertainties

Assumptions

(1) Steady-state analyses will be sufficient for TSPA-VA. Transient effects will be modeled when more information is available.

(2) The scale of the regional model captures essential details of the regional flow system (i.e., hydraulic heads and flux) for TSPA-VA. Additional details will be modeled at the site-scale. See D'Agnese and others (in press) for additional assumptions and limitations of the regional flow model.

Uncertainties

(1) At the regional model scale, the proportion of flux from different source areas or hydrogeologic units to a discharge point cannot be quantified with any degree of certainty. This uncertainty impacts issues such as dilution and radionuclide concentrations at discharge points.

(2) Because little information is available concerning effective porosity of regional hydrogeologic units, calculations of travel time based on the regional model will be speculative.

4.5.8 Potential Follow-up Work

(a) Match paleowater-table observations and constrain minimum and maximum flux and hydraulic conductivity that can be obtained from those conditions. Match estimated water ages along certain critical flow paths (such as Spring Mtns. to Devil's Hole).

(b) Evaluate the feasibility of determining the percentage of flux derived from different units and areas at a regional model scale.

(c) Evaluate the feasibility of transient model calibration.

(d) Further refinement of regional model in terms of vertical and areal distribution and use of an unconfined uppermost layer.

(e) Further refinement of the regional hydrogeologic framework model.

(f) Simulation of possible changes in regional water use (pumpage or surface-water diversions).

(g) Simulation of additional climate scenarios with the newly calibrated regional model.

4.5.9 Inputs/Feedbacks to Other WBS Elements

(a) To biosphere model - discharge areas and fluxes down-gradient, well-withdrawal scenarios.

(b) To site-scale SZ model - matching fluxes.

4.5.10 Potential Problems:

Schedule

- Scarce personnel resources (available personnel are already fully committed)
- Lack of good areal and vertical distribution of water-level, flux, and geochemical data
- Scaling differences between models
- Lack of data needed for transient model calibration
- Difference in finite-element and finite-difference models
- Status of site-scale flow model

4.6 GEOLOGIC STRUCTURE AND PROCESSES AFFECTING FLOW CHANNELIZATION

4.6.1 Participants:

Andrew Cohen, Chris Potter, Don Sweetkind, Mike Wilson, and George Zyvoloski

4.6.2 Objectives:

(a) Determine how the 3-D hydrogeologic structure and flow processes at Yucca Mountain control saturated zone flow channelization on the scale of hundreds of meters to kilometers (termed here as "large scale").
(b) Determine effects of fault offset, fault-zone properties, upwelling from Paleozoic formation, and geothermal heating on horizontal and vertical flow channelization.

4.6.3 Hypotheses:

(a) Large scale structural features significantly control flow channelization up- and down-gradient of the repository; and
(b) such channelization may be a dominant factor affecting transport characteristics on the scale of the accessible environment (5km), and therefore is an important process affecting 1) peak concentration of radionuclides at 5km from the repository; 2) time to peak concentration; 3) spatial distribution of radionuclide plume (both horizontal and vertical); and 4) spatial distribution of groundwater flux.

4.6.4 Products to TSPA-VA:

Numerical simulation results will show the effect of individual structural features/processes on vertical and horizontal channelization on the scale of the accessible environment. These include: 1) offset of hydrogeologic units separated by a) permeable fault zones; b) low permeability fault zones; c) offset-only faults; 2) upwelling from Paleozoic aquifer; and 3) geothermal heating. Results from a calibrated model will show the 3-D steady-state flow geometry within the model domain (see below). Two-dimensional model cross-sections will also be used for simulations. Particle tracking is used to examine flow geometry. Effective dispersivity resulting from the mechanical dispersion due to the large scale features will be presented. Sensitivity studies will show the relative impact of different features/processes on flow channelization, and those geologic features and processes relevant to transport calculations will be identified. This information is needed to support assumptions made in TSPA transport calculations, such as whether or not the effect of these features can be lumped into a single effective property. Potential questions that can be answered include a) does upwelling significantly affect vertical mixing, b) does geothermal heating produce significant convection, and c) are fluids originating at the water table confined to the upper 100 m of the saturated zone down-gradient due to flow geometry imposed by the faulted geologic structure?

4.6.5 Issues to be Covered:

The model considers the following saturated zone characteristics and processes: 1) the presence of high and low permeability faults which offset units; 2) the potential upwelling of fluids from the Paleozoic carbonate formation via conductive faults; 3) differences in fluid temperatures with depth due to thermal conduction and convection; 4) chemical and isotopic variation in saturated-zone water chemistry, and implications for flow pathways and travel times; and 5) the 3-dimensional hydrologic mixing and dilution produced by the above processes. These are selected for investigation because a) the effects of these features/processes on flow have primarily only been hypothesized to date, without confirmation of their importance; b) the block-bounding faults are the most prominent geologic features on the scale of the model domain.

4.6.6 Abstraction/Testing Plan

Approach

The Sub-Site-Scale 3-Dimensional Saturated Zone Flow Model will be used to perform hypothesis testing and sensitivity studies of the effects of the large-scale 3D geologic structure on flow channelization. The construction of this model, along with the proposed work described here, are part of a study already in progress at LBNL under WBS 1.2.3.3.1.3.3. This 3-D model explicitly accounts for unit thickness variation, fault offset, fault zones between units, geothermal flux, and fluid upwelling from the Paleozoic formation. The model covers an area of approximately 100 km^2. The boundaries of the model are approximately located at the boundaries of the "Accessible Environment," and encompass the saturated-zone well field. All block-bounding faults including and between the Solitario Canyon and Forty Mile Wash faults are modeled explicitly. The 3-D distribution of faults and geologic units is based on the 3-D Geologic Framework Model, version 2.0. Fault zone properties will be varied systematically but in accordance with understanding of individual fault zone properties as observed from the surface and in boreholes. The model will be calibrated with respect to water table elevations, temperature logs, and qualitatively by geochemical data.

Radionuclide transport is not modeled explicitly. Instead, flow geometry is the focus, as the emphasis is placed on flow channelization. The large hydraulic gradient to the north will be investigated in future work with the model.

Metrics:

(a) vertical fluxes in the regions of major faults
(b) effective dispersion as determined from particle tracking.

Work Covered in Existing Workscopes:

This work is covered by WBS 1.2.3.3.1.3.3.

Sources of Information:

The geologic structure represented in the model is based on the 3-dimensional geologic framework model, version 2.0. Data on water table elevations from SZ boreholes are used for calibration. Temperature logs from SZ boreholes, and implicitly, water table temperature are used to quantitatively calibrate the model. Isotopic and geochemical data collected in SZ boreholes are used qualitatively to constrain interpretations of simulation results.

Computer Codes to be Utilized:

TOUGH2 is used for model simulations. Nonisothermal, single continuum flow is considered.

Single continuum is appropriate for investigation of flow geometry during steady-state flow. The code is capable of dual permeability flow, but will not be used in this way for these simulations.

Roles and Responsibilities:
LBNL is responsible for model simulations. Andrew Cohen, Curtis Oldenburg, and Ardyth Simmons of LBNL will maintain communication with other modeling teams and geologists to ensure that current knowledge of geologic properties and modeling concerns and needs are meet.

Schedule:
The current work at LBNL which includes proposal products discussed here is "Sub-Site-Scale 3-Dimensional Numerical Saturated Zone Flow Model. The 1997 deliverable for this work is August 31.

4.6.7 Model Assumptions and Uncertainties

A single continuum model is used. The 3-D geologic structure between the water table and the base of the Lithic Ridge Tuff is modeled as confined flow. This assumption is valid since steady-state flow through a region with hydraulic gradient of 0.0001 is being considered. The main uncertainties are hydrologic properties of faults, and secondarily, of geologic units. The latter information will be extracted from pumping tests and borehole flow surveys. The former information is unknown, and will be varied to examine the potential effects on flow channelization of different fault properties in relation to the overall geologic structure. The model assumes vertical faults.

4.6.8 Potential Follow-up Work

The model is designed to enable transient, dual-permeability simulations. The model grid is already constructed so that the area near and around the C-hole complex is finely discretized such that pumping tests and the response at neighboring observation wells can be simulated.

4.6.9 Inputs/Feedbacks to Other WBS Elements

This work is directly related to transport modeling because channelization affects flow geometry. Therefore, one major product of the work is the identification of how particular geologic features/processes affect transport. This knowledge will help in developing conceptual models of transport on a large scale, and determining which features/processes can or can not be disregarded in transport simulations by other modeling teams, and ultimately by TSPA.

4.6.10 Potential Problems:

The very small gradient down-gradient of the repository will likely allow for multiple property variations to fit a "calibrated" model. The range of possible scenarios will be constrained by the use of temperature data calibration and qualitative agreement with borehole geochemical data. Use of pumping test data from C-hole tests will most likely not be used for calibration of the August, 1997 deliverable.

5. REFERENCES

Barnard, R.W., M.L. Wilson, H.A. Dockery, J.H. Gauthier, P.G. Kaplan, R.R. Eaton, F.W. Bingham and T.H. Robey, 1992. *TSPA 1991: An Initial Total-System Performance Assessment for Yucca Mountain*. SAND91-2795. Albuquerque, NM: Sandia National Laboratories. 386 p.

Czarnecki, J.B. and R.K. Waddell, 1984. *Finite-Element Simulation of Ground-Water Flow in the Vicinity of Yucca Mountain, Nevada-California*. Water Resources Investigations Report 84-4349. Denver, CO: U.S. Geological Survey. 42 p.

D'Agnese, F.A., Faunt, C.C., Turner, A.K., and Hill, M.C., in press, Hydrogeologic evaluation and numerical simulation of the Death Valley regional ground-water flow system, Nevada and California, using geoscientific information systems: U.S. Geological Survey Water-Resources Investigations Report 96-4300.

M&O, 1995. *Total Systems Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository*, B00000000-01717-2200-00136, Rev. 01, TRW Environmental Safety Systems, Las Vegas, NV.

Wilson, M. L., J. H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer and D.E. Morris, 1994. *Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993)*. SAND93-2675. Albuquerque, NM: Sandia National Laboratories.

Appendix A

INVITATION MEMO TO THE WORKSHOP

Sandia National Laboratories

Albuquerque, New Mexico 87185-1326

WBS 1.2.5.4.4
QA:NA

date: March 10, 1997

to: Distribution

from: Bill W. Arnold; Jack H. Gauthier; Pat Tucci; Bruce A. Robinson

subject: Invitation to TSPA-VA Saturated Zone Flow and Transport Abstraction/Testing Workshop

This memo serves as an invitation to a workshop conducted by the Performance Assessment (PA) group on abstractions of Saturated Zone (SZ) Flow and Transport for Total System Performance Assessment-Viability Assessment (TSPA-VA). This workshop provides an opportunity for process-level modelers and site-characterization staff to insure that their work is adequately represented in TSPA calculations. The workshop is intended to be a working meeting. Therefore, the number of participants is limited to keep the meeting as productive as possible (see page 5 for list). In addition to the participants a small number of observers are also invited. Their role is to observe, not to participate in the presentations, discussions and planning that will take place during the workshop. In contrast, all participants will have to do preparation work prior to the workshop. Many will have to give short proposal presentations during the workshop, and small working groups will be writing proposals during the workshop.

The workshop is being held in Denver, CO at the Federal Center in Building 25 (see Appendix K) on April 1, 2 and 3, 1997. **If you are unable to attend the workshop, please respond immediately.** Write-ups on assigned issues are due from the participants on March 17, 1997 (see Attachments F and I). Please also note that a block of rooms has been reserved at the Sheraton Denver West Hotel and that participants and observers must make reservations with the hotel by **March 17, 1997** to be guaranteed one of these rooms (see Attachment K).

This letter defines the goals and describes the process of the SZ Flow and Transport workshop. Additional important information is provided as a series of Attachments.

Introduction

This workshop is the eighth in a series of ten which have the ultimate goal of helping to develop a valid, defensible TSPA-VA using the most complete and current information available. In order to achieve these goals we need to incorporate reasonable models that reproduce the essential behavior of key processes important to long-term performance in a computationally efficient manner. In addition, we need to describe alternative conceptualizations and parameter sets that reflect the variability and uncertainty of the system. The TSPA-VA calculations and documentation need to be completed by June, 1998. During the 1997 fiscal year it is therefore necessary to completely define how TSPA calculations will be made, what input parameters will be used, and the uncertainty associated with these input parameters.

The SZ workshop is intended to bring together data collectors, process modelers, subsystem modelers, and TSPA modelers in order to address issues seen as important for TSPA-VA. A list of activities and products for each of the workshops is presented in Attachment A, along with what is expected from post-workshop activities. All participants in the workshop must stay focused on the goals of the workshop. That is, we are deciding how to handle issues for TSPA-VA calculations. We are *not* trying to resolve the issues. We would like to discuss what SZ flow and transport calculations have been completed to date and decide what still remains for input into TSPA-VA. We will all need to come to agreement on model inputs, parameters, geometries, and other issues at the site- and regional-scales. To assist those who are not used to thinking with a TSPA perspective, a TSPA outlook focused on SZ modeling is attached (Attachment B). It is critical for all the workshop participants to read this carefully and keep what is said in mind while preparing for the workshop.

What we need to accomplish this year is often referred to as "abstraction" and thus these workshops are called abstraction/testing workshops. "Abstraction" is defined by performance-assessment analysts as a process of capturing or simplifying very complex and multifaceted processes that occur over many spatial and temporal scales in a manner that permits the important aspects of the processes to be included in total-system performance calculations. "Testing" of these abstractions involves comparing the results of the simplified model to the results of the more complex process-level model to assure that the abstracted model adequately represents the behavior of the system. To help clarify the meaning of abstraction, examples of how abstractions have been conducted in past TSPA calculations are given in Attachment C.

Description of the SZ Flow and Transport Workshop

The SZ workshop will concentrate on the abstracting and testing of issues pertinent to SZ flow and radionuclide transport at Yucca Mountain that have a significant influence on long-term performance of the repository. In preparation for this workshop, TSPA and subsystem modelers have put together a list of these issues that need to be addressed in order to conduct appropriate abstractions for the SZ portion of TSPA-VA calculations (Attachment D). This list was prepared through consultation with site-characterization personnel to make sure that the list is inclusive and to obtain input on the best approach to addressing these issues. Suggested methods for coupling SZ flow and transport calculations to other components of TSPA-VA are presented in Attachment E. The goal of the workshop will be to address all of the issues listed in Attachment D. Areas that are not easily resolved or for which there is some disagreement between participants (herein referred to as problem areas) will be noted and methods of resolving these problem areas proposed and assessed.

In order to make the workshop successful, much work has gone into the planning and it is asked that the participants also conduct some detailed work prior to the workshop. Attachment F contains complete instructions for the workshop participants. As a mechanism to begin the discussion, and to start participants thinking about the issues involved in TSPA modeling of SZ flow and transport at Yucca Mountain, we present a series of "strawman" proposals in Attachment G. The proposals represent current ideas in the TSPA group and how we would go about modeling SZ flow and transport in the absence of the abstraction/testing workshop. Examination of the proposals shows that they are incomplete and that there are many issues that need to be resolved at this workshop or during the remainder of the fiscal year. Workshop participants are asked to completely review this strawman (Attachment G) and comment as appropriate. As a minimum, all participants (see below) should send in at least one proposal response on the sub-issue (see Attachment D) that they believe falls within their area of expertise or area of interest. If you would like to write a proposal on multiple topics, please do so and clearly indicate which topics you plan to discuss. Some people have been assigned specific area(s) in which to respond. This would count towards the required proposal write-up, but all are free to comment on any other issues of interest. Please see Attachment I to determine if you are required to write-up a proposal in a certain area. A short written proposal, following the outline format, on what each person can contribute to the issue(s) is requested in advance of the workshop (see Attachment F for complete instructions). If you feel that a potential issue has been omitted from Attachment D, address the omitted issue and submit a proposal for its inclusion in the workshop discussion. These proposals will be compiled and distributed to all of the participants before the workshop. If a strawman proposal is not controversial then it will be assumed to be acceptable for TSPA calculations. The pre-workshop preparation will allow the participants at the workshop to concentrate on the more complicated issues and arrive at plans on how to address them. Also as pre-workshop work, participants will be asked to prepare a short presentation of their proposal(s), described below.

A draft agenda for the workshop is presented in Attachment H. This agenda is expected to change based on the results of the comments we receive on the issues list and strawman proposals. For example, if general agreement is found on a particular issue, less time will be devoted to that issue. The format of the workshop is as follows. Each major issue (1 through 4 in Attachment D) will be considered in some detail. A TSPA representative will present a perspective on the major SZ issue. Each of the assigned proposals (within that major SZ issue) will be presented to the entire working group. After the proposal presentations, small working groups will (1) identify the major points that were brought out by the proposal and/or additional points that need to be included in the proposal to address TSPA-VA, (2) identify weaknesses (if any) of the proposals with respect to the TSPA-VA viewpoint AND suggested alternative methods to resolve the weaknesses, (3) repeat steps (1) and (2) for each sub-issue/proposal, and (4) prioritize the most important points for each major issue relative to specific criteria deemed to be important to disposal system performance and identify whether they are readily addressable or relatively intractable.

The resulting important points from the small groups will then be prioritized for full-group consensus. Each major issue will then contain a prioritized list of items that have been determined to be important to TSPA-VA by the entire group present. The proposals can then be adjusted to incorporate the prioritized small group responses. The revised proposal will then be reconsidered by the core teams to insure that all important issues have been completely addressed. This process will occur a total of 4 times in order to address each major issue in Attachment D.

In addition to identifying and presenting proposals based on the list of issues important to flow and transport in the saturated zone, another outcome of the workshop will be to define the abstraction approach for TSPA-VA, and a set of analyses to be done after the workshop to aid in developing the abstractions. This will result in identifying (groups of) individuals who will perform SZ analyses and new sensitivity studies. It must be understood that this effort will have to be coordinated with the abstraction/testing core team throughout the FY in order to insure that TSPA-VA goals and needs are being met. Any problem areas that may remain at the end of the workshop will be addressed and handled by the abstraction/testing core team and the TSPA core team, with continued input from the affected workshop participants. This process occurs during FY97 and into FY98 while TSPA sensitivity studies proceed.

Schedule of Workshop:

Tuesday, April 1, 1997	Day 1 of Workshop (all day)	8:00 am - 5:00 pm
Wednesday, April 2, 1997	Day 2 of Workshop (all day)	8:00 am - 5:00 pm
Thursday, April 3, 1997	Day 3 of Workshop (all day)	8:00 am - 12:00 pm
Thursday, April 3, 1997	Core Team Wrap-up Meeting	12:00 pm - 5:00 pm

(See Attachment H for a draft agenda)

List Of Participants:

<u>SZ Core Team:</u>

Bill Arnold	SNL
Jack Gauthier	SNL
Bruce Robinson	LANL
Pat Tucci	USGS

<u>TSPA Core Team:</u>

Bob Andrews	INTERA
Holly Dockery	SNL
Jack Gauthier	SNL
Jerry McNeish	INTERA
Dave Sevougian	INTERA
Mike Wilson	SNL

<u>Other Participants:</u>

George Barr	SNL
Andrew Cohen	LBNL
Ardyth Simmons	LBNL
John Czarnecki	USGS
Frank D'Agnese	USGS
Ed Kwicklis	USGS
Chunhong Li	INTERA
Sean McKenna	SNL
Arend Meijer	LANL
Zell Peterman	USGS
Chris Potter	USGS
Chris Rautman	SNL
Jake Turin	LANL
Ardyth Simmons	LBNL
Tony Smith	INTERA
Inez Triay	LANL
M. J. Umari	USGS
Vinod Vallikat	INTERA
Dave Vaniman	LANL
George Zyvoloski	LANL

Facilitator:

Susan Altman	SNL

List of Observers:

Larry Rickertsen	TRW
Abe Van Luik	DOE
Eric Smistad	DOE
Russ Patterson	DOE
Dwight Hoxie	USGS
Mike Chornack	USGS
Cynthia Miller-Corbett	USGS
Leon Reiter	NWTRB Representative
Jim Duguid	INTERA
Alva Parsons	SNL
Gilles Bussod	LANL
Rod Ewing	PA Peer Review Panel
Chris Wipple	PA Peer Review Panel
NRC Representative	
EIS/NEPA Representative	

List of Attachments:

Attachment A:	Specific Activities and Products of Each Abstraction/Testing Workshop
Attachment B:	TSPA Introduction
Attachment C:	Discussion of the Meaning of Abstraction
Attachment D:	Important Issues of SZ Flow and Transport
Attachment E:	Coupling of SZ Flow and Transport to Other Models Developed for TSPA-VA
Attachment F:	Preparation Work for Workshop Participants
Attachment G:	Strawman Proposals for Addressing Important SZ-Flow and Transport Issues for TSPA-VA
Attachment H:	Draft Agenda for the SZ Workshop
Attachment I:	Required Proposals by Workshop Participants
Attachment J:	References
Attachment K:	Conference Facilities and Hotel Information
Attachment L:	Schedule of Other Abstraction/Testing Workshops

Distribution:

MS1326	B.W. Arnold, 6851
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MS1326	M.L. Wilson, 6851

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	C. Faunt (USGS/Denver)
	Z. Peterman (USGS/Denver)
	C. Potter (USGS/Denver)
	M.J. Umari (USGS/Denver)
	A. Meijer (LANL)
	P.W. Reimus (LANL)
	H.J. Turin (LANL)
	G.A. Zyvoloski (LANL

cc:

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	A.E. Van Luik, DOE
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	W.J. Boyle, DOE
	S.J. Brocoum, DOE
	S.H. Hanauer, DOE
	D.T. Hoxie, USGS
	R.W. Craig, USGS
	J.A. Canepa, LANL
	G.S. Bodvarsson, LBNL
	Y. Tsang, LBNL
	L. Reiter

R. Ewing
C. Wipple
P. Witherspoon

YMP:1.2.5.4.3:PA:NQ/WA-0335
YMP CRF

Attachment A

Specific Activities and Products of Each Abstraction/Testing Workshop

1) Identify and group the important issues (e.g., processes and parameters) of the given abstraction/testing topic with respect to long-term performance of the repository. The suggested grouping is as follows based on the relative priority: essential, important, not critical, and to be determined. (The Features Events and Processes (FEPs) should be compared to the scenario trees that have been developed to ensure that no important issues have been overlooked.)

2) Prioritize the "to be determined" issues as to which are most important to be evaluated as a post-workshop activity. Develop alternative methods for evaluating importance of "to be determined" issues and document strengths and weaknesses of each alternative.

3) Present how the important issues and associated uncertainties have been incorporated in previous TSPAs. Discuss appropriateness of these methods and possible alternatives.

4) Decide upon a method for addressing and quantifying uncertainty in alternative process models and parameters of the abstraction/testing topic. (The eventual outcome of this method during post-workshop activities should be probabilities and/or probability distributions.)

5) Create a plan for developing and testing appropriate model abstractions of the most important processes. The plan should resolve (or outline a procedure to resolve) the following important issues:
   a) Which type of abstraction is most appropriate: response surface, lower-dimensional process model, analytical model/algorithm, etc.(or a combination of these)?
      i) The abstraction must be sufficiently accurate.
      ii) The abstraction must be capable of interfacing with TSPA software in a computationally efficient manner; i.e., we must be able to use it in a multi-realization probabilistic mode.
   b) How should spatial and temporal variability be represented in the abstraction?
      i) How is heterogeneity represented if dimensionality is reduced?
      ii) What degree of spatial/temporal discretization is acceptable in the abstracted model?

6) Define, or at least discuss, how the above abstractions will interface with other abstraction/testing topics in a consistent fashion: with respect to time, space, processes, and parameters.

7) Discuss how available resources and scheduling will affect post-workshop activities:
   a) How much time/personnel/funds is required and available to conduct post-workshop abstraction/testing activities?

b) How do abstraction/testing activities fit into both overall PA schedule and overall Site schedule?

c) Can some activities be performed that will satisfy both Site and PA deliverables?

d) Develop a tentative schedule for completion and delivery of post-workshop products.

Specific Outcomes and Products of Post-Workshop Abstraction/Testing Activities

1) Write workshop deliverable, which reports upon the activities and decisions of the workshop and the plans for post-workshop abstraction/testing activities that feed TSPA-VA.

2) Develop and test abstraction methods proposed by the workshop. Compare abstracted models to more detailed models (if available) to determine accuracy (acceptability) of abstractions. Errors in abstractions should be on the conservative side.

   a) Decide upon the degree of dimensionality reduction.

   b) Determine how to incorporate spatial and temporal variability.

   c) Test the interface with TSPA software and see if it is feasible to use the given abstraction in multi-realization fashion.

   d) Examine predictions of the abstraction compared to the process model. Does the abstraction represent uncertainty appropriately?

   e) Determine if the abstraction can be coupled with other abstraction such that coupled processes and synergistic effects are still accurately captured by the abstraction(s).

3) Write a section for the TSPA-VA report detailing the models and abstractions to be used for TSPA-VA. All decisions made should be documented, along with the sensitivity analyses and abstraction-testing that were performed. The workshop deliverable should serve as a starting point.

Attachment B

TSPA Introduction

The purpose of total-system performance assessment (TSPA) is to calculate various measures of repository safety, such as peak individual radiation dose, and to estimate the uncertainty in the calculations. Essentially, we want to estimate the radiation dose and put error bars around the estimate, just as any experimental result should always be accompanied by an error estimate. (There are other "performance measures" of interest as well, but for the rest of this discussion we'll just speak of peak doses.)

The uncertainty estimate complicates the problem and increases the difficulty of the task considerably. Suppose for the sake of discussion that we need to consider four design cases (e.g., with and without backfill, high and low thermal load). If we were confident enough of our models and their input parameters, we would just need to make four deterministic model calculations, so it would be feasible to use models so complicated that they take several weeks to run.

However, because of the uncertainty in models and input parameters, we must conduct a probabilistic assessment with multiple runs for each design case in order to look at the probability distribution of peak doses. Uncertainty in peak dose is usually expressed as a CCDF, or complementary cumulative distribution function. Such a distribution is equivalent to the more familiar probability density function, but it shows more explicitly what we really want to know: the probability of having high calculated doses.

The importance of examining system performance probabilistically is illustrated by the fact that the mean dose is often dominated by low-probability occurrences--that is, by "realizations" with one or more input parameters from the tails of their probability distributions. (Incidentally, the measure of risk that the National Academy of Sciences recommended using (National Research Council, 1995) is calculated from the mean of the peak-dose distribution.)

The need for multiple calculations leads to requirements for computational efficiency and reliability in the process calculations. An estimate of the number of performance calculations, schedule requirements, and computer resources for TSPA-VA provides a rough quantitative idea of the computational efficiency and reliability needed. Uncertainty in TSPA calculations may be broken into two pieces: (1) discrete scenarios, e.g. repository design options, waste package/EBS design options, geochemical environments, future climate; (2) uncertainty or variability in model parameters. We expect about 30 discrete scenarios for the TSPA-VA. For each discrete scenario, a suite of about 100 or more realizations may be needed to capture the effects of parameter uncertainty. Therefore, a complete TSPA will involve approximately 3,000 calculations of the system performance. Possible problems arising during the course of these calculations could cause the actual number of calculations required to double, implying 6,000 calculations of the system performance.

TSPA calculations are scheduled for a period of about three months (beginning in January of 1998 and ending in March of 1998), which is about 2,200 hours. The computer resources available for these calculations are estimated to be about the equivalent of five dedicated workstations. This gives a total of about 11,000 hours of processor time. Therefore, the processor time available for each realization is about 110 minutes. (For comparison, this is about an order of magnitude slower than the computation speed for an average realization in TSPA-95.) There are roughly nine separate processes in the TSPA calculations, corresponding to the nine workshops: UZ flow, waste package degradation, thermal hydrology, UZ radionuclide transport, waste form degradation, waste form mobilization, near field environment, SZ radionuclide transport, and biosphere. It is likely that some (if not all) of these processes will be captured in a very simple way for TSPA such that computation for these items is small. If we conservatively assume four detailed process calculations are performed per realization, then the average time available for each detailed process calculation is on the order of 30 minutes. This estimate is based on continuous, round-the-clock, end-to-end, performance assessment calculations. A variety of inefficiencies will likely reduce this by another factor of three. Therefore, we may expect process calculations in TSPA to be limited to an average of about 10 minutes of processor time. Furthermore, the process calculations must be reliable in the sense that they will nearly always converge to the correct solution without special adjustments to the calculations.

Results of TSPA-93 and TSPA-95 were found to be sensitive to SZ flow and transport when calculating doses over a 1,000,000 year period. Of particular importance were parameters related to dilution; e.g., the cross-sectional area of flow (an estimate of lateral dispersion) and the groundwater flux. The SZ was found to be relatively unimportant to cumulative releases and over a 10,000 year period. This finding could, however, be an artifact of the way the system was modeled - the SZ was considered as a single-continuum, porous medium and plutonium was only transported as a solute. Thus, plutonium was retarded in the SZ until it decayed to very low concentrations. Colloidal transport or channelized flow could have altered these results.

Our SZ-flow and -transport needs for TSPA-VA can be summarized as follows:

1. We must be able to run hundreds of model calculations of the entire disposal system, including container corrosion, waste-form degradation and radionuclide release, unsaturated-zone flow and radionuclide transport, saturated-zone flow and transport, and biosphere transport and dose to individuals.
2. The calculations must cover at least 10,000 years, and some of them will cover 1,000,000 years.
3. The SZ-flow calculations must include effects caused by changes in climate.
4. The model(s) we use for TSPA-VA will have to be defensible in terms of their consistency with available experimental and field data.

Please keep the above criteria in mind when considering which models are appropriate for use in TSPA. The simplest choice would be a detailed process model for SZ flow and transport that would explicitly model all the relevant processes In practice, however, it is doubtful that such a model could meet the computational performance requirements for speed and reliability that are needed for TSPA-VA calculations. Given this constraint, we must decide on the best approach for "abstraction," which is to say an appropriate set of approximations or simplifications that will allow the calculations to be completed within the time available and at the same time represent the essential behavior of the system. Abstraction is discussed further in Attachment C.

Attachment C

Discussion of the Meaning of Abstraction

Definition of Abstraction

As a first step, let us try to remove the "abstractness" from the terms "abstraction" and "abstraction/testing", as used by Performance Assessment. The term abstraction is often used to mean a "simplified model" or the procedure for developing such a simplified model. Perhaps a clearer definition of abstraction is "model". All physical-chemical models are an abstraction of the one reality to a greater or lesser degree. At the simplest level, the "abstraction/testing" procedure would consider two models of a given physical-chemical process, a complex model and a simple model (there may actually be a spectrum of models going from the most complex, and presumably most accurate, to the most simple), and compare the system response predicted by the two models. If the simple model response reasonably bounds (i.e., predicted peak concentration is equal to or higher than) the complex model over the range of uncertainty of the model parameters and boundary/initial conditions, then the simple TSPA model can be said to be validated viz-a-viz the presumably "calibrated" complex model.

Calibration of Models and the Use of Reasonably Conservative Models

All models need to be calibrated and validated against experimental data. In many cases, the most simplified (or most abstracted) TSPA model might just as well be calibrated against the available data as the most complex (or process-level) 3-D model. However, often as a matter of preference the simple model is calibrated against the complex model rather than against the data itself. (For some very simple models, such as the RIP TSPA model, certain state variables are not explicitly used in the simple model, so the simple model cannot really be calibrated, per se.)

Even the most complex process-level models of Yucca Mountain cannot really be validated, due to the lack of data. Thus, a reasonably conservative simple model seems a valid approach-for example, 1-D flow where this would result in conservative estimations of the release and/or peak dose. An obvious caveat to this example is that 1-D flow does not consider the dilution afforded by lateral dispersion, which might be appropriate for highly channelized flow field. However, one would have to use a so-called "alternative conceptual model" for at least some of the PA calculations (realizations) in order to incorporate the uncertainty associated with dimensionality reduction.

Definition of "Alternative Conceptual Models"

This brings us to a clarification of the often used phrase "alternative conceptual model". As used in the previous paragraph, this just refers to a form of uncertainty and/or simplification in the modeling of the system or process behavior. If there is a single agreed-upon TSPA model that can allow for both vertical flow through the zeolites and bypassing of them, through the inclusion of uncertainty in model parameters and/or boundary/initial conditions, then there is no need for a so-called alternative conceptual model.

The phrase "alternative conceptual model" often seems to imply that two or more "alternative" models are equally good representations of the underlying reality. However, this is rarely the case, because as mentioned in the opening paragraph, all models are abstractions or simplifications of varying degree of the underlying physical-chemical processes (we don't use quantum mechanics to describe unsaturated groundwater flow). Thus, one of these two or more alternatives is more of a simplification than the other. For example, the equivalent continuum model (ECM) of fracture/matrix flow and the dual permeability model (DKM) of fracture/matrix flow are often referred to as alternative conceptual models. However, these two models are really just different levels of simplification (with the ECM being the simplest, since it is based on the additional assumption of capillary equilibrium between the two continua). As such, we do not necessarily need both of these models for TSPA calculations. In particular, if the desired degree of uncertainty (and accuracy) in the system response can be adequately represented in either one or the other model, through variations in boundary/initial conditions and phenomenological coefficients, then that model alone is sufficient. There are some likely situations where this is not the case for the ECM and DKM, for example, the case of transient flow and/or transient boundary conditions. This would argue for the DKM model (the more complex of the two) as being more appropriate. However, that brings us back to one of the primary reasons for using simplified models: computational resources and efficiency when running calculations in a multiple realization format. This in turn brings us to the question of how to ascertain whether a TSPA model provides "an adequate representation" of the system response over a wide range of uncertainty in boundary/initial conditions and phenomenological coefficients. In this context, one important workshop task is to identify how to validate the simple models against the complex model. Criteria for validation must include metrics for how "well" the various processes are captured or addressed in the simpler model. (See below.)

Model Validation/Calibration as a Function of Process Simplification

To prevent the workshop from becoming mired in an endless and largely fruitless discussion of currently unresolvable "issues", it is important to classify issues as to how they relate to both model abstraction and total system performance. Broadly speaking there is really only one issue: model validation. For the purposes of attacking this issue from a performance-assessment (and also "abstraction") perspective, it is convenient to discuss it in two parts: (1) how model validation is a function of (or is affected by) process simplification and (2) how model validation is a function of uncertainty. With regard to the former, the important point is to quantify how accurately the key physical-chemical processes and boundary/initial conditions are represented in the various models. To this end, a large part of the workshop discussions will revolve around the components of the various models themselves (rather than around "issues"): processes included in the models, boundary and initial conditions, coupling to other models, methods for calibration/validation of the models and submodels (both "process-level" and simplified TSPA models). For SZ transport the appropriate processes to discuss are matrix diffusion, mechanical dispersion, sorption, precipitation/dissolution, radionuclide decay, flow in 3-D, etc. Boundary conditions include the boundary heads (including the water-table height) or fluxes. Initial conditions include all the initial parameter values. For example, perched water is not an issue per se, nor is it a process. It is an initial condition of the fluid saturation in the pores (or it could be a later state condition of the fluid saturation, for some realizations of the phenomenological coefficients and boundary/initial conditions). Coupling to other models would include the coupling to thermohydrological processes, to UZ transport, and possibly to the biosphere.

Presentations should discuss how both the most complex and simple models include or account for the various processes and boundary/initial conditions. This requires a definite proposal for a simple TSPA model. Furthermore, there should be a presentation/discussion of processes and boundary/initial conditions not adequately addressed in the complex and simple models, and a ranking of if/how/which processes need to be included in complex and TSPA models. This should be done in light of the effect of these things on system performance (and also keeping in mind the limitations on computer resources). First, the absent processes need to be addressed in the process models. Then the absent processes need to be addressed in the TSPA models. For TSPA models, some processes may have been intentionally left out, or represented by a simpler model. The effect of this omission or simplification of an important process needs to be quantified. If the workshop decides that some of these omitted processes need to be included, or simplified processes need to be represented more thoroughly (in either the complex or simple SZ transport models), then a discussion of time/personnel/resources is required to decide the feasibility of this for TSPA-VA.

Some time in the workshop will be devoted to a discussion of model calibration of the more complex models, primarily to educate all participants so that everyone can help decide the validity of the simpler TSPA models.

Model Validation/Calibration as a Function of Uncertainty

Regarding uncertainty, which is caused by lack of data for parameters (phenomenological coefficients) and boundary/initial conditions, and lack of knowledge of the appropriate mathematical representation of the process(es), the workshop must address the major sources of this model uncertainty and how to include the uncertainty in both the complex model and the simple model. Parameter uncertainty seems somewhat more quantifiable than so-called conceptual-model uncertainty, which is really uncertainty regarding the level of detail needed to represent certain processes, such as fracture/matrix interaction, for the purposes of predicting peak dose to humans. Specifically, one must address how parameter uncertainty translates to process uncertainty, i.e., how input uncertainty translates to uncertainty in the system response, which is a function of the particular process model.

The uncertainty in some model parameters, such as bulk permeability, seems straightforward to quantify, based on well tests. On the other hand, the uncertainty in other model parameters is very difficult or impossible to quantify, since these model parameters represent abstractions of reality that are not directly measurable by experiments (or, also that there are too many parameters in the model to assign unique values to the various parameters). One example is matrix/fracture coupling.

Inherent in validating a simple TSPA model against a complex process-level model is to validate it over the entire uncertain range of the parameters and boundary/initial conditions, or equivalently, over the entire range of likely system response. This would seem to require as many runs of the complex model as the simple model for the purposes of calibration. Deciding upon the necessary number of runs is a post-workshop activity, and proposing criteria for making this decision is a useful outcome of the workshop itself. As with any physical model of reality (e.g., Newton's 2nd law), we can only validate the model at a few values of the parameters with a few experiments, and then use the model to predict the system response at other values of the parameters. Ideally, this should be done in an interpolation sense, rather than an extrapolation sense, but that may not always be possible. As mentioned previously, in the case of simple TSPA models, the model validation will generally consist of comparison to the more complex "process-level" models, rather than comparison to the experimental data themselves. In this validation process, it is clear that the simple model response will not be the same as the complex model response. Theoretically, the complex model response should be more accurate, but given the lack of data, that is not necessarily so. In any case, since we believe the more complex models to be more accurate (or at least that they have a higher degree of spatial-temporal resolution), we want the simple model responses to "bound" the more complex model responses, i.e., to always give equal or higher values for the doses. We need to build confidence that significant dose peaks (i.e., those that occur temporally on the order of human behavior and human life span) are captured adequately by the simple models.

To summarize, the workshop participants should identify those values of the model parameters at which to compare/validate the simple models against the "calibrated" complex models. In conjunction with this, the workshop should identify/quantify uncertainty ranges for the parameters and boundary/initial conditions of the complex and simple models.

Discussion of Response Surfaces

It may be decided during post-workshop analyses that the proposed simple models are inadequate. Perhaps they have so few measurable parameters, or the dimensionality and discretization have been reduced so much, that they cannot adequately predict system response over the supposed uncertainty range. Or perhaps, they do not allow a high enough degree of coupling to other workshop models, such as thermohydrologic models. In this case, the only possible abstraction or simplification alternative may be to develop response surfaces based on the complex model. Here we mean that the complex model is run relatively few times to develop a curve fit of the nonlinear system response as a function of time, space, and the key model input parameters. Then, the system response for other values of the input parameters is interpolated from the response function. (Ideally, extrapolation would never be attempted.) This method is in contrast to running the simple model at any and all values of the input parameters.

However, the use of response surfaces seems more amenable to processes other than SZ flow and transport, such as thermohydrology. In the latter, the response surface is a function relationship or table lookup of temperature (T) and relative humidity (RH) as a function of time, space, and certain system parameters, such as percolation rate. Temperature and relative humidity from the response surface are then used directly in a waste-package degradation model. Furthermore, these T and RH response surfaces are based directly upon a set of initial/boundary conditions specific to the desired repository system, for example, a specific areal heat loading (or emplacement density of the waste packages). SZ response surfaces would be represented as mass concentration or rate at some distance downgradient, as a function of time, space, and various system parameters (for example, flux).

Variability

Another, possibly separate issue is spatial-temporal variability, which is related to (1) the probabilistic versus deterministic nature of the physical-chemical processes themselves; (2) simplification of the spatial-temporal domain due to lack of knowledge (uncertainty) about the boundary/initial conditions; (3) simplification of the spatial-temporal domain due to constraints on computational resources. When validating the various models, the necessary or desired degree of variability must always be considered in the calibration process.

Summary of Possible Abstractions

Most of the possible abstractions of simple models have been discussed above. Here we summarize these and give examples from previous TSPAs.

Dimensionality reduction and/or spatial-temporal averaging

A commonly used simplification in past TSPAs was to represent the SZ as 1-D. This simplification clearly ignores lateral dispersion. For TSPA-VA, the possibility of 2-D (or even 3-D) flow and transport should be considered. Regarding spatial temporal averaging, in past TSPAs the lateral domain was sometimes represented with several 1-D flow tubes.

Simplified process models

As described earlier, all models are abstractions of one degree or another. However, the term abstraction is often reserved for the simplest of these models. In TSPA-1995, the simple abstraction used for fracture/matrix interaction was the Markovian particle transition model incorporated in the RIP TSPA code (Golder, 1994). In this model, fracture/matrix flux is constant over the vertical extent of each hydrogeologic unit. Radionuclide particles from an upstream hydrogeologic unit are apportioned to the immediate downstream unit according to the constant (steady-state) fraction of the total liquid flux that is flowing in the fractures and matrix of that unit. Then as the particles traverse the unit, the interaction between the fractures and matrix is assumed to occur as a random Markov process, wherein a particle will randomly transition from one continuum to the other based on a Poisson distribution for the travel length. (The so-called lambda parameter is the inverse of the average travel length, or equivalently, the average rate of an exponential decay function.) This simple model of fracture/matrix interaction was not calibrated to a more "sophisticated" model such as DKM, but given the several free parameters in the DKM, it still may be a valid approach.

Response surfaces

As described above, response surfaces have been used frequently in TSPAs. TSPA-93 (Wilson et al., 1994) calculations involved development of a three-dimensional, site-scale flow model of the SZ that considered two alternative conceptual models of flow related to the large-hydraulic gradient, a fault-controlled model and a carbonate-aquifer-drain model. Five to eight one-dimensional flow tubes (corresponding to representative UZ flow and transport columns) were used in the abstraction of SZ behavior, with two classes of velocity and dispersivity distributions derived from the three-dimensional flow and transport modeling. This was accomplished by fitting 1-D advection/dispersion solutions to the results of the 3-D flow and transport modeling. Radionuclide concentrations at the downstream end of the flow tubes were calculated by assuming complete mixing across an area defined by the transverse dispersivity and a somewhat arbitrary range of mixing depth (10 to 500 m).

Summary

All of the above abstraction options have potential drawbacks. It might take too many model runs to develop an acceptable response surface (the discussion in Attachment B about the number of runs needed to determine the uncertainty caused by the key parameters applies as well to development of a response surface). In reducing the dimensionality we could miss important effects related to the dimension, such as lateral dispersion. And the danger of developing simple models to explore particular effects is that other important effects may be left out, such as coupling to other physical-chemical processes. Additional discussion of abstraction issues may be found in Chapter 3 of the TSPA-VA Plan (M&O, 1996).

Clearly, in the abstraction process there must be a balance between the complexity of the abstracted models and the number of times they can be run. A very complex model such as a 3-D SZ model with thermal effects can be used either directly or to generate response surfaces, but because of the limited number of runs possible, the uncertainty might not be represented well. A simpler model or a reduced-dimensionality version of the complex model can be run enough times to cover the range of uncertainty, but the flow might not be represented properly. Part of the abstraction process is to test or validate the abstractions to assure that they are acceptable. For example, if a reduction in dimension to 1-D is the abstraction method chosen, a selection of cases with a variety of input parameters must be run in both 1-D and 3-D to find out whether the predicted doses are acceptably similar.

In both the development and the testing of abstractions for TSPA-VA, performance assessment needs the support of site-characterization personnel and process modelers so that we can optimize their models in a realistic fashion for TSPA calculations.

Attachment D

Important Issues of SZ Flow and Transport

We have identified four issues with subtopics that we would like the SZ flow and transport workshop participants to think about. The issues are listed below as four major headings and the important issues that make up each heading. These issues will be addressed in the workshop in the form of proposal presentations and discussions as described in the main body of this letter. Workshop participants are requested to prepare statements (a minimum of one proposal) on how they feel the issues should be addressed and what they can contribute to addressing the issues. As a starting point, strawman proposals for each issue are included in Attachment G.

1. Conceptual Models of SZ Flow

   1.1 Alternative conceptual models (e.g., of the large hydraulic gradient)
   1.2 Hydraulic properties of faults
   1.3 Vertical flow
   1.4 Distribution of recharge
   1.5 Regional discharge

2. Conceptual Models of SZ Geology

   2.1 Flow channelization
   2.2 Spatial distribution of hydraulic conductivity
   2.3 Geologic and mineralogic framework

3. Transport Processes and Parameters

   3.1 Dispersivity
   3.2 Matrix diffusion (effective porosity)
   3.3 Sorption
   3.4 Colloid transport

4. Coupling to Other Components of TSPA

   4.1 Climate change
   4.2 Thermal and chemical plume
   4.3 Well withdrawal scenarios
   4.4 Coupling with UZ transport

Attachment E

Coupling of SZ Flow and Transport to Other Models Developed for TSPA-VA

The SZ flow and transport component of the TSPA calculations is intermediate between the UZ flow and transport component and the biosphere component of the analysis. The coupling of SZ flow and transport to other components is relatively straightforward because processes in the SZ are generally decoupled from the relevant processes in the other components, with some important exceptions. This is in contrast to some other components of the TSPA analysis (e.g., UZ flow and UZ thermohydrology), which may be intimately coupled.

The primary coupling between UZ flow and transport and the SZ simulations is through the radionuclide mass flux at the water table. The UZ component of the analysis provides a time-dependent radionuclide source term for the SZ transport calculations. This radionuclide source term for SZ transport calculations may also have significant spatial variability, depending on the type and resolution of the UZ transport component. There may also be significant coupling of flow between the UZ and SZ flow simulations, especially at higher infiltration rates. Past TSPA calculations have assumed that there is minimal impact on the local SZ flow system by infiltration through the UZ. However, recently reported estimates of infiltration at Yucca Mountain are relatively high and may require that local recharge to the SZ flow system be consistent with the values used in the UZ flow component of the analysis.

Simulations of the climate change must be consistent between the UZ flow and transport component of the analysis and the SZ flow and transport component. Obviously, the effects of climate change should be applied to both the UZ and SZ over the same time periods. In addition, the effects of climate change influence the coupling between UZ flow and transport and the SZ component by rise of the water table. A rise in the water table (estimates indicate 80 to 100 m) decreases the transport pathlength from the repository to the water table, may alter the flow system in the shallow SZ, and may provide a "slug" of radionuclides for transport in the SZ that were in transit in the UZ prior to the water table rise. If natural discharge areas from the SZ are considered in the TSPA analysis, water table rise due to climate change could affect the locations of these discharge areas and would thus influence the coupling between the SZ flow and transport component and the biosphere component of the analysis.

The coupling between the SZ component of the TSPA analysis and the biosphere model is through the concentration of radionuclides in the groundwater delivered to the biosphere. This coupling may be unidirectional if groundwater is supplied to the biosphere by low-discharge wells that have minimal impact on the ambient SZ flow system or by springs. If high-capacity wells are considered, however, dilution by pumping may have a significant impact on the simulated radionuclide concentrations passed to the biosphere component of the analysis.

Attachment F

Preparation Work for Workshop Participants

1) Read this memo carefully. (Look to the Strawman write-up for ideas and background)

2) Each participant is required to write a short proposal on at least one of the subtopics listed in Attachment D (or on an area that may have been omitted from Attachment D). Check to see if you have been selected for a pre-assigned topic (refer to Attachment I to see if your name is next to an issue). You may write additional proposals for any other areas of interest or concern as listed in the attachment.

3) Prepare the proposal write-up of the issue(s) for which you have been assigned or have a specific interest or have performed previous work and any other issue(s) that you would like to comment on.

   We require that all participants send a short write-up (approximately 1 page) on the issue(s) for discussion. These write-ups will be collected and compiled before the workshop and redistributed to all the workshop participants, also before the workshop. This will allow the workshop organizers to ascertain where the most discussion will be necessary and plan accordingly. It will also allow all of the workshop participants to come to the workshop thinking about the important issues and aware of the other participants' opinions.

   The proposal write-ups should follow this format: (1) list the issue from Attachment D (or identify a new issue) that you are to address, (2) provide a problem statement and a previous-work summary (what has been done by you or others in this area), (3) propose your future work and sensitivity analyses for feeding TSPA-VA needs, and (4) provide a format for how you feel your proposal and work can be incorporated by TSPA-VA (you may want to contact a TSPA representative before the workshop to clarify the tie-in of your work). We welcome comments from all of the workshop participants on any issue of their interest.

4) Send write-ups by **Monday, March 17, 1997**. Write-ups are to be emailed to **bwarnol@nwer.sandia.gov** or **jhgauth@nwer.sandia.gov**, preferably in ASCII format.

5) Prepare for the proposal presentations

   Presentations should be short. We have a lot to cover in a small amount of time. As a guideline keep your presentation to 5 minutes and no more than 3 viewgraphs. If you feel it is not possible to cover what is necessary in that amount of time call Bill Arnold at (505) 848-0894 or Jack Gauthier at (505) 848-0808 by March 14, 1997. As with the proposal write-ups, presentations might discuss your opinion of the strawman and what analysis ideas you can provide, what data are available, what your modeling experience or field observations have taught you, what information can be extracted from certain models, and how your work will tie into TSPA-VA needs.

6) Make travel arrangements to attend the workshop. **Please bring a laptop if you have one, or notify Bill Arnold or Jack Gauthier to obtain one or make prior arrangements before the meeting.**

Attachment G

Strawman Proposals for Addressing Important SZ-Flow and Transport Issues for TSPA-VA

As a mechanism to begin the discussion, and to get all participants started thinking about the issues involved in TSPA modeling of SZ flow and transport at Yucca Mountain, we present discussion and "strawman" proposals for the issues listed in Attachment D. The following represents current ideas in the TSPA group and how we would interpret SZ flow and transport issues without the benefit of the workshop discussions. Many of these interpretations remain to be translated into specific proposals for use in TSPA-VA. It is our expectation that such concrete proposals will result from the SZ flow and transport workshop.

1. Conceptual Models of SZ Flow

1.1 Alternative conceptual models

A key component of any conceptual model of SZ flow at the Yucca Mountain site is the cause of the large hydraulic gradient to the north of the potential repository. Because the large hydraulic gradient is located upgradient from the potential repository its presence may or may not be relevant to the performance of the repository. The results of TSPA-93 (Wilson et al., 1994) were not very sensitive to differences between two conceptual models of the large hydraulic gradient that were considered. It is difficult, however, for the project to argue that we have adequate understanding of processes in the SZ without considering plausible alternative conceptual models of this feature. It is also necessary to assess the impacts of possible stresses on the system (e.g., climate change and repository heat) to the durability of the large hydraulic gradient.

Models of SZ flow processes (e.g., discrete fracture vs. continuum) can be considered as alternative conceptual models of flow. The important consideration is actually the spatial scale (if any) at which the simplifying assumption of continuum behavior is valid.

1.2 Hydraulic properties of faults

Site-scale modeling of the SZ in some TSPA calculations (Wilson et al., 1994) has relied on inferences about the hydraulic conductivities of faults near the repository to produce calibrated flow models. Large changes in the magnitude of the hydraulic gradient of the SZ seem to be associated with some structural features, but the relationship between the faults and SZ flow is highly interpretive. Inverse groundwater flow modeling on the regional scale suggests that some NE/SW trending (higher permeability) and some NW/SE trending (lower permeability) fault zones are important to regional flow in the SZ (D'Agnese et al., 1996).

1.3 Vertical flow

Very little information is available on vertical hydraulic gradients in the SZ and possible vertical flow in the system. Data from well UE-25 p#1 indicates that there is a significant upward gradient from the Paleozoic carbonate aquifer to the volcanic tuff aquifer. Whether this represents a local feature of the flow system, or a more widespread confining unit between these aquifers, is unknown. Variations in temperature at the water table and geothermal flux indicate that there may be significant vertical flow in the SZ (Sass et al., 1988). Inferences on vertical flow from hydrochemical data may be useful in bounding the behavior of the system. The degree of interaction of flow in the vertical direction in the SZ has important implications for the amount of dilution by vertical dispersion.

1.4 Distribution of recharge

The distribution of recharge for regional-scale flow modeling has been derived from a modified Maxey-Eakin method (D'Agnese et al., 1996). This method predicts little or no recharge occurring at the repository area. However, recent estimates of infiltration at the Yucca Mountain site (Hudson and Flint, 1996) suggest that there may be significant recharge to the SZ in some areas at the site. The influence of possible recharge in the immediate vicinity has not been incorporated in previous site-scale SZ flow modeling.

1.5 Regional discharge

There is significant uncertainty regarding the ultimate discharge areas of flow in the SZ from the area beneath Yucca Mountain. Alternative modeling studies have indicated that the ultimate discharge point(s) for flow from the Yucca Mountain area may be Franklin Lake Playa or Death Valley (or a combination of both). It is possible that radionuclides transported to these discharge areas may interact with the biosphere by plant and animal uptake at springs or by wind erosion of playa surfaces containing precipitated radionuclides. Although the focus of TSPA-VA calculations will be on discharge of radionuclides from the SZ via pumping wells, it is still unclear whether the regional discharge area pathways must also be considered.

2. Characterization of the Model Domain

2.1 Flow channelization

The question of flow channelization in the SZ is significant at a number of scales and bears directly on our representation of dilution. All flow modeling of the SZ that has been performed to date has assumed continuum behavior of the medium. Well-test data suggest that this assumption is probably not valid for scales of less than, at least, 100's of meters.

The most important impact on the downgradient radionuclide concentrations in the SZ could come from flow channelization along larger-scale discrete structural features. Such features may or may not correspond to continuous, mappable structures at the surface, such as major faults. A likely candidate for such a flow-channelization feature would be zones of relatively continuous brecciation and tensile faulting, such as observed at the surface in the area of the south ramp of the ESF (Day et al., in review). If similar zones in the SZ provide continuous zones of enhanced hydraulic conductivity over scales of 1,000 m, channelization of flow and transport could be significant at the 5 km travel distance. Relatively rapid pressure response in well H-4 and ONC-1 to pumping in the C-well complex raises the likelihood of this possibility.

2.2 Spatial distribution of hydraulic conductivity

Additional data are clearly needed to fully characterize the distribution and variability of hydraulic conductivity in the SZ. The amount of dilution by dispersion is directly related to the spatial variability of hydraulic conductivity. Characterization of the distribution of hydraulic conductivity also has direct bearing on the validity of assumptions about the appropriate conceptual models of flow and transport processes (e.g., continuum vs. discrete flow and dual-porosity vs. effective porosity transport). The SZ flow modeling that has been performed to date relies on the assumption that hydraulic conductivity correlates well with hydrostratigraphic units; the limitations of this correlation should be further explored. Stochastic analyses using heterogeneous material properties, similar to those that have been used in UZ flow modeling (Arnold et al., 1995; Altman et al., 1996), could make use of available data on the spatial distribution of hydraulic conductivity to simulate a more realistic representation of variability of media in the SZ.

2.3 Geologic and mineralogic framework

Geologic framework models have been developed in support of YMP at the site scale (Zelinski and Clayton, 1996), the sub-regional scale (Czarnecki et al., 1996), and the regional scale (D'Agnese et al., 1996). The site-scale geologic framework model has substantially greater stratigraphic resolution (especially in the UZ at Yucca Mountain), but has much more restricted areal extent (and depth) than the sub-regional-scale model. An important question is the degree of consistency between these two models. Also of concern is the question of whether the sub-regional-scale geologic framework model has sufficient spatial resolution to accurately represent flow in the SZ to a nearby well (e.g., 5 km downgradient of the repository). In addition, a mineralogic framework model has been developed at the site-scale (Chipera et al., 1997), which is based on the units and geometry of the site-scale geologic model.

3. Transport Processes and Parameters

3.1 Dispersivity

Assuming that our conceptual model of continuum behavior is valid for the fractured media in the SZ and that we can apply a Fickian model of dispersion, there exists considerable uncertainty in parameter values for longitudinal and transverse dispersivity. Recent tracer test results from the C-well complex indicate effective longitudinal dispersivity of about 4 to 50 m for travel distances of 30 to 100 m. An analysis of theoretical macrodispersivity based on air permeability data from the TSw indicates an average value of about 14 m for the longitudinal dispersivity (Altman et al., 1996). Tracer test results from the Paleozoic carbonate aquifer yield an estimate of 15 m longitudinal dispersivity for a travel distance of about 120 m (Claassen and Cordes, 1975).

Field studies at numerous sites and theoretical considerations indicate that dispersivity is scale dependent and increases with travel distance. Synthesis of measurements of dispersivity over a large range of scales provides an "order of magnitude" estimate of the relationship between dispersivity and travel distance (Gelhar et al., 1985). Projecting the field scale measurements from the Yucca Mountain area to travel distances of 5 to 30 km indicates that the appropriate value of dispersivity for transport calculations is on the order of 100 to 500 m.

Of equal or greater importance to the maximum concentration simulated for SZ transport is the value of transverse dispersivity used. Little or no information is expected on transverse dispersivity from field tests. The "rule of thumb" often applied is that transverse dispersivity is approximately one tenth of the longitudinal dispersivity, although there are few data to support this assumption in fractured media.

3.2 Matrix diffusion (effective porosity)

Diffusion of solutes from fractures into the matrix of the volcanic aquifer is expected to be a process which contributes significantly to the effective retardation of radionuclide movement in the SZ. Numerical simulations indicate approximately complete diffusive exchange between fractures and matrix for travel times of greater than about 100 years using representative material properties (Robinson, 1994). In addition, recent tracer tests, using solutes of varying coefficients of dispersion, have demonstrated that matrix diffusion is operating, even on the relatively short time-scales of these tests.

The important consideration for TSPA-VA calculations is how to most appropriately and efficiently incorporate the process of matrix diffusion into the analysis. One approach is to explicitly simulate this process with a dual-porosity model, which may be computationally impossible for numerous Monte Carlo realizations of the system. Another approach is to use a single continuum model and a value of effective porosity. It is important to realize that the effective porosity concept would only be valid for certain length- and time-scales. The suggested abstraction approach for this issue is to perform sensitivity analyses using the dual-porosity conceptual model to substantiate or derive values of effective porosity for use in TSPA calculations.

3.3 Sorption

Sorption of radionuclides in the SZ may play an important role in retardation and the attenuation of peak concentration. Recent tracer test results at the C-wells and from laboratory studies suggest that sorption both in the matrix and on fracture surfaces (Triay et al., 1996) are significant and verifiable processes. Important questions include the spatial distribution of mineralogy conducive to sorption (see issue 2.3) and how to derive an effective sorption coefficient for use in a single continuum model of the flow system.

3.4 Colloid transport

Colloid facilitated transport has the potential to "bypass" processes (i.e., matrix diffusion and sorption) that retard the movement of radionuclides in the SZ. Colloids occur in the natural system and may serve as sorptive sites for radionuclides. In addition, colloids from degradation of the waste forms and repository materials may be introduced to the SZ if they remain in the infiltrating groundwater during passage through the UZ. Filtration of colloids may be a process which significantly attenuates radionuclide transport on colloids. Results from tracer experiments using microspheres at the C-well complex may be useful in quantifying the process of filtration.

Models for incorporating colloid movement into existing transport simulations using both a process-based formulation (Gauthier, 1995) and a simplified, effective formulation (Triay et al., 1996) have been proposed. The issue of colloid transport has been given relatively high priority by investigators in the UZ transport area. It is suggested that an approach similar to the one being developed for colloid transport in the UZ be used in SZ transport calculations.

4. Coupling to Other Components of TSPA

4.1 Climate change

The effects of wetter climatic conditions on the water table elevation beneath the repository have been largely inferred from isotopic data and from investigations of paleospring deposits. These inferences, as well as estimates of changes in SZ flow rates and patterns and changes in discharge areas, remain somewhat uncertain. These effects can probably be further substantiated by additional regional-scale flow modeling.

An additional impact of climate change could be the relatively sudden mobilization of radionuclides in transit between the lower water table and the pluvially induced higher water table. This effect could be incorporated into TSPA calculations by UZ transport modeling of the radionuclide fluxes at the present water table and at an elevation approximately 100 m above the present water table. The inventory of radionuclides between these two surfaces would be delivered to the SZ transport module in TSPA when climate change is simulated to occur.

4.2 Thermal and chemical plume

The possible effects of higher temperatures and chemical alterations of groundwater in the SZ due to the presence of the repository include transient changes to the SZ flow system and durable mineralogical changes to the medium. Preliminary modeling of the thermohydrologic effects to the SZ flow system indicate that temperature changes of >20°C at the water table may occur beneath and downgradient of the repository for up to 10,000 years (Ho et al., 1996). We have only limited data on the possible long-term effects of these alterations to the medium.

One effect of the thermal plume in the SZ flow system is that groundwater velocities are increased somewhat (by less than a factor of 2) in the region directly beneath the repository. It may be possible to incorporate this effect by using a small multiplication factor for groundwater velocity in the area beneath and downgradient of the repository. Alternatively, this effect may be considered unimportant relative to much larger uncertainties concerning the SZ flow system.

Independent scoping calculations or coupled thermal-chemical-hydrologic modeling are necessary to evaluate the impacts of chemical changes (e.g., dissolution-precipitation reactions) on the medium in the SZ. It may be possible to devote some resources at this time to these scoping evaluations, refer to them in TSPA-VA, and defer incorporation (if warranted) into the TSPA calculations to TSPA-LA.

4.3 Well withdrawal scenarios

The well withdrawal scenarios employed in TSPA provide a coupling between SZ flow and transport simulations and biosphere models, which are used to calculate radiological dose. The geographic placement of wells, depth of completion, and discharge rates in the models may have very large effects on the maximum simulated radionuclide concentrations delivered to the biosphere model. To a large extent, decisions regarding these scenarios are regulatory. However, because strict regulatory guidance is not available and because well withdrawal scenarios should be based on hydrologically plausible assumptions, members of the SZ workshop are being asked for some guidance on this issue.

The simplest scenario would be to assume a low-discharge well that would have minimal impact on the SZ flow system and to place the well in the area of the highest radionuclide concentration at some distance from the repository. Such a well could be simulated by simply recording the maximum concentration simulated at that location. This scenario would correspond to a domestic- or stock-well. Alternatively, a high-capacity well would need to be incorporated into the SZ flow and transport model because of the alterations it would produce in the flow system. This type of scenario more closely corresponds to pumping for municipal or irrigation purposes. An important consideration is that TSPA models should maintain the flexibility to incorporate guidance on well withdrawal scenarios from regulators when and if it becomes available.

4.4 Coupling with UZ transport

The radionuclide source term used in SZ transport simulations in TSPA is produced by the UZ transport model. Successful coupling of the SZ model to the UZ model depends on consistency between the simulations. One aspect of that consistency is the spatial resolution of the respective numerical models. The resolution of the grid in the SZ model at the water table below the repository should be at least as fine as that used in the UZ transport model. In addition, if there is a discrepancy in dimensionality of the UZ and SZ models (e.g., a 2-D profile model of the UZ and a 3-D SZ model), an approximation of the interface must be devised.

The most straightforward assumption concerning the coupling of transport in the UZ and the SZ is that radionuclides are delivered at the water table for SZ transport. This assumption of continuum behavior in the SZ is at odds with observations in numerous wells. The drilling record for well SD-12 shows that just below the water table at that location, little or no hydraulic communication exists between fractures over a vertical distance of 10's of meters. Radionuclides may be transported well below the water table before they are available for movement in the fracture network in the SZ. It may be more realistic to introduce the radionuclide flux from the UZ transport simulations over a range of depths below the water table in the SZ flow and transport modeling, if that flux is delivered by fracture flow in the UZ model.

Attachment H

Draft Agenda for the SZ Workshop

Tuesday, April 1, 1997

Overview Introduction	Bob Andrews	
Overview of workshop objectives	8:30 - 8:45	
Discussion of resources for the abstraction work between PA/Site/etc.		
Workshop Introduction	Bill Arnold, Susan Altman, Pat Tucci	
Goals of workshop		
Format of workshop	8:45 - 9:00	
Ground rules		
PA Perspective Introduction	Mike Wilson	
Explanation of past TSPA outlook	9:00 - 9:45	
TSPA plans for the future		
Questions that TSPA needs answered before TSPA-VA		
NRC Concerns		
Break	9:45 - 10:00	
Review the important issues to SZ Flow and Transport	Bill Arnold	
Introduce the 4 major issues	10:00 - 10:15	
Presentation and review of proposals for major issue 1	10:15 - 12:15	
TSPA perspective of the major issue		
Proposal presentations by participants		
Small group (4 groups) review of proposals and prioritize points		
Lunch	12:15 - 1:15	
Presentation and review of proposals for major issue 2	1:15 - 2:45	
TSPA perspective of the major issue		
Proposal presentations by participants		
Small group (4 groups) review of proposals and prioritize points		
Break	2:45 - 3:00	
Presentation and review of proposals for major issue 3	3:00 - 5:00	
TSPA perspective of the major issue		
Proposal presentations by participants		
Small group (4 groups) review of proposals and prioritize points		

Wednesday, April 2, 1997

Presentation and review of proposals for major issue 4 TSPA perspective of the major issue Proposal presentations by participants Small group (4 groups) review of proposals and prioritize points	8:00 - 10:00
Break	10:00 - 10:15
Prioritization of all sub-issues across all major issue categories Establishment of major proposal categories Assignment of participants to proposal teams	10:15 - 12:00
Lunch	12:00 - 1:15
Summary of existing workscopes	Pat Tucci and Bruce Robinson 1:15 - 1:45
Proposal teams brainstorming on abstraction/testing proposals	1:45 - 3:15
Break	3:15 - 3:30
Presentations of preliminary proposals to all participants Feedback on preliminary proposals from all participants and readjustment of proposals	3:30 - 5:00

Thursday, April 3, 1997

Proposal teams produce written abstraction/testing proposals	8:00 - 11:15
Summary of work to be done after the Workshop and closing remarks Comments from observers	11:15 - 12:00
Lunch	12:00 - 1:00
Core teams wrap-up	1:00 - 5:00

Attachment I
Required Proposals by Workshop Participants

Table 1: Proposal Areas and Participant Responsibilities

Major Issue	Sub-issue		
1. Conceptual Models of SZ Flow	(1.1) Alternative conceptual models	George Barr John Czarnecki George Zyvoloski	
	(1.2) Hydraulic properties of faults	George Barr Ardyth Simmons	
	(1.3) Vertical flow	Andrew Cohen Zell Peterman	
	(1.4) Distribution of recharge	Frank D'Agnese Pat Tucci	
	(1.5) Regional discharge	John Czarnecki Frank D'Agnese	
2. Conceptual Models of SZ Geology	(2.1) Flow channelization	Chris Potter Bill Arnold	
	(2.2) Spatial distribution of hydraulic conductivity	Sean McKenna M.J. Umari	
	(2.3) Geologic and mineralogic framework	Chris Rautman Dave Vaniman	
3. Transport Processes and Parameters	(3.1) Dispersivity	Bruce Robinson Chunhong Li	
	(3.2) Matrix diffusion (effective porosity)	Bruce Robinson Jake Turin	
	(3.3) Sorption	Inez Triay Mike Wilson	
	(3.4) Colloid transport	Arend Meijer Jerry McNeish	
4. Coupling to Other Components of TSPA	(4.1) Climate change	Frank D'Agnese Jack Gauthier	
	(4.2) Thermal and chemical plume	George Barr	
	(4.3) Well withdrawal scenarios	Bill Arnold Tony Smith	
	(4.4) Coupling with UZ transport	Ed Kwicklis Dave Sevougian	

Attachment J

References

Altman, S.J., B.W. Arnold, C.K. Ho, S.A. McKenna, R.W. Barnard, G.E. Barr, and R.R. Eaton. 1996. *Flow Calculations for Yucca Mountain Groundwater Travel Time (GWTT-95)*, SAND96-0819. Albuquerque, NM: Sandia National Laboratories.

Arnold, B.W., S.J. Altman, T.H. Robey, R.W. Barnard, and T.J. Brown. 1995. *Unsaturated-Zone Fast-Path Flow Calculations for Yucca Mountain Groundwater Travel Time Analyses (GWTT-94)*. SAND95-0857. Albuquerque, NM: Sandia National Laboratories. 169 p.

Claassen H.C. and E.H. Cordes. 1975. "Two-well recirculating tracer test in fractured carbonate rock, Nevada." *Hydrologic Sciences Bulletin*, v. 20, no. 3, 367-382.

Czarnecki, J.B, Faunt, C.C., Gable, C.W., and Zyvoloski, G.A. 1996. "On the development of a three-dimensional finite-element ground-water flow model of the saturated zone, Yucca Mountain, Nevada": Colorado School of Mines, Poster Papers, ModelCARE 96, International Conference on Calibration and Reliability in Groundwater Modeling, Colorado School of Mines, Golden, Colorado, USA, September 24-26, 1996, pp. 51-59.

D'Agnese, F.A., C.C. Faunt, A.K. Turner, and M.C. Hill. 1996. *Hydrogeologic Evaluation and Numerical Simulation of the Death Valley Regional Ground-Water Flow System, Nevada and California, Using Geoscientific Information Systems*. Water-Resources Investigation Report 96-xxxx (in review). Denver, CO: U.S. Geological Survey.

Day, W.C., C.J. Potter, D.S. Sweetkind, R.P. Dickerson, and C.A. San Juan. (in review). Bedrock Geologic Map of the Central Block Area, Yucca Mountain, Nevada. Miscellaneous Investigations Series MI-xxxx. Denver, CO: U.S. Geological Survey.

Gauthier, J.H. 1995. "Proposed models of colloid-facilitated transport for total-system performance assessment," *Proceedings of the Sixth Annual International Conference on High-Level Radioactive Waste Management, Las Vegas, Nevada, April 30-May 5, 1995*. La Grange Park, IL: American Nuclear Society.

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*. EPRI EA-4190 Project 2485-5. Palo Alto, CA: Electric Power Research Institute. 116 p.

Golder Associates, Inc. 1994. RIP Performance Assessment and Strategy Evaluation Model: Theory Manual and User's Guide, Version 3.20, Redmond, WA: Golder Associates.

Ho, C.K., N.D. Francis, B.W. Arnold, Y. Xiang, S.A. McKenna, S. Mishra, G.E. Barr, S.J. Altman, X.H. Yang and R.R. Eaton. 1996. *Thermo-Hydrologic Modeling of the Potential Repository at Yucca Mountain Including the Effects of Heterogeneities and Alternative Conceptual Models of Fractured Porous Media*, Sandia National Laboratories Milestone Report T6536.

Hudson, D.B. and A.L. Flint. 1996. *Estimation of Shallow Infiltration and Presence of Potential Fast Pathways for Shallow Infiltration in the Yucca Mountain Area, Nevada*, U.S. Department of Energy Technical Report, TIS#960242.

M&O, 1995. *Total Systems Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository*, B00000000-01717-2200-00136, Rev. 01, TRW Environmental Safety Systems, Las Vegas, NV.

M&O. 1996. *Total System Performance Assessment - Viability Assessment (TSPA-VA) Plan*. Civilian Radioactive Waste Management System, Management and Operating Contractor Report B00000000-01717-2200-00179, TRW Environmental Safety Systems, Las Vegas, NV.

National Research Council, 1995. *Technical Bases for Yucca Mountain Standards*, National Academy Press, Washington, DC.

Robinson, B.A. 1994. "A Strategy for Validating a Conceptual Model for Radionuclide Migration in the Saturated Zone Beneath Yucca Mountain," *Radioactive Waste Management and Environmental Restoration*. Vol. 19, no. 1-3, 73-96.

Sass, J.H., A.H. Lachenbruch, W.W. Dudley, Jr., S.S. Priest, and R.J. Munroe. 1988. *Temperature and Thermal Conductivity, and Heat Flow Near Yucca Mountain, Nevada: Some Tectonic and Hydrologic Implications*. U.S. Geological Survey Open-File Report 87-649. Denver, CO: U.S. Geological Survey.

Triay, I.R., A. Meijer, J.L. Conca, K.S. Kung, R.S. Rundberg, and E.A. Strietelmeier. 1996. *Summary and Synthesis Report on Radionuclide Retardation for the Yucca Mountain Site Characterization Project*. Milestone 3784. Los Alamos, NM: Los Alamos National Laboratory.

Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, 1994. *Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993)*. SAND93-2675. Albuquerque, NM: Sandia National Laboratories.

Zelinski, W.P. and R.W. Clayton. 1996. *A 3D Geologic Framework and Integrated Site Model of Yucca Mountain: Version ISM1.0*. Civilian Radioactive Waste Management System, Management and Operating Contractor Report B00000000-01717-5700-00002.

Attachment K

Conference Facilities and Hotel Information

WORKSHOP LOGISTICS

The workshop will be held in Lecture Halls A&B, Building 25, at the Denver Federal Center. A map of the Federal Center is attached. You will need a picture ID to enter the Federal Center - a driver's license or Government ID will work.

A block of rooms has been reserved at the Sheraton Denver West Hotel, 360 Union Blvd, Lakewood, CO 80228, (303) 987-2000. The room rate for the workshop is for the government per diem rate of $92, including tax. Workshop attendees should make their own reservations at the hotel by March 17, when the rooms will be released. Tell them it's for the U.S. Geological Survey/Yucca Mtn. Project. If you have any problems making reservations, call Pat Tucci (USGS, Denver) at 303-236-5050, x.230.

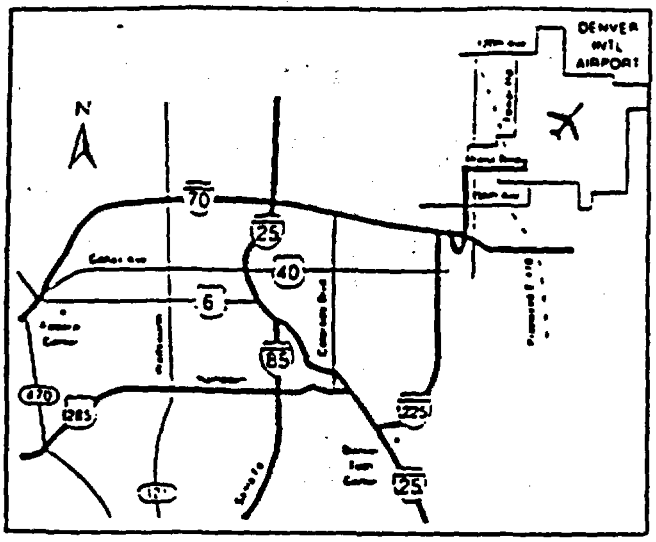
The hotel is just outside of the Federal Center, about 1/2 mile from Bldg. 25 (see attached map). You can get to the hotel by using Golden West Shuttle ($30 round trip) or by an approximate 45-60 minute drive from the airport. A flyer is attached with directions from the airport and with information on the shuttle. The hotel also has a van that will bring you into the Federal Center in the morning. If the weather's good, which it often is in Denver, it's not a bad walk from the hotel to Bldg. 25 (you'll still need to show your ID to the guard at the gate).

There are plenty of restaurants nearby, and a list of suggested places to eat will be provided at the workshop. We're trying to arrange for coffee and bagels at the workshop room in the mornings, and there is a cafeteria with a limited menu in Building 25. Another cafeteria, with a more extensive menu, is in Building 41.

There is one phone in the meeting room, and a pay phone in the lobby. There are no facilities in Building 25 for receiving messages. Messages may be left with the USGS office in Building 53 (303-236-5050, x. 222), and someone will deliver accumulated messages to Building 25 a couple of times a day (just before lunch and late in the afternoon).

More information concerning workshop logistics will be available at the workshop. If you have any questions concerning logistics, call Pat Tucci.

Airport Information



Directions from DIA Airport

I-70 west to I-25 south. From I-25, exit 6th Avenue westbound to the Simms St./Union ~~St.~~ Blvd. Exit. Turn left at the exit. Hotel is on the left after a couple of traffic lights.

Airport Transportation

Golden West Shuttle - Now Open 24 Hours - (303) 342-9300
Rate: $30 round trip

- Advance Reservations Required
- Airport Counter is located on level 5 near Info Booth in the center of the Main Terminal

Schedule

MONDAY - FRIDAY
TO DIA 4:30 a.m - Early Bird Special
Regular service every 30 minutes from 6:00 a.m. until 11:00 p.m
FROM DIA:
Every 30 minutes from 7.30 a m until 11:00 p m

SATURDAY
TO DIA Every hour from 5:00 a m until 9:00 p m
FROM DIA Every hour from 8.00 a.m until 11.00 p.m.

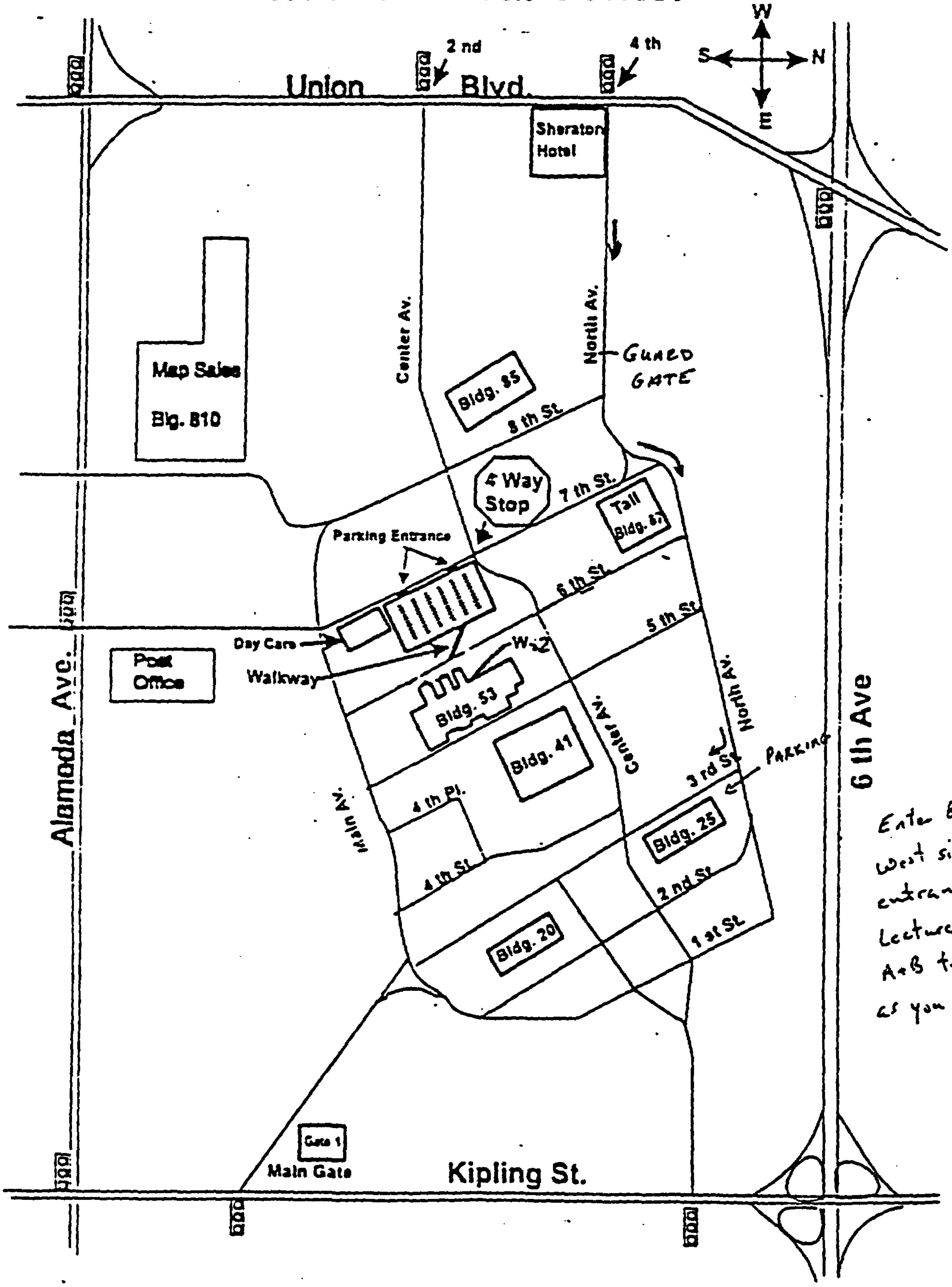
SUNDAY
TO DIA
Every hour from 5:00 a.m. until 3:00 p.m.
Then every 30 minutes until 11:00 p.m.
FROM DIA:
Every hour from 8:00 a.m. until 3:00 p.m.
Then every 30 minutes until 11:00 p.m.

HOLIDAYS
Call for Holiday Schedule

Shuttle service is scheduled after hours upon request

Please allow a minimum of 1 hour for travel time

Denver Federal Center



Enter Bldg 25 on west side main entrance. Lecture Halls A+B to the left as you come in.

Attachment L

Schedule of Other Abstraction/Testing Workshops

Workshop Subject	Date
Unsaturated Zone Flow	December 11-13, 1996
Waste Package Degradation	January 8-10, 1997
Thermo-Hydrology	January 21-23, 1997
Unsaturated Zone Radionuclide Transport	February 5-7, 1997
Waste-Form Degradation and Mobilization	February 18-21, 1997
Near Field Environment	March 4-6, 1997
Criticality	March 18-20, 1997
Saturated Zone Flow and Transport	April 1-3, 1997
National Environmental Protection Act (NEPA)	May 6-8, 1997
Biosphere	June 3-5, 1997

Appendix B

PRE-WORKSHOP MEMO TO THE PARTICIPANTS

Sandia National Laboratories

Albuquerque, New Mexico 87185-1326

WBS 1.2.5.4.4
QA:NA

date: March 21, 1997

to: Distribution

BWA

from: Bill W. Arnold; Jack H. Gauthier; Pat Tucci; Bruce A. Robinson

subject: TSPA-VA Saturated Zone Flow and Transport Abstraction/Testing Workshop

This purpose of this memo is to assist participants in the Saturated Zone (SZ) Flow and Transport Workshop with their preparation for this workshop. As a reminder, this workshop is sponsored by the Total Systems Performance Assessments (TSPA) group with the Yucca Mountain Project, was described in detail in a memo dated 3/10/97, and is scheduled to be held at the **Denver Federal Center April 1 to 3, 1997**. This memo contains instructions for preparing presentations for participants (Attachment A), a list of assigned presentations on the issues (Attachment B), a revised agenda for the workshop (Attachment C), and the participant proposals and issue write-ups (Attachment D) provided in response to the SZ Workshop invitation memo.

Please call us or contact us by e-mail if you have any questions or suggestions concerning the SZ Workshop or your role in it (Bill Arnold, tel. (505) 848-0894, e-mail: **bwarnol@nwer.sandia.gov** and Jack Gauthier, tel. (505) 848-0808, e-mail: **jhgauth@nwer.sandia.gov**.

We want to remind all participants and observers that a **picture ID is required for entry to the Denver Federal Center**. During the workshop, messages can be left for attendees with the secretary at 303-236-5050 ext. 222; Fax messages can be phoned to 303-236-5050. These messages and Fax messages will be received at a separate location at the Federal Center and will be delivered to the workshop approximately twice daily.

List of Attachments:

Attachment A:	Instructions for Preparing Presentations
Attachment B:	List of Presentations
Attachment C:	Revised Agenda for the SZ Workshop
Attachment D:	Participant Proposals and Issue Write-ups

Schedule of Workshop:

Tuesday, April 1, 1997	Day 1 of Workshop (all day)	8:30 am - 5:00 pm
Wednesday, April 2, 1997	Day 2 of Workshop (all day)	8:00 am - 5:00 pm
Thursday, April 3, 1997	Day 3 of Workshop (all day)	8:00 am - 12:00 pm
Thursday, April 3, 1997	Core Team Wrap-up Meeting	12:00 pm - 5:00 pm

List Of Participants:

SZ Core Team:

Bill Arnold	SNL
Jack Gauthier	SNL
Bruce Robinson	LANL
Pat Tucci	USGS

TSPA Core Team:

Bob Andrews	INTERA
Holly Dockery	SNL
Jack Gauthier	SNL
Jerry McNeish	INTERA
Dave Sevougian	INTERA
Mike Wilson	SNL

Other Participants:

George Barr	SNL
Andrew Cohen	LBNL
John Czarnecki	USGS
Frank D'Agnese	USGS
Ed Kwicklis	USGS
Chunhong Li	INTERA
Sean McKenna	SNL
Arend Meijer	LANL
Zell Peterman	USGS
Chris Potter	USGS
Chris Rautman	SNL
Jake Turin	LANL
Ardyth Simmons	LBNL
Tony Smith	INTERA
Inez Triay	LANL
M. J. Umari	USGS
Vinod Vallikat	INTERA
Dave Vaniman	LANL
George Zyvoloski	LANL

Facilitator:

Susan Altman	SNL

List of Observers:

Larry Rickertsen	TRW
Abe Van Luik	DOE
Eric Smistad	DOE
Russ Patterson	DOE
Dwight Hoxie	USGS
Mike Chornack	USGS
Cynthia Miller-Corbett	USGS
Leon Reiter	NWTRB Representative
Victor Palciauskas	NWTRB Representative
Richard Parizek	NWTRB Representative
Jim Duguid	INTERA
Alva Parsons	SNL
Gilles Bussod	LANL
Rod Ewing	PA Peer Review Panel
Chris Wipple	PA Peer Review Panel
NRC Representative	
EIS/NEPA Representative	

Distribution:

MS1326	B.W. Arnold, 6851
MS1326	S.J. Altman, 6851
MS1326	G.E. Barr, 6851
MS1326	H.A. Dockery, 6851
MS1326	J.H. Gauthier, 6851
MS1326	M.L. Wilson, 6851
MS1326	C. Li, (INTERA)
MS1324	S.A. McKenna, 6115
MS1324	C.A. Rautman, 6115
	B.A. Robinson (LANL)
	P. Tucci (USGS/Denver)
	R.W. Andrews (INTERA/Las Vegas)
	J.A. McNeish (INTERA/Las Vegas)
	D. Sevougian (INTERA/Las Vegas)
	V. Vallikat (INTERA/Las Vegas)
	J. Duguid (INTERA)
	A. Cohen (LBNL)
	A. Simmons (LBNL)
	J.B. Czarnecki (USGS/Denver)

F. D'Agnese (USGS/Denver)
C. Faunt (USGS/Denver)
Z. Peterman (USGS/Denver)
C. Potter (USGS/Denver)
M.J. Umari (USGS/Denver)
C. Miller-Corbett (USGS/Denver)
W.W. Dudley (USGS/Denver)
A. Meijer (LANL)
P.W. Reimus (LANL)
H.J. Turin (LANL)
G.A. Zyvoloski (LANL)

cc:

MS1326	R.W. Barnard, 6851
MS1324	P.B. Davies, 6115
MS1399	M.C. Brady, 6314
MS1395	L.E. Shephard, 6800
MS0734	A.M. Parsons, 6472
MS1328	A.R. Schenker, 6849
	L.D. Rickertsen, M&O/TRW
	J. L. Younker, M&O/TRW
	L.R. Hayes, M&O/TRW
	A.E. Van Luik, DOE
	E.T. Smistad, DOE
	R.L. Patterson, DOE
	W.J. Boyle, DOE
	S.J. Brocoum, DOE
	S.H. Hanauer, DOE
	D.T. Hoxie, USGS
	R.W. Craig, USGS
	J.A. Canepa, LANL
	G.S. Bodvarsson, LBNL
	Y. Tsang, LBNL
	L. Reiter (NWTRB)
	V. Palciauskas (NWTRB)
	R. Parizek (Penn. State University)
	J. Duguid (INTERA)
	R. Ewing
	C. Wipple
	P. Witherspoon

YMP:1.2.5.4.4:PA:NQ/WA-0335
YMP CRF

Attachment A

Instructions for Preparing Presentations

The guidelines listed below are intended to facilitate the functioning and documentation of the SZ Flow and Transport workshop. There is a relatively long list of speakers (see Attachment B) and only a short amount of time available for each presentation. Experience at previous workshops has shown the value of "standardizing" the documentation of these presentations.

1a. **Proposal and Issue presentations are to be 5 minutes in length.** Please limit your number of viewgraphs to 3 (2 for the technical issues presentation and 1 as a title page). The title page should include the following:

- (i) your presentation title
- (ii) the "major issue" and "sub-issue" addressed in your presentation (e.g., "3. Transport Processes and Parameters", "3.1 Dispersivity")
- (iii) your name
- (iv) your affiliation
- (v) the date of your presentation

1b. **TSPA presentations are to be 10 minutes in length.** Please limit your number of viewgraphs to 6 (5 for the technical issues presentation and 1 as a title page). The title page should include the following:

- (i) your presentation title
- (ii) the "major issue" addressed in your presentation (e.g., "3. Transport Processes and Parameters")
- (iii) your name
- (iv) your affiliation
- (v) the date of your presentation
- (vi) clearly indicate that it is a TSPA presentation

2. **All speakers should bring 50 copies of their viewgraphs.** The photocopies should be stapled and already have three-hole punch holes. These copies should be given to the workshop facilitator (Susan Altman) before the presentations begin in each major issue category so they can be distributed to everyone at the meeting before the talks begin. **Please note that we will not have the time or clerical resources necessary to make photocopies at the workshop. Please come to the meeting prepared.**

Attachment B

List of Presentations

Major Issue Category 1: Conceptual Models of SZ Flow

John Czarnecki	1.1	Alternative conceptual models
Bill Dudley	1.1	Alternative conceptual models
George Barr	1.2	Hydraulic properties of faults
Andrew Cohen	1.3	Vertical flow
Frank D'Agnese	1.4	Distribution of recharge
Pat Tucci	1.4	Distribution of recharge
John Czarnecki	1.5	Regional discharge
Frank D'Agnese	1.5	Regional discharge
George Zyvoloski	1.6	Grid sensitivity

Major Issue Category 2: Conceptual Models of SZ Geology

Chris Potter	2.1	Flow channelization
Bill Arnold	2.1	Flow channelization
Dave Vaniman	2.1	Flow channelization
Sean McKenna	2.2	Spatial distribution of hydraulic conductivity
M.J. Umari	2.2	Spatial distribution of hydraulic conductivity
Dave Vaniman	2.3	Geologic and mineralogic framework
Chris Rautman	2.3	Geologic and mineralogic framework

Major Issue Category 3: Transport Processes and Parameters

Bruce Robinson	3.1	Dispersivity
Chunhong Li	3.1	Dispersivity
Mike Wilson	3.1	Dispersivity
Jake Turin	3.2	Matrix diffusion (effective porosity)
Bruce Robinson	3.2	Matrix diffusion (effective porosity)
Ines Triay	3.3	Sorption
Jake Turin	3.3	Sorption
Jake Turin	3.4	Colloid transport

Major Issue Category 4: Coupling to Other Components of TSPA

Frank D'Agnese	4.1	Climate change
George Barr	4.2	Thermal and chemical plume
Bill Arnold	4.2	Thermal and chemical plume
Bill Arnold	4.3	Well withdrawal scenarios
Jerry McNeish	4.3	Well withdrawal scenarios
Bruce Robinson	4.4	Coupling with UZ transport
Ed Kwicklis	4.4	Coupling with UZ transport

Attachment C

Revised Agenda for the SZ Workshop

Tuesday, April 1, 1997

Participant and Observer Introductions	Susan Altman, Pat Tucci	
Site logistics		8:30 - 8:40
Overview Introduction	Bob Andrews	
Overview of workshop objectives		8:40 - 8:55
Discussion of resources for the abstraction work between PA/Site/etc.		
Workshop Introduction	Bill Arnold, Susan Altman	
Goals of workshop		8:55 - 9:10
Format of workshop		
Ground rules		
PA Perspective Introduction	Jack Gauthier	
Explanation of past TSPA outlook		9:10 - 9:45
TSPA plans for the future		
Questions that TSPA needs answered before TSPA-VA		
NRC Concerns		
Break		9:45 - 10:00
Review the important issues to SZ Flow and Transport	Bill Arnold	
Introduce the 4 major issues		10:00 - 10:15
Presentation and review of proposals for major issue 1		10:15 - 12:15
TSPA perspective of the major issue		
Proposal presentations by participants		
Small group (4 groups) review of proposals and prioritize points		
Lunch		12:15 - 1:15
Presentation and review of proposals for major issue 2		1:15 - 2:45
TSPA perspective of the major issue		
Proposal presentations by participants		
Small group (4 groups) review of proposals and prioritize points		
Break		2:45 - 3:00
Presentation and review of proposals for major issue 3		3:00 - 5:00
TSPA perspective of the major issue		

Proposal presentations by participants
Small group (4 groups) review of proposals and prioritize points

Wednesday, April 2, 1997

Presentation and review of proposals for major issue 4 TSPA perspective of the major issue Proposal presentations by participants Small group (4 groups) review of proposals and prioritize points	8:00 - 10:00
Break	10:00 - 10:15
Prioritization of all sub-issues across all major issue categories Establishment of major proposal categories Assignment of participants to proposal teams	10:15 - 12:00
Lunch	12:00 - 1:15
Summary of UZ flow and transport proposals	Susan Altman and Bruce Robinson 1:15 - 1:40
Summary of existing SZ workscopes	Pat Tucci and Bruce Robinson 1:40 - 2:00
Proposal teams brainstorming on abstraction/testing proposals	2:00 - 3:15
Break	3:15 - 3:30
Presentations of preliminary proposals to all participants Feedback on preliminary proposals from all participants and readjustment of proposals	3:30 - 5:00

Thursday, April 3, 1997

Proposal teams produce written abstraction/testing proposals	8:00 - 10:30
Team presentations of final draft proposals	10:30 - 11:15
Summary of work to be done after the Workshop and closing remarks Comments from observers	11:15 - 12:00
Lunch	12:00 - 1:00
Core teams wrap-up	1:00 - 5:00

Attachment D

Participant Proposals and Issue Write-ups

1. Conceptual Models of SZ Flow

1.1 Alternative conceptual models

John Czarnecki, USGS

Large Hydraulic Gradient:

Several possible mechanisms can be invoked to characterize the cause of the approximately 300 m change in hydraulic head over a distance of approximately 2 km north of Yucca Mountain. These mechanisms include but are not limited to: (1) faults that contain nontransmissive fault gouge or that juxtapose transmissive tuff against nontransmissive tuff; (2) the presence of a different type of lithology that is less subject to fracturing; (3) a change in the direction of the regional stress field and a resultant change in the intensity, interconnectedness, and orientation of open fractures on either side of the area with the large hydraulic gradient; (4) an apparent large gradient resulting from a disconnected, perched or semi-perched water body; or (5) a highly permeable buried fault that drains water from tuff units into a deeper regional carbonate aquifer. Modeling of case 1 was essentially done in the model of Czarnecki (1985), which was extended to examine the removal of the barrier to flow resulting from an inferred tectonic event which increased the transmissivity 1.5 orders of magnitude. The results for these transient analyses (never published) were: (1) a maximum water table rise beneath the potential repository block on the order of only 40 meters; (2) a dramatic increase (~order of magnitude) in downgradient flux, decades after the actual event; (3) a direct link between the timing of the water table rise and the porosity used in the simulation; (4) the magnitude of the water table rise was independent of the porosity value used; and (5) a net decrease in the water table altitude in the vicinity of the design repository long after the abrupt increase in transmissivity. A further extension of the modeling was begun to examine the system with an abrupt increase in hydraulic conductivity coupled with an increased recharge resulting from wetter climatic conditions, but had to be terminated. Increased recharge simulation produced a water table rise of about 130 meters (Czarnecki, 1985) for what was considered to be the maximum probable increase in recharge. It would seem that this combination would have the greatest likelihood for inundation of the potential repository, although the likelihood of these two mechanisms even occurring is unknown.

A closer examination of conditions in borehole USW G-2 (Czarnecki and others, 1993, 1994) resulted in the advancement of possible perched water conditions to explain the large hydraulic gradient. Evidence for this condition is supported by: (1) a 12 m decline in the water level in G-2 over its hole history; (2) water wet borehole walls and observed dripping water in the air filled part of the borehole above the basal vitrophyre of the

Topopah Spring member, the same; (3) a decrease in the thermal gradient in the borehole with time; (4) observed downward flow in the water-filled part of the borehole from pulsed-heat flow surveying; (5) a moderate hydraulic conductivity in the Calico Hills Formation; (6) a less-than-full recovery (0.5 m) of the water level following hydraulic testing; and (7) apparent partial saturation within the Calico Hills formation based on analyses of borehole geophysical logs, with a coincidental return to full saturation at an altitude of ~730 m (top of the Crater Flat tuff).

Borehole UZ-14 may be a good analog to conditions in USW G-2 had the latter been cased off when initial water production occurred. In the case of UZ-14, so called 'perched water' was encountered above the basal vitrophyre of the Topopah Spring member. This zone was cased off so that coring could commence without affecting the ambient condition of the core which would be affected by cascading water. Drilling through what should have been the saturated zone resulted in no water production until an altitude of about 630 meters, at which depth a water-filled fracture with the Bullfrog Member of the Crater Flat tuff transmitted water into the borehole The apparent saturation based on laboratory determinations from cuttings/core between the apparent perched water body and the bottom of the hole in UZ-14 showed at or near 100% saturation, in contrast to the geophysically derived saturation values for USW G-2. One possible explanation is that the so-called 'perched water' in borehole UZ-14 actually represents the beginning of the saturated zone. If correct, the apparent large hydraulic gradient would be 0.8 versus 0.15.

A comparison between geophysically derived saturation values and those derived from laboratory analyses should be done. These data exist for borehole UZ-14, although laboratory saturation determinations stopped when a hold was placed on cuttings/core from UZ-14. In addition, no water chemistry exist for the extant water in borehole UZ-14, a necessary comparative data point to those for the 'perched water' samples.

For USW G-2, a full test plan had been developed which is only minimally completed. G-2 needs to be reconfigured so that hydraulic testing and hydraulic head monitoring can be done in the Crater Flat tuffs.

The drillpad for borehole WT-24 was constructed between UZ-14 and USW G-2, but drilling never commenced. Construction and testing of this hole if done carefully and with sufficient depth will identify possible perched water occurrence and the mechanism behind the cause of the large hydraulic gradient.

Several conceptual models are being considered in the site saturated-zone model, among which is that of a perched, separate flow system to explain the conditions in USW G-2, WT-6, and UZ-14.

References:

Czarnecki, J. B., 1985, Simulated effects of increased recharge on the ground-water flow system of Yucca Mountain and vicinity, Nevada-California: U.S. Geological Survey

Water-Resources Investigations Report 84-4344, 33 p.

Czarnecki, J.B., O'Brien, G.M., Nelson, P.H., Sass, J.H., Nelson, P.H., Bullard, J.W., and Flint, A.L., 1994, Is there perched water under Yucca Mountain in borehole USW G-2?: Trans. American Geophysical Union, EOS, vol. 75, no. 44, pp. 249-250.

Czarnecki, J.B., Nelson, P.H., O'Brien, G.M., Sass, J.H., Thapa, Bhaskar, Matsumoto, Yoshitaka, and Murakami, Osamu, 1995, Testing in borehole USW G-2 at Yucca Mountain: The saga continues: Trans. American Geophysical Union, EOS, vol. 76, no. 7, p. F190.

1.2 Hydraulic properties of faults
Bill Arnold, SNL

No direct measurements of the hydraulic properties of faults in the SZ have been made at the Yucca Mountain site. As stated in the strawman proposal, inferences concerning the permeabilities of individual faults have been based on the spatial coincidence of faults with large changes in the hydraulic gradient and on regional flow modeling results. In this sense, the inclusion of faults as low permeability barriers to flow is one of several possible alternative conceptual models of the flow system. A more important question, from the perspective of repository performance may be the hydraulic properties of faults in the region downgradient of the repository. Although the faults in the low hydraulic-gradient region to the south and east of the potential repository do not show any dramatic impact on the potentiometric surface, this may be due to their location in a region of low gradient. The entire low gradient area may be hydaulically controlled by features exterior to the area. This would tend to mask the effects of individual faults within the low gradient area, even if their hydraulic properties were significantly different from the surrounding medium.

In the absence of information on the hydraulic properties of individual faults, properties of these features could be added to flow models in a stochastic manner. A conceptual model of the possible range of fault permeabilities would have to be developed and could be related to fault orientation. A stochastic representation of fault properties overlaps with the question of flow channelization and the spatial distribution of hydraulic conductivity at smaller scales. It may be possible to develop a single stochastic description of the medium in the SZ at all of these scales simultaneously.

1.3 Vertical flow
Andrew Cohen, LBNL

Problem Statement:

Numerical simulations show that the presence of faults can produce upward and downward fluid flow near and at faults, regardless of fault zone properties. Therefore, the effect of faults in general may be to enhance vertical dispersion. This phenomenon must be more fully understood and its effects quantified in order to properly predict downgradient mixing.

Previous Work Summary:

A cross-sectional model based on the geologic structure of the saturated zone was developed in 1996 to investigate the effect of faults, geothermal heating, and variation of hydrologic properties on flow geometry (Cohen, A., Najita, J, Karasaki, K., and A. Simmons, Conceptual model development of saturated zone flow in the vicinity of C-holes, Yucca Mountain, Nevada, Milestone #OBO3M, E.O. Lawrence Berkeley National Laboratory, 1996, 89 pp.). Simulations showed that significant vertical flow in the upward and downward directions can occur near and at faults, regardless of fault zone hydrologic properties. Fault zones with significant permeability compared to the surrounding units act as flow pathways through which fluids can migrate from lower to higher units or vice-versa. In addition, faults that simply offset units, and that do not possess internal permeability, also produce vertical flow between formations. A fluid parcel may move downward or upward for distances on the order of the fault displacement or more. Furthermore, these vertical flows occur without imposing vertical pressure gradient boundary conditions.

Proposed Work:

Flow simulations that consider the complex geologic structure at the site in three dimensions are now being conducted using the 3-D Sub-Site-Scale Saturated Zone Flow Model (LBNL). These simulations will in part be used to further investigate the vertical flow produced by the presence of faults and their respective properties. This model explicitly accounts for the offset of hydrogeologic units and fault zone properties. Simulations that consider different fault and near-fault property scenarios will be carried out to determine the dominant mechanism(s) that control vertical flow near faults (e.g. fault zone properties, degree of offset, contrast of unit permeabilities and porosities, etc.). We will investigate the relationship between the potential vertical dispersion near faults and the flow parameters found to be most significant.

1.4 Distribution of recharge
Pat Tucci, USGS

Problem:

The distribution and rates of areal recharge to the site saturated zone flow system are not well known, and are usually the least understood of model-input variables. Net infiltration through the potential repository is the primary mechanism for transport of radionuclides to the accessible environment. The amount of this infiltration that reaches the water table is needed to provide a source concentration for transport models. Models of flow and transport in these environments are particularly sensitive to the recharge parameter.

Previous Work:

Most previous models of the area assumed no recharge on Yucca Mountain. All recharge was either applied to Pahute Mesa to the north (or as boundary inflow on the north), and/or as infiltration along Fortymile Wash. Czarnecki and Waddell (1984) simulated recharge along Fortymile Wash of about 22,000 m^3/d. Czarnecki (1985) used recharge rates of 2.0, 0.5, and "minor" in his subregional model, including Yucca Mountain. D'Agnese and others (in press), simulated recharge of about 2,000 m^3/d in the Pahute Mesa area, but did not include recharge along Fortymile Wash, in their regional model. However, that recharge value is about an order of magnitude less than simulated inflow along the boundaries of the site model area.

Osterkamp and others (1994) estimated recharge along Fortymile Wash of about 12,000 m3/day, which included about 800 m^3/day along Yucca Wash and 200 m^3/d along Drillhole Wash. More recent work by Savard (in review) estimates a recharge rate of about 300 m^3/day as a minimum rate.

Recent work by Flint and others (in review) concludes that some recharge does occur on parts of Yucca Mountain. Average annual rates of infiltration range from zero to more than 80 mm/yr depending on location, and average about 4.5 mm/yr. This conclusion may be supported by recent analysis of chloride-36 isotope data from the ESF.

Proposed Work:

New Data: (1) Proposed artificial infiltration studies along Fortymile Wash should be completed; (2) Continue with infiltration studies at Yucca Mountain and with isotope sampling in the ESF and in selected wells; (3) Obtain better estimates of regional discharge, which may provide better estimates of regional recharge.

Sensitivity Analyses: Use values ranging from 0-4.5 mm/yr on Yucca Mountain, and values ranging from 300 m^3/d to 22,000 m^3/d for Fortymile Wash. If other values are output from the site UZ model, use those as well (with a range comparable to their uncertainty in the values. Use boundary fluxes from the regional model that range over the uncertainty in those values.

Application to TSPA-VA:

The site model will have a high degree of uncertainty, because recharge and permeability will be highly correlated. The site model will have a very non-unique solution, because the model includes no natural discharge areas that can be used to help "tie down" recharge values. ANYTHING that we can do to increase our confidence in recharge values will increase our confidence in output from the site model and any models based on that model.

1.4 Distribution of recharge
Frank D'Agnese, USGS

Problem Statement/Previous Work:

Recharge is one of the least understood parameters, and perhaps, one of the most difficult to estimate. This is most easily attributed to issues of scale. Important features at the site scale are negligible at the regional scale. Uncertainty is high; sensitivity is high.

The best way to reduce this uncertainty is to better characterize:

-Discharge at large ET areas
-Discharge through pumping
-Discharge at regional springs

The major source of recharge to the regional ground-water flow system is from precipitation on the highest mountains within the region. On a more local scale, runoff to major drainages is likely. Some recharge occurs from recycled irrigation and domestic waters, as well as seepage of spring discharge back into the ground-water system. For simplification these are ignored.

The current regional ground-water model uses a modification of the empirical Maxey-Eakin first-approximation method. This method is highly dependent on elevation data, surface hydrogeology, and vegetation distributions. Areas of high recharge occur at the highest elevations, on well-drained soils, in areas of dense vegetation.

Future Work/Sensitivity Analyses:

The best way of improving recharge parameters in the regional model is to improve discharge observations. Additional simulations utilizing regional vegetation maps along with improved observations of discharge flux may increase the number of zones used to classify recharge. This may also allow some stream-flow rerouting simulations to allow recharge along major drainages.

How it fits into TSPA-VA:

Improves the definition of recharge areas, fluxes and processes. This improvement leads to better parameter value estimates and confidence intervals and reduces uncertainty in fluxes and flow-paths to accessible environment and site model.

1.5 Regional discharge
John Czarnecki, USGS

Traditional representations of the potentiometric surface from Yucca Mountain to points south show a systematic decrease in the potentiometric surface toward Franklin Lake playa (Alkali Flat) in Inyo County, California. Field estimates of discharge at the playa were made using a variety of techniques (Czarnecki, 1990) including the use of the eddy-correlation technique which estimated discharge at between 1 and 3 mm/d throughout the year. This value was confirmed by more recent analyses by D'Agnese using GIS techniques to estimate discharge.

Lack of data precludes the assessment of possible flow paths from Yucca Mountain to a possibly connected discharge location in Death Valley via the Funeral Mountains. Specifically, insufficient piezometric data exist up to the eastern range front of the Funeral Mountains to construct a potentiometric surface. Further, the extent and hydraulic characteristics of possible Paleozoic carbonate rocks underlying the basin-fill sediments of the Amargosa Desert has not yet been determined.

A dual piezometer borehole (NT-1) was drilled initially as an exploration drillhole by a mining company, and is the closest and deepest borehole to the eastern rangefront of the Funeral Mountains. Water-level monitoring stopped shortly after the hole was completed making it difficult to establish hydraulic head in either the deep or shallow saturated zone (initial heads were higher in the deeper piezometer indicating upward flow). No water samples were ever obtained. An attempt to obtain hydrochemical and potentiometric data from each piezometer would be an important cost-effective addition to the sparse data from that area.

An additional deep borehole Felderhoff-Federal 25-1 was drilled as a wildcat oil well about 3 miles south of Amargosa Valley. The USGS participated in logging the hole during its construction. The hole was competed with drillable plugs. One cost-effective option would be to drill out plugs in Felderhoff-Federal 25-1 and instrument with packers/ sliding sleeves. This is a 5000 ft deep hole which penetrated 3000 feet of Pz carbonates, and is only 10 km south of Yucca Mountain. At the time the hole was drilled (4/91) it looked like it would cost under $65,000 to do the conversion, but that was with the rig on the hole (included 4 packers/5 sleeves/5,000 ft of tubing/ and 3 days of rig time).

References:

Czarnecki, J.B., 1990, Geohydrology and evapotranspiration at Franklin Lake playa, Inyo County, California: U.S. Geological Survey Open-File Report 90-356, 96 p.

1.5 Regional discharge
Frank D'Agnese, USGS

Problem Statement/Previous Work:

Only one evapotranspiration discharge study has been conducted within the Death Valley ground-water basin that utilizes extensive field measurements and estimates flux rates using various techniques (Czarnecki, 1990). This series of independent measurements allowed for the development of a reasonable estimate for evapotranspiration (ET) discharge at Franklin Lake Playa of 22,800 m^3/d (+/-25%).

Most previous (pre-characterization) studies of ground-water resources in the Death Valley region have estimated ground-water ET discharge by delineating areas of phreatophytes on airphotos and applying empirically derived mean consumptive-use rates for those species of phreatophytes at the discharge site (Walker and Eakin, 1963; Rush, 1968; Malmberg and Eakin, 1962; Glancy, 1968; Malmberg, 1967). Although a useful first approximation, these estimates contain large (often an order of magnitude) potential errors.

Current regional ground-water modeling results only use these empirical/field ET discharge volumes to compare with model results. Recent modifications to MODFLOWP allow for the inclusion of these rates in the model as flow observations to constrain the inverse solution. Recent model results clearly show that ET accounts for 66% of total flux through the system. Using detailed ET estimates from related DOE studies at Franklin Lake Playa, Ash Meadows, and Oasis Valley may constrain the model sufficiently to improve sensitivity analyses.

Future Work/Sensitivity Analyses:

Obtain Ash Meadows ET flux map from Las Vegas subdistrict USGS. Develop Franklin Lake Playa ET flux map from Czarnecki (1990). Develop MODFLOWP Flow Observation files for each ET area for which flux data exists. Represent each cell of model representing ET area as head-dependent boundary. Conduct inverse parameter estimation runs using flow observations as additional constrains to the inverse problem. Evaluate changes to potentially improved parameter estimates, parameter sensitivities, and confidence intervals. Conduct similar exercises utilizing Oasis Valley and Death Valley saltpan data when available.

How it fits into TSPA-VA:

Improvement of model parameter sensitivities and estimated parameter value confidence intervals. Reduces uncertainty in fluxes and flow-paths to accessible environment and site model.

2. Characterization of the Model Domain

2.1 Flow channelization
Jack Gauthier, SNL

Problem Statement and Previous Work:

Benson et al. (1983) reported discrete "producing zones" in well pump tests. They also reported a number of isotopic/chemical measurments. Of interest is that measurements often differed. Further, at H-1, where data were collected both when the hole was partially drilled and when it was completed, C-14 suggested that older water was above younger water. A similar conclusion can be drawn from data taken from G-4 (where most water came from depth) and H-4 (where water came from several locations, including near the surface).

These data indicate that SZ flow is heterogenous and that the SZ is not well mixed on time scales of 10+ ky. All TSPA calculations to date have been performed with the assumption that the SZ acts like a single porous medium (actually, several). Highly channelized flow should significantly increase transport velocity, decrease lateral (and longitudinal) dispersion, reduce matix diffusion, and result in higher concentrations in localized regions downgradient.

Proposed Future Work and Sensitivity Analysis:

A modest program to collect isotopic/chemical data in packed-off intervals of selected boreholes should be initiated. SZ transport models, and hence flow models, should be calibrated to these data. (Better yet, the models should be used now to predict the measurements.) At a minimum, SZ flow and transport models should be calibrated to the Benson et al. data.

Format for incorporation into TSPA-VA:

TSPA transport models should be dual-continuum with a probabilistically defined matrix/ fracture coupling factor. Input fluxes should be consistent with estimates from the process models of the cross-sectional area that contributes to flow.

References:

Benson, L.V., J.H. Robison, R.K. Blankennagel, and A.E. Ogard, Chemical composition of ground water and locations of permeable zones in the Yucca Mountain area, Nevada, U.S. Geological Survey Open File Report 83-854, 19p., 1983.

2.1 Flow channelization
Dave Vaniman, LANL

Problem Statement and Previous Work:

Several fractured intervals in the SZ are characterized by mineralization and Liesegang structures indicative of long-term flow and transport. In several instances these altered fractures correspond to depths where packer tests indicate high flow. Current fracture-flow experiments indicate particularly high retardation of some problem radionuclides, particularly Np, along such transmissive fractures. Do these fracture features reliably indicate channels of present transmission, and can they be modeled as such?

Proposed Future Work and Sensitivity Analysis:

For TSPA-VA, preliminary data connecting sorption (including microautoradiography results), flow volumes/rates, and mineralogy from pre-QA core may be available in a form amenable to simplified abstraction. In the longer term, for performance confirmation, a more complete variety of transmissive fractures must be considered and the question of vertical linkage between transmissive intervals should be considered.

Format for incorporation into TSPA-VA:

A 3-D model of channelization may be used for comparison with the 3-D mineralogic model and with specific, detailed mineralogic studies of altered SZ fractures from highly transmissive intervals. Such a comparison might be spread across several milestones due by the end of FY97.

2.2 Spatial distribution of hydraulic conductivity
Sean McKenna, SNL

Problem Statement:

The spatial distribution of hydraulic conductivity in the saturated zone of Yucca Mountain is heterogeneous. The effects of this heterogeneity on the migration and dilution of radionuclides exiting the potential repository has not been examined in detail. Previous models of the saturated zone at Yucca Mountain have considered the distribution of hydraulic conductivity to be homogeneous within each of a small number of hydro-stratigraphic units. Recent work on the geologic framework model (Clayton, et al., 1997) allows for the discretization of the saturated zone stratigraphy into approximately 30 lithologic units. This fine stratigraphic resolution allows for the inclusion of small but potentially significant hydrostratigraphic layers in saturated zone flow models.

Proposed work:

I propose to model the saturated zone flow system at Yucca Mountain in the area of the repository block at a fine scale with both mean values of hydraulic conductivity in each of the hydrostratigraphic units and also with spatially variable hydraulic conductivity in the units. The goal of this work is to evaluate the amount of dilution or focusing of flow paths that occurs within the saturated zone. In light of that goal, it is proposed to use an advective particle tracking scheme to examine the dilution/focusing of the flow paths as a proxy for full contaminant transport modeling. Additionally, the grid resolution of the model will be varied to examine the effects of scaling on flowpath dilution/focusing.

Tie to TSPA-VA:

The results of this work will allow PA to determine the amount of resolution in the geologic framework model that is necessary to include within the PA transport calculations. This work will also allow PA analysts to determine whether or not it is necessary to include intra-unit heterogeneity in the PA transport calculations.

References:

Clayton, R.W., W.P. Zelinski and C.A. Rautman, 1997, *DRAFT ISM2.0: A 3D Geologic Framework and Integrated Site Model of Yucca Mountain*, Rev0B, CRWMS M&O, Las Vegas, Nevada.

2.3 Geologic and mineralogic framework
Dave Vaniman, LANL

Problem Statement and Previous Work:

There are two fundamental problems in the geologic and mineralogic framework of flow and transport in the SZ.: 1) Relatively few drill holes are available for SZ characterization. QA samples are available from the upper SZ beneath the exploration block from 5 recent holes (UZ-16, UZ-14, SD-7, 9, and 12) but characterization of the deeper SZ (below the Bullfrog Tuff) is largely restricted to pre-QA core and cuttings. 2) Comparisons between transmissive intervals and mineralogic zones are presently limited to pack-and-pump data from pre-QA cores.

Proposed Future Work and Sensitivity Analysis:

For TSPA-VA, it should be possible to link SZ transmission models from several of the newer drill holes with quantitative mineralogy results. In the future, beyond TSPA-VA and into confirmation testing, more comparisons between transmissive zones, non-transmissive zones, and XRD-measured mineral abundances are needed.

Format for incorporation into TSPA-VA:

The comparisons with transmissive intervals could be incorporated as part of the revised 3-D mineralogic model due 9/30/97 (milestone SP321AM4).

3. Transport Processes and Parameters

3.1 Dispersivity
Chunhong Li, INTERA

Depending on the flow condition, dispersion could play an important role in the transport of radionuclides in the saturated zone. High dispersivities in the longitudinal and the transversal directions can effectively spread the plume in both directions, thus reduce the peak concentration of the solute reaching the down stream observation wells. Therefore, determine the range of despersivities and evaluate their influence on the transport process in the saturated zone will help the TSPA-VA analysis.

Zyvoloski et al (1996) applied the Neuman (1990) correlation function to estimate the scale dependent dispersivity in the SZ. They found that using the correlation function for an accessible environment of 25 Km, the estimated dispersivity could reach 1400 m. But for conservative reason, they used longitudinal dispersivity in the range of 100 to 500 m in their simulations.

But the estimated dispersivity and the effects of dispersion also depends on the conceptual models and other physical and chemical processes in the SZ. Those factors include discrete network model vs. continuum model, flow velocity in the SZ (Peclet number), adsorption, and matrix diffusion, etc. Thus, for TSPA-VA analysis, the effect of dispersion should be investigated in combination with other physical and chemical processes.

To bound the effect of dispersion, we can select a range of dispersivity under different scenarios to estimate the influence of dispersion on the simulated transport process of radionuclides. Such exercise will also enable us to investigate the sensitivity and uncertainty of dispersivity on the SZ transport process.

References:

Neuman, S.P., Universal scaling of hydraulic conductivities and dispersivities in geologic media, Water Resources Res., 1191-1211, 26(8), 1990.

Zyvoloski, G., J. Czarnecki, B. Robinson, C. Gable, and C. Faunt, Milestone: 3624 - Saturated zone radionuclide transport model, LA-EES-5-TIP-96-011,August 29, 1996, Los Alamos National Laboratory, Los Alamos, New Mexico.

3.1 Dispersivity
Mike Wilson, SNL

It is probably just an oversight, but it is not stated in the "strawman" write-up that dispersivity is only included in the transport model to compensate for heterogeneities that are not explicitly modeled. Thus, large dispersivity values (hundreds of meters) are only appropriate in a simplified model that does not have the right large-scale structure (stratigraphic layering, faults, etc.). An example is the saturated-zone modeling done by George Barr for TSPA-1993. Taking his breakthrough curves at the 5-km accessible-environment boundary, I showed that they implied dispersivities of 100 m to 170 m, for his six cases (Table 11-6 of our TSPA-1993 report). The idea then is that a featureless 1-D model with dispersivity of 150 m (say) would give results similar to a 3-D model with the right large-scale structure but zero dispersivity.

In fact, however, there may be reason to use higher dispersivity values even in a detailed 3-D model. The dispersivity values above (100 m to 170 m) reflect the effective dispersivity of the given model assumptions, including the assumptions of equivalent-continuum behavior and confined-aquifer behavior with aquifer thickness of 200 m. If flow is actually highly channeled, the topology of the channel network could determine the effective dispersivity -- and that aspect of the large-scale structure is not captured in the model.

3.1 Dispersivity
Bruce Robinson, LANL

Problem Statement:

We don't have hard numbers at the range of dispersivity values to use in model calculations at the scale of SZ transport to the accessible environment. C-Wells results are a good start, but we will always be forced to extrapolate interwell tracer test results to larger scales. Furthermore, the nature of the dispersion model and the assumed value of transverse dispersivity may critically influence the model results. A sensitivity analysis on a simple flow system is needed to separate the dispersion and transport model parameters to determine which are critical, and which can be held constant in TSPA calculations.

Proposal Approach:

Use a simplified 3D steady state flow field and vary the radionuclide source term from the UZ and the transport parameters systematically to perform a sensitivity analysis that can be used to decide which parameters should be retained as sensitive parameters in TSPA calculations. The radionuclide source term would be generated from a series of UZ flow and transport simulations to provide a time-dependent function for input to this simplified SZ model. The SZ dispersion terms to vary are the longitudinal and transverse dispersivities. The sorption parameter is Kd. The effective porosity is also variable since the entire matrix may not be accessible to transporting radionuclides. This parameter will also allow the "fluid travel time" to be varied without changing the flow field calculation. Sensitivity will be quantified to determine which parameters are most important and need to be explicitly varied in TSPA realizations, and which can be assumed constant. Base case values will be set as follows:

dispersivity: minimum bound on longitudinal dispersion set using C-Wells transport results, transverse value set assuming a range of long. to trans. dispersivity ratios (say, 50:1 to 3:1 ?)

sorption coefficient: 0 for conservative radionuclide, 1 for weakly sorbing radionuclide, 50 for strongly sorbing radionuclide

effective porosity: minimum bound is the assumed fracture porosity, typically of order .0001. The maximum is the matrix porosity, based on a model of pervasive matrix diffusion of radionuclides into the rock matrix.

Radionuclide Source Term: Select a range of UZ breakthrough curves for key radionuclides at the water table, capturing the range of variability likely to come out of UZ transport models.

1.3, 2.1, 2.2, 3.1) Vertical flow, flow channelization, distribution of hydraulic conductivity, transverse dispersivity.
Dave Sevougian, INTERA

I do not have a specific proposal, but want to reiterate that from a TSPA perspective, dilution in the SZ is a very important performance factor. Therefore, any of these phenomenon that affect mixing on a large scale are very important to repository performance. Thus, if we are to include them in TSPA-VA, we need input from the SZ process modelers and data gatherers on appropriate methods and parameter values.

3.2 Matrix diffusion (effective porosity)
Bruce Robinson, LANL

Problem Statement:

It is uncertain whether to use dual porosity or effective continuum models for SZ flow and transport models. Permeability is likely to be controlled by fractures, whereas matrix diffusion models typically predict, and available field data support, dual porosity models for transport. If the fracture porosity is used to simulate transport, the travel times through the saturated zone will be underpredicted by several orders of magnitude compared to the results assuming that the relevant porosity is the matrix porosity. Robinson (1994) examined the conditions likely to be present in transport of radionuclides through the SZ, concluding that the matrix porosity is likely to be closer to the appropriate one to be used in radionuclide migration simulations in the SZ. We now have additional information to augment the work of Robinson (1994) in assessing the validity of an single continuum, effective porosity model.

Sensitivity analysis: assuming the range of values for diffusion coefficient and fracture aperture consistent with the C-Wells reactive tracer experiments, along with the range of possible groundwater flow velocities consistent with SZ flow modeling studies, systematically estimate the effective porosity using the type curve analysis of Robinson (1994). If the resulting analysis suggests that pervasive matrix diffusion is likely, then the matrix porosity distribution can be assumed for transport, and a continuum model can be employed for TSPA. If there is a range of effective porosities between that of fracture porosity and matrix porosity determined from the sensitivity analysis, then a more sophisticated dual porosity model should be developed, and if it is determined to be too computationally intensive for TSPA use, it should be compared to a simplified single continuum model. For the single continuum model, the effective porosity could be based on a node-by-node analysis of the flow velocity, diffusion coefficient, and fracture aperture to determine a spatially dependent effective porosity. To justify the use of the simplified single continuum model, agreement between it and the dual porosity model would be required. Note that this stage of the analysis would only be required if the simplified effective porosity analysis was proven to be incorrect (or non-conservative).

3.2 Matrix diffusion (effective porosity)
Jake Turin, LANL

Problem Statement:

Previous process modeling has demonstrated that matrix diffusion may potentially have a profound beneficial impact on repository performance through retardation and attenuation of solute concentrations. Before the recent C-Wells reactive tracer test results, we had no clear evidence that matrix diffusion really operates on the field scale. Preliminary analysis of the C-Wells results seems to indicate unequivocal evidence of field-scale matrix diffusion. The challenge is to confirm these preliminary analyses and to provide estimates of matrix-diffusion parameters and parameter uncertainty in a timely fashion, so that these results can be confidently integrated into the TSPA efforts.

Strategy:

Existing analysis of the C-Wells results have relied on LANL's RELAP code, a powerful analytical tool that permits rapid parameter estimation at the cost of certain simplifying assumptions, including 1-D linear flow through a single homogeneous dual-porosity medium. More extensive analysis should be performed using the FEHM numerical model. This analysis should focus on the significance (if any) of RELAP's assumptions. In particular, the FEHM analysis should look at the effects on tracer breakthrough curves (BTCs) of radial flow, multi-dimensionality, and aquifer heterogeneity. If these phenomena are shown to have significant effects on predicted BTCs, new matrix diffusion parameter estimates based on the C-Wells results will be derived. If, on the other hand, detailed FEHM analysis results substantially agree with the RELAP results, the RELAP results can be applied to TSPA-level predictions with increased confidence, and the simpler RELAP code can be used for future analyses.

3.3 Sorption
Jake Turin, LANL

Problem Statement:

We have extensive laboratory data on radionuclide sorption, but until recently, no field-scale measurements to enable us to confidently apply these data to field conditions. The recent C-Wells test of lithium transport, combined with supporting lab studies of lithium sorption to Bullfrog Tuff, provide us with the first concrete evidence that laboratory measurements can provide reliable predictions of field transport. Thus far, our analysis of these data has been limited to 1-D linear flow through a homogeneous medium with linear equilibrium sorption.

Strategy:

To reduce uncertainty in our results, the analysis should be extended to a more realistic and complex regime using the FEHM numerical model. In particular, the FEHM analysis should look at the effects on tracer breakthrough curves (BTCs) of radial flow, multi-dimensionality, aquifer heterogeneity, sorption nonlinearity, and sorption nonequilibrium. If these phenomena are shown to have significant effects on predicted BTCs, new matrix diffusion parameter estimates based on the C-Wells results will be derived. If, on the other hand, detailed FEHM analysis results substantially agree with previous results, those results can be applied to TSPA-level predictions with increased confidence, and the simpler code can be used for future analyses.

3.4 Colloid transport
Jake Turin, LANL

Problem Statement:

Colloid transport of radionuclides remains a potential "wild-card" in SZ transport predictions. The recent C-Wells reactive tracer test produced a reliable and detailed breakthrough curve (BTC) for transport of 0.36-um microspheres through 30 m of fractured Bullfrog Tuff. Approximately 11% of the injected microspheres were recovered within 2650 hours of pumping, and recovery continues to increase. This BTC provides the most reliable evidence of the potential for SZ colloidal transport at the field scale in the vicinity of Yucca Mountain, and any conceptual model of colloidal transport must at least be consistent with these data. In particular, the low microsphere recovery relative to the conservative tracer recoveries (55%-60%) suggests that an effective colloid removal or retardation process exists.

Strategy:

The successful C-Wells reactive tracer test has provided direct evidence of field-scale colloidal transport. We propose a thorough analysis of the microsphere BTC using the FEHM code, comparable in scope to that proposed for the solutes under sub-issue 3.2 and 3.3. The combination of solute and colloid BTCs from the same test greatly constrain the analysis and will increase the confidence in the results. Specifically, the conceptual model and transport parameters for the colloids must be consistent with that for the solutes, adjusted for the large size and negligible diffusivity of the colloids.

Preliminary analysis indicates that C-Wells colloid transport predictions based on solute behavior without matrix diffusion will greatly overestimate colloid concentrations and recovery. The proposed detailed analysis will investigate alternative removal or retardation models, including simple linear filtration, aperture-dependent filtration, and time-dependent deposition/resuspension. FEHM is currently capable of modeling these and other processes. Results of these analyses will feed TSPA analyses by providing more realistic transport parameters for colloid-facilitated radionuclide migration in the SZ. Furthermore, these analyses will lay the groundwork for planning future field-scale colloid transport tests, should they be deemed necessary.

4. Coupling to Other Components of TSPA

4.1 Climate change
Jack Gauthier, SNL

Problem Statement and Previous Work:

Paleospring deposits and Sr-ratios from drill core suggest that the water table was approximately 100-m higher during the Younger Dryas (11.5 to 13 ky BP) and the last glacial cycle (18+ ky BP). This perturbation to the potentiometric surface could cause a significant change to SZ flow (direction and velocity). The pluvial climates that could have caused such a water-table excursion have not been particularly rare.

Proposed Future Work and Sensitivity Analysis:

SZ flow models should be exercised to determine conditions that could cause significant water-table excursions. The models should be calibrated to known paleospring deposits. Resulting flow fields should be used by transport models to investigate implications for performance (peak concentration, travel time).

Format for incorporation into TSPA-VA:

TSPA SZ models should incorporate perturbed SZ flow and transport during periods of wetter climates.

4.1 Climate change
Frank D'Agnese, USGS

Problem Statement/Previous Work:

Simulations of the effects of climate change on the Death Valley region are currently being conducted. These simulations assess the effects of two wetter climates:

(1) a VERY wet climate occurring 21 ka.
(2) a slightly wetter climate assumed to occur in the future when CO_2 gases attain concentrations of twice the present level.

These simulations are extremely generalized because of the lack of calibration data. A "reasonableness check" is used in lieu of calibration. Simulations are deemed reasonable if they result in adequate numerical stability, water budget closure, and conform to current hypotheses about paleohydrology.

Future Work/Sensitivity Analyses/How it fits into TSPA-VA;

Ultimately, results from regional simulations could be used as boundary conditions for site past/future climate simulations.

4.2 Thermal and chemical plume
John Czarnecki, USGS

A possibly overlooked effect of increased heat on the effect of flow on the saturated zone was the observation of decreased hydraulic conductivity by several orders of magnitude with time as heated J-13 water was passed through pressure-loaded core (Lin, 199x, LLNL report). The mechanism for this decrease in hydraulic conductivity likely involves the silica dissolution of the asperities, specifically the pressure loaded points within an asperity, causing the sidewall pressure to close the asperity. Asperities examined using an SEM appeared to have been smoothed, supporting the silica dissolution mechanism.

If the mechanism invoked to explain the large hydraulic gradient is one of a lateral contrast in hydraulic conductivity, then it might be possible to envision a similar mechanism below and downgradient from the thermal footprint of the design repository area, in which permeability decreases. If so, this 'plug' could conceivably back up water (like a large rock in a stream), causing a systematic rise in the water table under current climatic conditions.

References:

Lin, Wunan, 1989, Laboratory study of fracture healing in Topopah Spring tuff: Implications for near field hydrology in Nuclear waste isolation in the unsaturated zone: FOCUS '89, Las Vegas, NV, 18-21 Sept. 1989, 23 p.

4.3 Well withdrawal scenarios
Jerry McNeish, INTERA

Problem Statement/Previous Work Summary:

In TSPA-95, the dose to man scenario was a simple drinking water scenario. The receptor was assumed to drink 2 liters/day from a well at the accessible environment. The well was assumed to be screened over a 50 m depth in the SZ. No dilution due to wellbore mixing was included. No dilution due to withdrawal of groundwater above or below the screened interval was included. It is intended that the TSPA-VA dose to man scenarios will incorporate more realism in the well withdrawal portion of the calculation and evaluate the effect of the modifications on the overall dose.

Proposed Future Work/Sensitivity Analyses:

As the strawman proposes, a few pumping scenarios could be developed for a few well configurations. The range of these scenarios will depend on the range of regulatory alternatives expected. Local scale modeling of the mixing (thus dilution) of the release plume with the other groundwater pumped could be conducted. Such parameters as pumping rate, length of screened interval, depth of vertical mixing, zone of influence, and distance to accessible environment could be varied.

Proposed Abstraction:

The abstraction from the sensitivity analyses could provide both a wellbore mixing factor and a regional aquifer mixing factor depending on the pumping scenario being analyzed. Depending on the results of the sensitivity analysis, the TSPA-VA could include a couple of these pumping scenarios in the calculations.

4.3 Well withdrawal scenarios
Dave Sevougian, INTERA

With regard to well-withdrawal, TSPA-1995 assumed that the entire SZ plume was contained within a 50-m screened interval of a pumping well at 5 km downgradient of the repository. Depending on the dispersion model used in TSPA-VA (e.g., for very little vertical mixing), this depth could be important. We also need input on how well-withdrawal may differ at the 5 km and 30 km withdrawal distances.

4.4 Coupling with UZ transport
Bruce Robinson, LANL

Problem Statement:

The method for coupling the UZ and SZ transport models must capture the relevant processes and outcomes, yet be computationally efficient. In principal, a completely coupled UZ-SZ flow and transport model is required to exactly capture the behavior of the entire geologic barrier system, but computational efficiency issues preclude the development and use of such a model at this time for PA. A convolution method has been used in the past (Zyvoloski et al., 1996, LANL YMP Milestone 3624) to put these two models together, and should be used in TSPA-VA if it can be demonstrated to be robust enough.

The essence of the convolution technique is captured in the following steps:

Step 1: compute the SZ flow and transport behavior for a system in which a known radionuclide input function is assumed, such as a step change in input concentration at $t = 0$. The relevant data from this step is the breakthrough curve at selected positions corresponding to the accessible environment;

Step 2: compute the UZ radionuclide mass flux versus time reaching the water table. If this function is spatially variable, capture this effect by subdividing the water table lower boundary into regions and computing the breakthrough curves for each region;

Step 3: compute the concentration-time behavior at the accessible environment using the convolution integral, which takes the "generic" response curve from Step 1 and convolutes the UZ breaktrough curve from Step 2. If subregions were defined in Step 2, the overall C vs. t response at the accessible environment is obtained by superposition of the individual curves.

The advantage of this approach is that the UZ and SZ model results can be computed independent of one another, with a simple numerical integration convolution step to couple the two together. The two models need not be performed on the same model domain (but we must know where to input radionuclides in the SZ, so we must know how they "link up" in space), and they need not be run with the same flow and transport model options (i.e. particle tracking could be used for the UZ, and finite element solute transport could be used for the SZ if this were desirable). Most importantly for TSPA, it would not be necessary to perform an individual model calculation for each realization. If for example it was determined that a fewer SZ model runs were necessary to capture the uncertainty of the system, a catalog of SZ simulations could be created ahead of time that would be sampled from for each realization, but only the convolution step would have to be performed in the Monte Carlo TSPA simulations. The "response surface" for the SZ would be sampled from for each realization, but in this case the "response" would be based on a 3D flow and transport realization that would capture all of the complexities present in the SZ flow and transport model. The pitfalls of response surfaces are avoided by building the complexity of the process-level model into the model without simplification.

The principle disadvantage of this approach is that only linear processes can be treated using convolution and superposition. Since the convolution function is based on the SZ model, any nonlinearities in the SZ flow and transport system would have to be linearized to use this approach. Processes such as climate-related transient flow, TH effects on SZ flow and transport, and nonlinear sorption would have to be studied and tested to assess the validity of this method.

Proposal: Test the validity of the convolution method

1. Verification of the numerical approach. For conditions in which the convolution approach should give identical results to a more complex, coupled model (i.e. steady state flow, linear transport models, etc.) there needs to be a demonstration that coupling via convolution gives the same results as a more complex, coupled model. The more complex model would be a 3D SZ model with an assumed time-dependent radionuclide concentration at various locations at the water table surface. Computation of the concentration versus time at the accessible environment should agree nearly exactly with a

convolution method in which the response to a unit concentration input condition is used to generate the SZ response curve. This would prove that the numerics of the approach have been properly implemented.

2. "Validation" of the convolution method. This type of test requires that some nonlinear or more complex model result could be conservatively captured using the convolution approach. A complex process would be simulated in full detail, and then the approximate convolution approach would be used to determine if the results are adequate. To state at this time which processes would need to be tested would be to pre-judge the results of the Abstraction/Testing Workshop. But for example, if climate-related transient flow in the SZ is taken to be important, then the convolution method strictly speaking would not be valid, but perhaps a bounding analysis could be performed to justify its use for TSPA-VA.

4.4 Coupling with UZ transport
Dave Sevougian, INTERA

Given the current degree of characterization of property heterogeneity in the SZ beneath the repository, I do not agree with the statement that the "resolution of the grid in the SZ model at the water table below the repository should be at least as fine as that used in the UZ transport model." I believe that in the current incarnations of the UZ and SZ flow models, that the SZ flow model is considerably coarser. I'm unsure about the SZ transport model. At any rate, depending on the heterogeneity of the breakthrough plume from the UZ to the SZ, it may be quite appropriate to use coarser discretization for the SZ model. Of course, this decision is also a function of how accurately we need to model fracture/ matrix interaction in the SZ (e.g., over what distance is complete matrix diffusion achieved). More data is required to determine how well the fracture and matrix continua are coupled with each other and within themselves. The hypothesis of whether the UZ source term should be considered a line source at the water table or distributed plane or volume source over a certain vertical distance should be easily testable with a few runs of a highly discretized FEHM grid, or even more simply with an analytical solution, which can predict the effect on the mixing depth. Coupling of UZ and SZ in past TSPAs is discussed in detail in Attachments C (pp. C-5 and C-6) and E, which discuss discretization and also the effect of climate change on the water table height. My proposal for TSPA-VA coupling would consist of the obvious: feeding the radionuclide mass flux rate (g/area/ time) at the base of the UZ as a boundary condition for the influx to the SZ model. Specifics of the spatial-temporal coupling and discretization cannot be decided upon until the results of the post-workshop analyses are completed. It will depend on the specific abstraction decided upon as a result of these analyses.

Appendix C

AGENDA FOR THE WORKSHOP

Revised Agenda for the SZ Workshop

Tuesday, April 1, 1997

Participant and Observer Introductions — Susan Altman, Pat Tucci
- Site logistics — 8:30 - 8:40

Overview Introduction — Bob Andrews
- Overview of workshop objectives — 8:40 - 8:55
- Discussion of resources for the abstraction work between PA/Site/etc.

Workshop Introduction — Bill Arnold, Susan Altman
- Goals of workshop — 8:55 - 9:10
- Format of workshop
- Ground rules

PA Perspective Introduction — Jack Gauthier
- Explanation of past TSPA outlook — 9:10 - 9:45
- TSPA plans for the future
- Questions that TSPA needs answered before TSPA-VA
- NRC Concerns

Break — 9:45 - 10:00

Review the important issues to SZ Flow and Transport — Bill Arnold
- Introduce the 4 major issues — 10:00 - 10:15

Presentation and review of proposals for major issue 1 — 10:15 - 12:15
- TSPA perspective of the major issue
- Proposal presentations by participants
- Small group (4 groups) review of proposals and prioritize points

Lunch — 12:15 - 1:15

Presentation and review of proposals for major issue 2 — 1:15 - 2:45
- TSPA perspective of the major issue
- Proposal presentations by participants
- Small group (4 groups) review of proposals and prioritize points

Break — 2:45 - 3:00

Presentation and review of proposals for major issue 3 — 3:00 - 5:00
- TSPA perspective of the major issue

Proposal presentations by participants
Small group (4 groups) review of proposals and prioritize points

Wednesday, April 2, 1997

Presentation and review of proposals for major issue 4 TSPA perspective of the major issue Proposal presentations by participants Small group (4 groups) review of proposals and prioritize points	8:00 - 10:00
Break	10:00 - 10:15
Prioritization of all sub-issues across all major issue categories Establishment of major proposal categories Assignment of participants to proposal teams	10:15 - 12:00
Lunch	12:00 - 1:15
Summary of UZ flow and transport proposals	Susan Altman and Bruce Robinson 1:15 - 1:40
Summary of existing SZ workscopes	Pat Tucci and Bruce Robinson 1:40 - 2:00
Proposal teams brainstorming on abstraction/testing proposals	2:00 - 3:15
Break	3:15 - 3:30
Presentations of preliminary proposals to all participants Feedback on preliminary proposals from all participants and readjustment of proposals	3:30 - 5:00

Thursday, April 3, 1997

Proposal teams produce written abstraction/testing proposals	8:00 - 10:30
Team presentations of final draft proposals	10:30 - 11:15
Summary of work to be done after the Workshop and closing remarks Comments from observers	11:15 - 12:00
Lunch	12:00 - 1:00
Core teams wrap-up	1:00 - 5:00

Appendix D

LIST OF ATTENDEES OF THE WORKSHOP

SATURATED ZONE FLOW AND TRANSPORT
ABSTRACTION / TESTING WORKSHOP

USGS, Denver, Colorado - April 1-3, 1997

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Appendix E

PRESENTATION VIEWGRAPHS FROM THE WORKSHOP

Saturated Zone Flow and Transport Model Abstraction/Testing Workshop
Objectives and Constraints

Robert W. Andrews
Manager, M&O Performance Assessment
April 1, 1997

Outline

- Viability Assessment Components
- Approach and Schedule for TSPA-VA
- Definition of Abstraction
- Goals of Abstraction/Testing Activities
- Goals of Abstraction Workshops
- Roles and Responsibilities
- Constraints

Viability Assessment Components

"(1) *the preliminary design concept for the critical elements for the repository and waste package;*

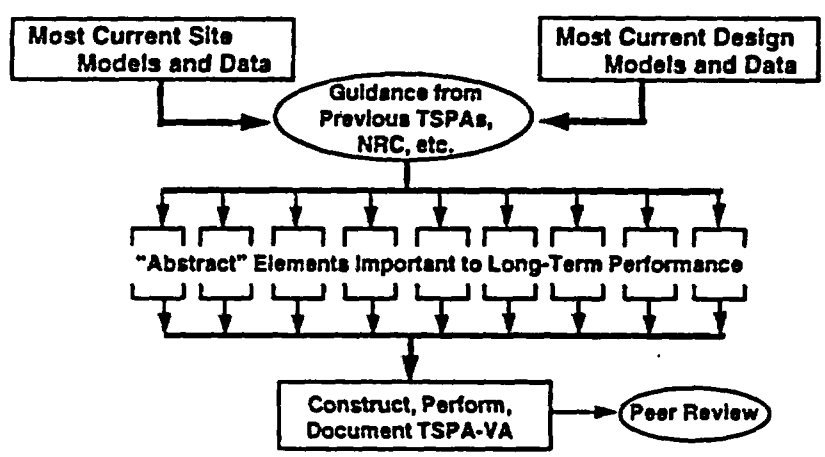
(2) a total system performance assessment, based upon the design concept and the scientific data and analysis available by September 30, 1998, describing the probable behavior of the repository in the Yucca Mountain geological setting relative to the overall system performance standards;

(3) *a plan and cost estimate for the remaining work required to complete a license application; and*

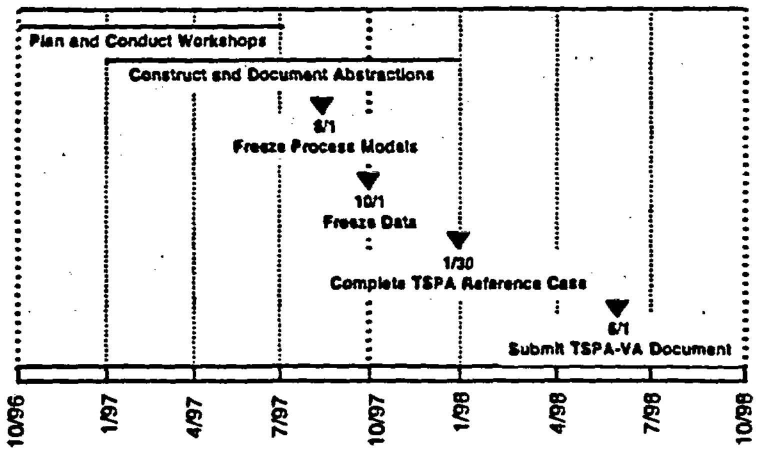
(4) *an estimate of the costs to construct and operate the repository in accordance with the design concept."*

(FY 1997 Energy and Water Appropriations Act)

Approach for TSPA-VA



Generalized Schedule for TSPA-VA



What is an "Abstraction"?

- a simplified/idealized model that reproduces or bounds the essential elements of a more detailed process model
  - inputs to abstracted model may be a subset of those required for process model
  - model may be reduced dimensions or a response function derived from intermediate results
  - model must capture uncertainty and variability
  - abstracted model must be tested against process models to assure validity

Abstraction/Testing: Basis

- TSPA-type analyses are probabilistic/stochastic
  - Goal is to retain key aspects of process model affecting post-closure performance while producing results usable in multiple realization probabilistic models
  - Essential elements (e.g., output) of some process models can be represented in a simplified form, thus increasing the computational efficiency of the TSPA

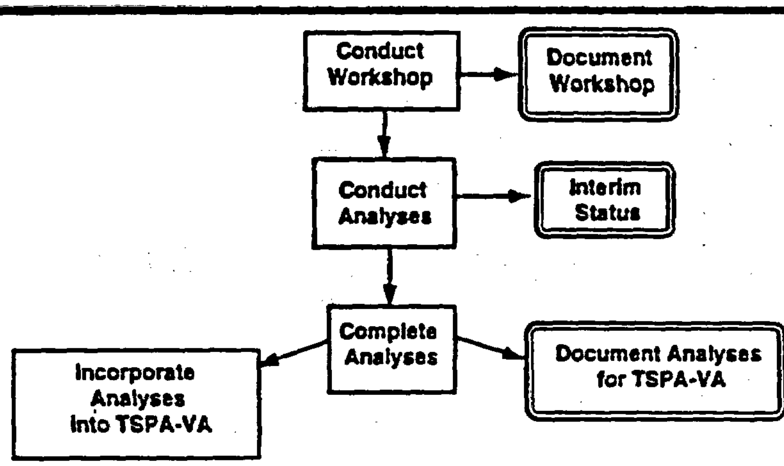
Abstraction Requires Collaboration

- Assure the most current understanding (observations and models) is incorporated
- Assure integration across major Project products used as the foundation (=confidence) of TSPA-VA
- Assure that issues are identified and can be addressed quantitatively/qualitatively in TSPA-VA

Goal of Abstraction/Testing Activities

- Develop a valid, defensible TSPA-VA:
  - Assure completeness/representativeness of models used in TSPA analyses with respect to important aspects of process model(s).
  - Assure appropriate issues (=alternative hypotheses) are identified, quantified and evaluated in TSPA.
  - Assure model development effort is focussed on most important issues with respect to performance
  - Assure bases for assumptions are well defined, justified and documented.

Format of Abstraction/Testing Activities



Schedule for Abstraction/Testing Workshops

Workshop Topic	Workshop Date	Workshop Lead	Workshop Location
Unsaturated Zone Flow	12/10-12/96	S. Altman	Albuquerque
Waste Package Degradation	1/8-10/97	J. Lee	Las Vegas
Thermohydrology	1/21-23/97	N. Francis/ C. Ho	Albuquerque
Unsaturated Zone Transport	2/5-7/97	J. Houseworth	Albuquerque
Waste Form Alteration and Mobilization	2/19-21/97	W. Halsey	Livermore
Near-Field Environment	3/5-7/97	D. Sassani	Berkeley
Criticality	3/18-20/97	R. Barnard	Las Vegas
Saturated Zone Flow and Transport	4/1-3/97	B. Arnold	Denver
NEPA	TBD	A. Smith	Las Vegas
Biosphere	6/3-5/97	A. Smith	Las Vegas

Goals of Abstraction Workshops

- Develop a comprehensive list of issues related to each process that need to be addressed for TSPA
- Prioritize the list of issues according to a consistent set of performance measures or criteria
- Develop analysis plans to address top priority issues (parameter set, numerical analyses, analytical analyses, literature searches, etc.)

Goal is not to resolve *key issues/uncertainties*

Roles and Responsibilities

- TSPA Core Team (TCT): assure approach is implementable in TSPA and process models are consistent
- Abstraction Core Team (ACT) : coordinate abstraction activities and assure integration with process model development
- Abstraction analysts - conduct sensitivity/uncertainty analyses
- Process model analysts - provide most current process model understanding
- Observation interpreters/synthesizers - assure most current interpretations are included in process model

Responsible Staff

TSPA Core Team:

Mike Wilson
David Sevougian
Jack Gauthier
Jerry McNeish

SZ Flow and Transport Model Abstraction Core Team:

Bill Arnold
Pat Tucci
Bruce Robinson
Jack Gauthier

Technical Constraints

- Easy to focus on conceptual uncertainties, more difficult to define appropriate methods to address these uncertainties
- Weighing of alternative hypotheses
- Alternative data interpretations
- Reasonably limiting the degree of conservatism

Programmatic Constraints

- 8 months of abstraction analyses by about 2 FTEs plus appropriate levels of M&I (plus about 0.5 FTE support provided by 1.2.3)
- Parallels in-situ testing, site-scale SZ flow and transport model revision/documentation, SZ hydrology synthesis, possible SZ flow and transport model expert elicitation and associated deliverables
- Abstraction/testing results completed by 11/97 (mid-point status in 7/97) [analyses documented by 12/97]
- TSPA-VA documented 6/98 (analyses completed 3/98)
  - TSPA-VA process will be peer reviewed

Summary

- TSPA-VA is owned by all
- Confidence/completeness/consistency in models is our collective responsibility
- Collaboration is required to assure success
- Workshop is just the beginning of the process towards generating a reasonable TSPA-VA
- At the workshop, we need to focus on approaches to evaluate issues not just identification of uncertainties

Civilian Radioactive Waste Management System
Management & Operating Contractor

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E-10

Saturated Zone Flow and Transport Abstraction/Testing Workshop

Workshop Introduction

BILL W. ARNOLD
SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NM
April 1, 1997

Sandia National Laboratories

Goal of the Abstraction/Testing Activities

- To develop a valid, defensible Total System Performance Assessment for Viability Assessment (TSPA-VA) using the most complete and current information available.

Method to Achieve Valid TSPA-VA

- **Incorporate reasonable models that reproduce the *essential behavior* of *key processes* important to *long-term performance* in a computationally efficient mode.**

- **Describe alternate conceptualizations and parameter sets that reflect the variability and uncertainty of the system.**

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Workshop Goals

- **Develop a comprehensive list of issues for saturated zone (SZ) flow and transport.**

- **Prioritize these issues using criteria linked to long-term performance of the repository.**

- **Develop SZ flow and transport modeling/testing strategies and post-workshop work plans (proposals) that will support TSPA-VA.**

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Workshop Agenda

Tuesday Morning	Introduction and TSPA Perspective Presentations of Issues (Category 1)
Tuesday Afternoon	Presentations of Issues (Category 2) Presentations of Issues (Category 3)
Wednesday Morning	Presentations of Issues (Category 4) Global Prioritization of Issues
Wednesday Afternoon	Review of Existing Workscopes Development of Abstraction/Testing Proposals
Thursday Morning	Documentation of Abstraction/Testing Proposals Workshop Wrap-up
Thursday Afternoon	Core-team Wrap-up

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Schedule

- SZ flow and transport workshop documentation:
  May 31, 1997 ? Level 3 milestone
- Status review:
  August 19, 1997 Level 4 milestone
- Complete TSPA-VA sensitivity analyses:
  September 8, 1997 ? Level 4 milestone
- Complete TSPA-VA abstraction/testing documentation:
  December 30, 1997 ? Level 3 milestone

TSPA Introduction

Jack Gauthier
SZ Abstraction/Testing Workshop
1 April 1997

Contents

- Purpose etc.
- Abstraction
- TSPA-93 Modeling and Abstraction
- Next?

Purpose etc.

Purpose of TSPA

- Determine if a repository at YM would comply with NRC (EPA) postclosure performance regs.
- Given that the regs don't exist, determine if a repository would be "safe."
- Provide guidance to site characterization and design.

Strategy of TSPA

- Quantify what we know
- Quantify what we don't know

TSPA Modules

Undisturbed	Disrupted
UZ flow	volcanism
NFE	tectonics
WPD	human intrusion
WFM	criticality
UZ transport	
SZ flow	
SZ transport	
Biosphere	

How PA Interacted with Site Before

- Painfully
- Very painfully

Why Are We Here?

- Identify SZ issues
- Prioritize SZ issues
- Develop analysis plans to address issues
- (We are not here to solve the issues.)

Abstraction

Why Abstract?

- We must be able to run hundreds of model calculations of the entire system.
- The calculations must cover at least 10,000 years, and some will cover 1,000,000 years.
- The calculations must include time-varying boundary conditions caused by changes in climate and possibly thermal effects.
- We must have the flexibility to allow for different conceptual models.

The Basic Issues

- UZ/SZ coupling (connectivity, climate change, etc.)
- Travel times (flux, matrix diffusion, decay, etc.)
- Mixing (flux, dispersion, channeling, matrix diffusion, concentrating areas, etc.)

Methods of Abstraction

- Response surface
- Dimension reduction
- Simplified model

Response Surface

- Use process models directly to create a functional relationship between input and output; e.g., lookup table, pdf, etc.
  - example – dilution factor as a function of water-table elevation and distance from source
- Pro — very fast and easy to use
- Con — inflexible

Dimensionality Reduction

- Use process models directly in the Monte Carlo simulations, but in 2-D or 1-D rather than 3-D.
- Other simplifications may be made as well (e.g., isothermal, single-phase calculations; heterogeneity reduction).
- The simplified process model should be compared with the full process model—comparison in terms of performance (e.g., calculated peak dose), not details of the flow field.
- Pro — tractable calculations
  — results are easier to check
- Con — omission of potentially important behavior

Simplified Model

- Develop models according to primary process
  - example – channelized flow model
  - example – single porous media
- Should be compared with process models
- Pro — evaluation of alternative conceptual models
- Con — validation

Overview of TSPA-1993 SZ Detailed Model

- 3-d detailed model
- 8 km by 8 km by 200 m
- confined aquifer
- 5 strata
- single porous media — 20% porosity

Overview of TSPA-1993 SZ Detailed Model (cont.)

- *diversionary and non-diversionary conceptual models*
- Solitario Canyon and Drill Hole Wash faults necessary
- 3 source locations for transport (Bullfrog, Prow Pass, Calico Hills)
- breakthrough curves output at 5 horizons at AE
- isothermal
- no climate change (except water table assumed to rise)

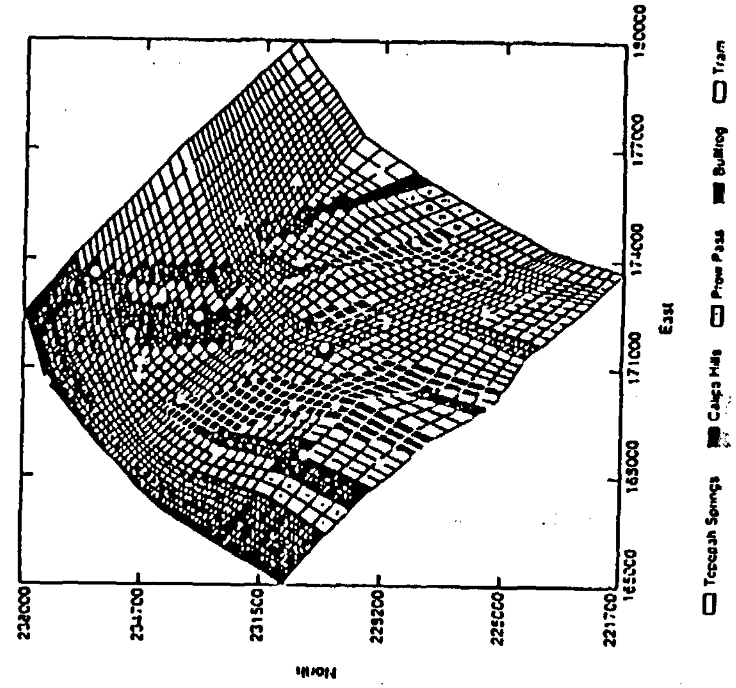


Figure 11-1. Geologic units intercepted by the water table (interpreted from Fridrich et al., 1991). Stars indicate well locations. Ordinate and abscissa values are Nevada state plane coordinates in meters.

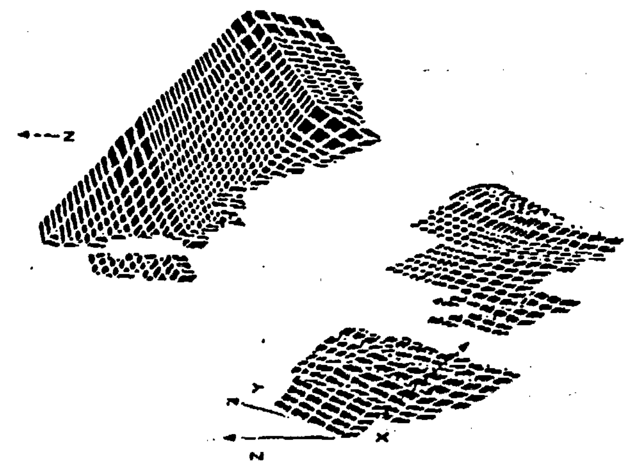


Figure 11-2. A three-dimensional view of the Topopah Spring unit below the water table, as constructed by translation.

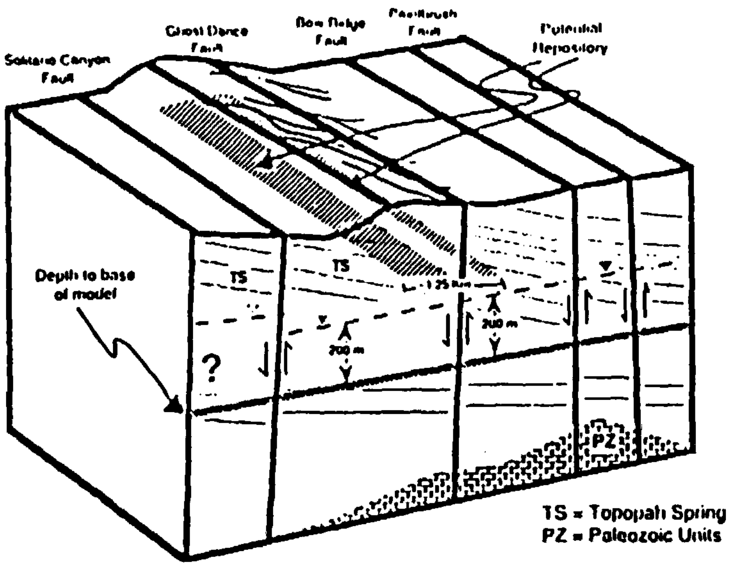


Figure 11-3. A schematic diagram showing the three-dimensional relationship among the potential repository, the stratigraphic units, and the major faults. Also shown is the depth of the base of the saturated-zone model developed for TSPA-93.

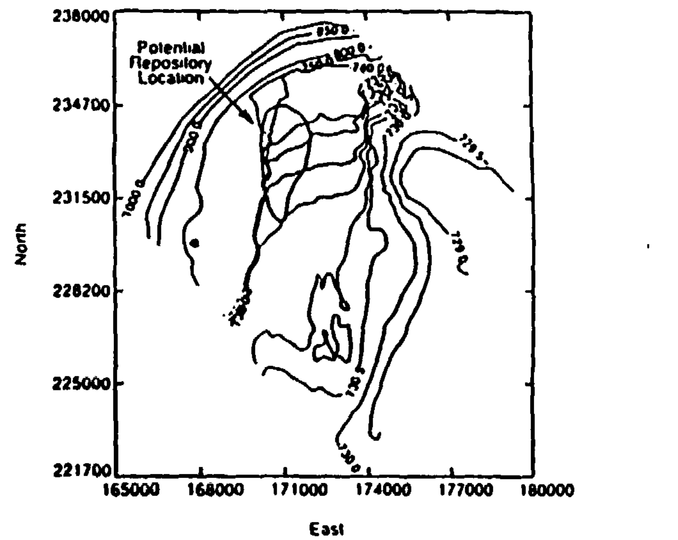


Figure 11-6. The potentiometric surface map based on calculated values of head for the case described in Table 11-2. Contour labels are meters above mean sea level. Coordinates are Nevada state plane coordinates (in meters).

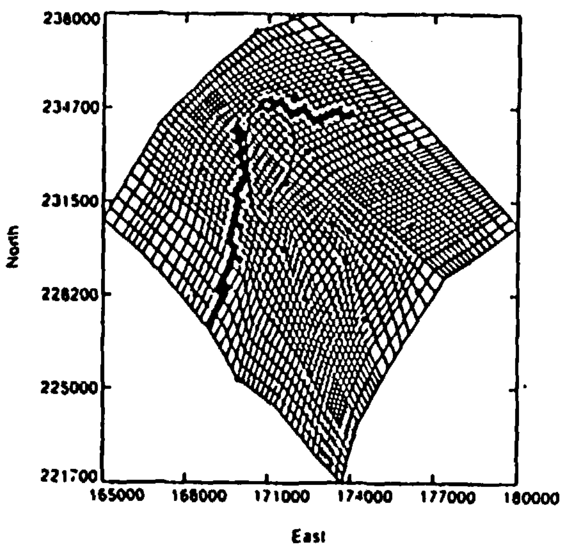


Figure 11-4. The approximate location of the potential repository, Solitario Canyon Fault Zone, and Drill Hole Wash Fault Zone on the calculational grid of Figure 11-1. Coordinates are Nevada state plane coordinates (in meters).

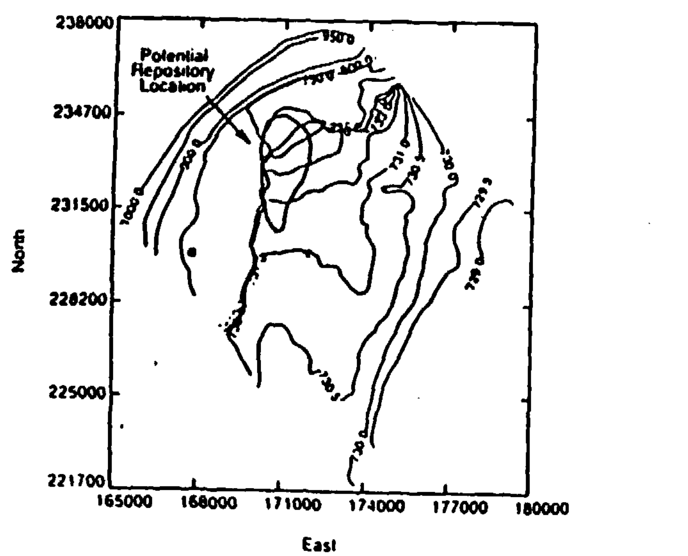


Figure 11-15. The potentiometric surface map based on calculated values of head for the case described in Table 11-4. Contours are altitude in meters. Coordinates are Nevada state plane coordinates (in meters).

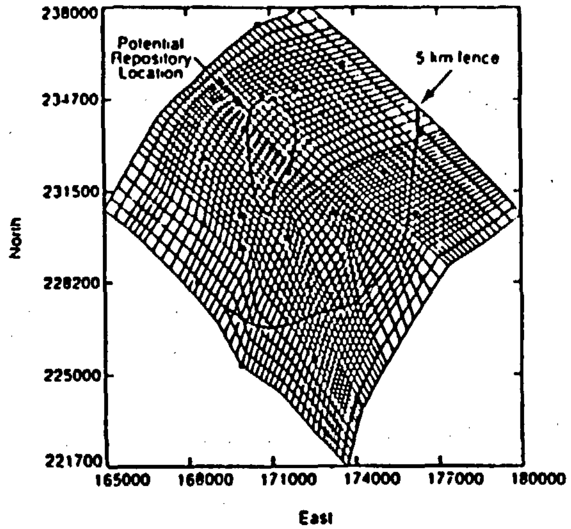


Figure 11-7. Approximate location of the 5-km fence at which breakthroughs are calculated. Coordinates are Nevada state plane coordinates (in meters)..

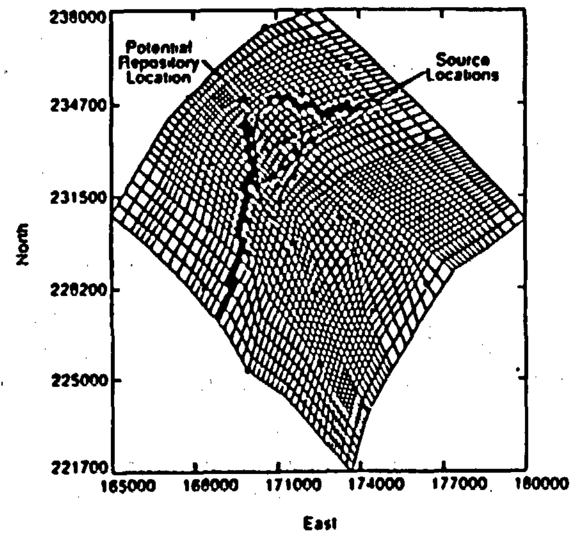


Figure 11-8. Locations of the three contaminant sources for transport calculations, shown as filled elements. Coordinates are Nevada state plane coordinates (in meters).

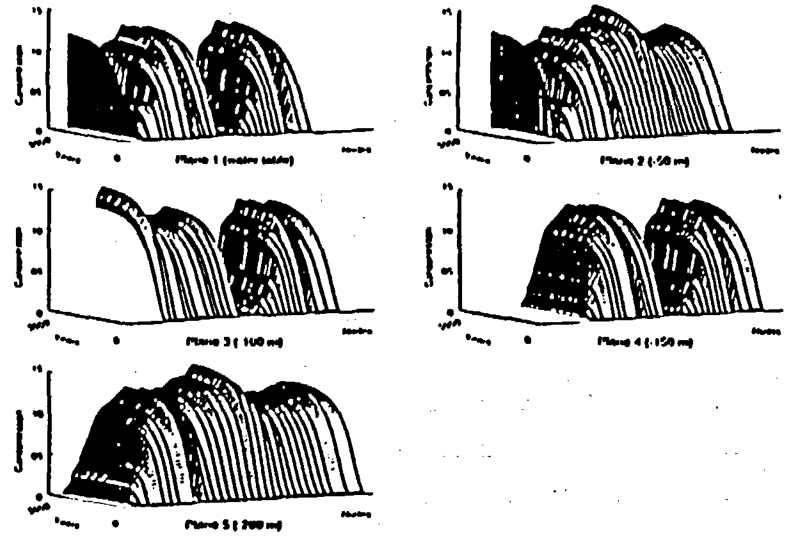


Figure 11-9 Breakthrough curves along the 5-km fence for a source of unit concentration located at the water table in the Prow Pass. Each set of curves is for a different depth below the water table.

TSPA-1993 SZ Abstracted Model

- Velocity calculated for each "fence" cell using distance from source divided by time to 50% max conc, and weighted by conc flux
- Velocity distribution approximated by using an advection/dispersi equation, using the mean velocity, and adjusting the dispersivity to produce a qualitative match
- Single flow tube created for each UZ column

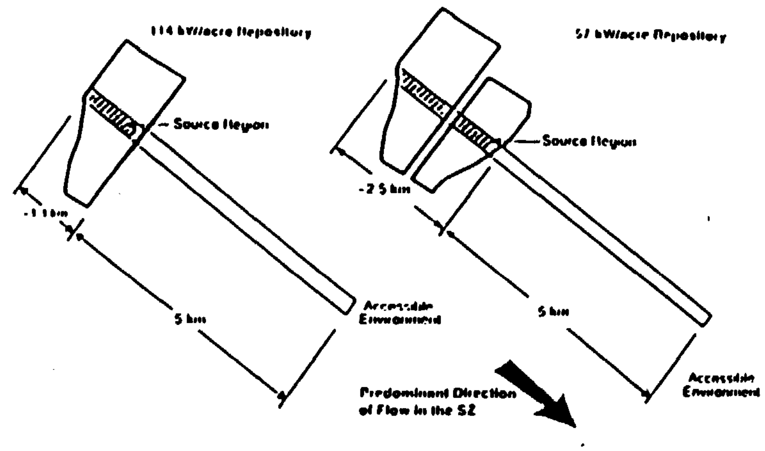
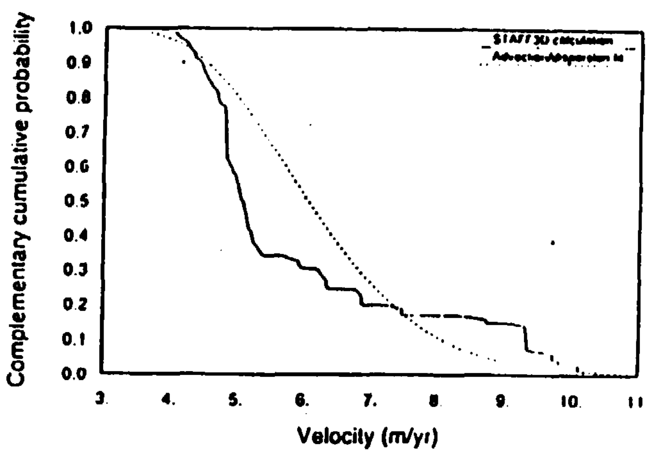


Figure 15-8. Layout of the one-dimensional flow tube used to describe the saturated zone for a weeps-model calculation.

TSPA-1993 SZ Abstracted Model (cont.)

- Velocity assumed to be uniformly distributed between low and high means of the diversionary and nondiversionary cases
- Dispersivity assumed to be uniformly distributed between 100 and 500 m
- Assuming a transverse dispersivity and a mixing depth: transport cross-sectional area was calculated to be uniformly distributed between 2×10^4 and 2×10^6 m^2



1-20. Distribution of effective velocities for Prow Pass source, no drain

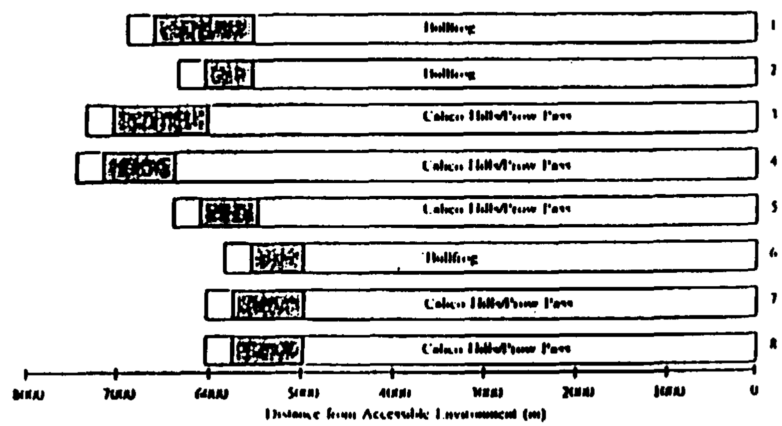


Figure 14-6. Saturated-zone flow tubes for 57-kW/acre cases. Unsaturated-zone releases are injected in the cross-hatched regions.

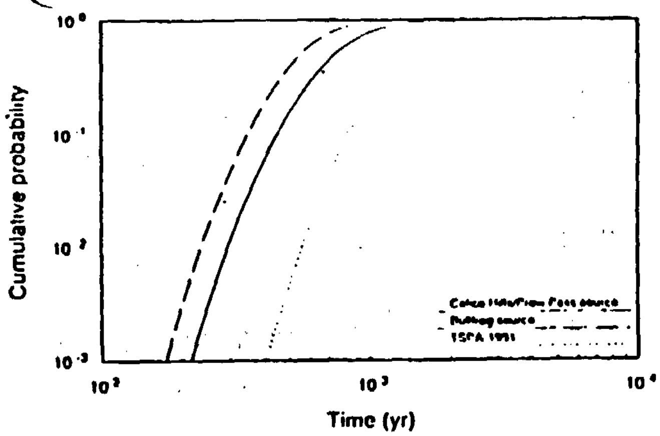


Figure 11-26. Comparison of SZ transport times for TSPA-91 and TSPA-93.

Table 11-6. Effective velocity and dispersivity for the six SZ cases.

Case	Velocity (m/yr)	Dispersivity (m)
Prow Pass source, no drain	5.9	130
Bullfrog source, no drain	8.7	170
Calico Hills source, no drain	6.0	110
Prow Pass source, drain	10.8	150
Bullfrog source, drain	12.5	100
Calico Hills source, drain	10.3	150

Table 11-7. Velocity and dispersivity distributions for TSA simulations.

Model parameter	Distribution
CH/PP* velocity (Cols. 3-5, 7, 8)	uniform from 5.5 to 11 m/yr
BF† velocity (Cols. 1, 2, 6)	uniform from 8.5 to 12.5 m/yr
Dispersivity	uniform from 100 to 500 m

*Calico Hills/Prow Pass source.
†Bullfrog source.

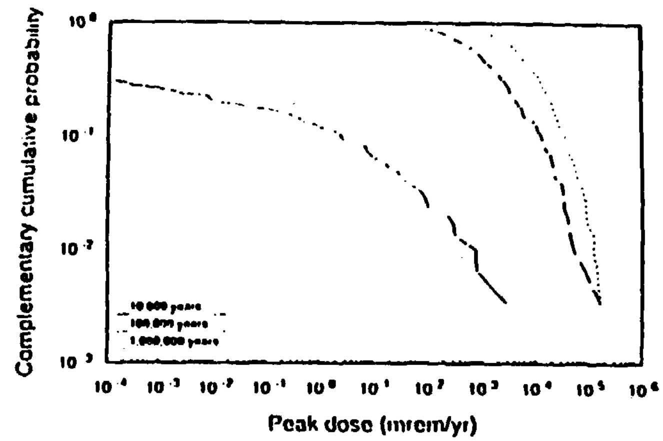


Figure 14-27. CCDFs for three time periods (57 kW/acre, vertical emplacement). Top: normalized cumulative aqueous release. Bottom: peak individual drinking-water dose rate.

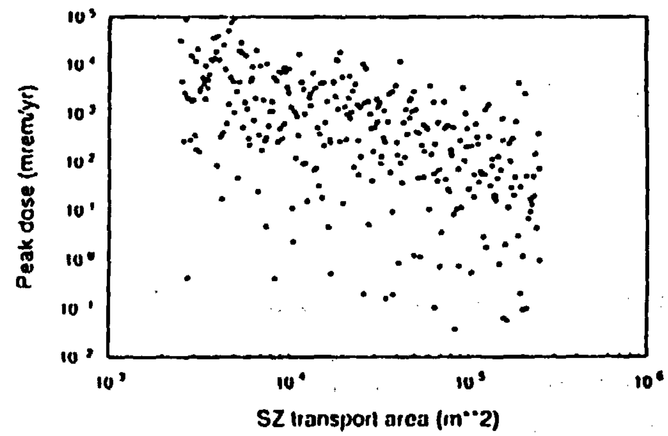


Figure 14-35. Scatter plot of peak individual drinking-water dose rate over 1,000,000 years vs. saturated-zone transport area (57 kW/acre, vertical emplacement, Column 8).

Key Aspects of SZ Flow and Transport (Based on Past TSPAs)

- Travel Time (flux, decay, etc.)
- Dilution (flux, dispersion, etc.)

Next?

NRC Concerns

- Future water-table levels
- Large Hydraulic gradient
- Dilution factors and channelization
  - use hydrochemical data and tracer test to validate models
  - better define mixing during well pumping (e.g., total withdrawal idea)

SZ Needs for TSPA-VA

- We must be able to run hundreds of model calculations of the entire system.
- The calculations must cover at least 10,000 years, and some will cover 1,000,000 years.
- The calculations must include time-varying boundary conditions caused by changes in climate and possibly thermal effects.
- We must have the flexibility to allow channeling.

What TSPA Can Use

- List of key issues
- Prioritization
- Methods to address key issues
  - TSPA models
  - sensitivity studies

What TSPA Can Use (cont.)

- Points for a response surface?
  - dilution-factor distribution
  - travel-time distribution
- Parameters for a 1-d model?
  - velocities or travel times
  - breakthrough curves
  - cross-sectional areas
- Simplified model?

Data Needs

- Fracture distribution and properties (via well tests)
- Measurement of heads and permeabilities and temperature (LHG, faults, revisit existing wells) as a function of depth
- Tracer tests around faults, Dune Wash (STC), H-4 through ONC-1 to C-wells
- Measure isotopes and chemistry as a function of depth

The End

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Saturated Zone Flow and Transport Abstraction/Testing Workshop

Review of SZ Flow and Transport Issues

BILL W. ARNOLD
SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NM
April 1, 1997

Objectives:

- Inform all workshop participants of the current understanding of these issues.
- Develop a comprehensive list of issues relevant to SZ flow and transport.
- Prioritize these issues based on criteria related to long-term performance of the repository.
- Discussion of these issues is <u>not</u> intended to definitively resolve the issues. Focus of the discussions should be on prioritization and the question of how TSPA calculations can incorporate uncertainty associated with the highest priority issues.

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Conceptual Models of SZ Flow

- Alternative conceptual models
- Hydraulic properties of faults
- Vertical flow
- Distribution of recharge
- Regional discharge
- Grid sensitivity
- Implications of isotopic and hydrochemical data

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Conceptual Models of SZ Geology

- **Flow channelization**
- **Spatial distribution of hydraulic conductivity**
- **Geologic and mineralogic framework**

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Transport Processes and Parameters

- Dispersivity
- Matrix diffusion (effective porosity)
- Sorption
- Colloid transport
- Radionuclide solubility

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Coupling to Other Components of TSPA

- Climate change
- Thermal and chemical plume
- Well withdrawal scenarios
- Coupling with UZ transport

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TSPA Introduction to Issue 1: Conceptual Models of SZ Flow

Jack Gauthier
SZ Abstraction/Testing Workshop
1–3 April 1997

Subissue 1.1
Alternative Conceptual Models

- Cause of the LHG
- Role of faults*
- Channelization (REV)*
- Outflows*
  - present (Death Valley or Franklin Lake Playa)
  - pluvial
- Future conditions (e.g., water-table levels)*

Subissue 1.2
Hydraulic Properties of Faults

- Barriers or conduits*
- What faults must be considered*
- Will tectonics signficantly change present fault properties

Subissue 1.3
Vertical Flow

- Is upwelling from the carbonates significant
- Is the upwelling distribution significant
- How does water flow where the tuffs pinch out
- What are the implications for mixing

Subissue 1.4
Distribution of Recharge

- Is there significant recharge at YM
  - present
  - future
- Do recharge zones change with time (climate)

Subissue 1.5
Regional Discharge

- Death Valley or Franklin Lake Playa*
- Future springs
- Future Forty Mile Creek

* Being considered for TSPA-VA

1. Conceptual Models of SZ Flow

1.1 Alternative conceptual models

John B. Czarnecki
U.S. Geological Survey

April 1, 1997

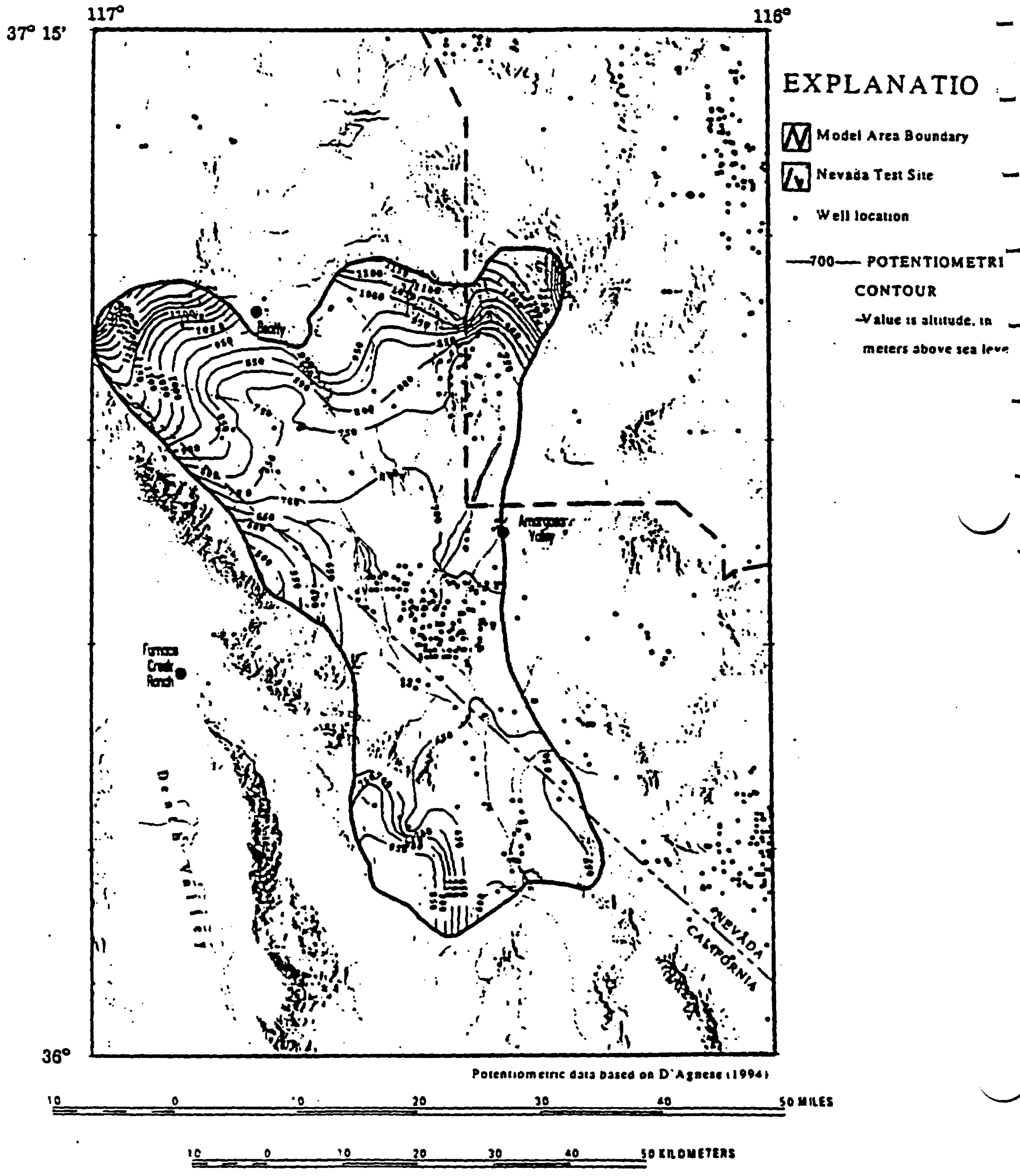


Figure 2. —Potentiometric surface.

Large Hydraulic Gradient: Possible Causes

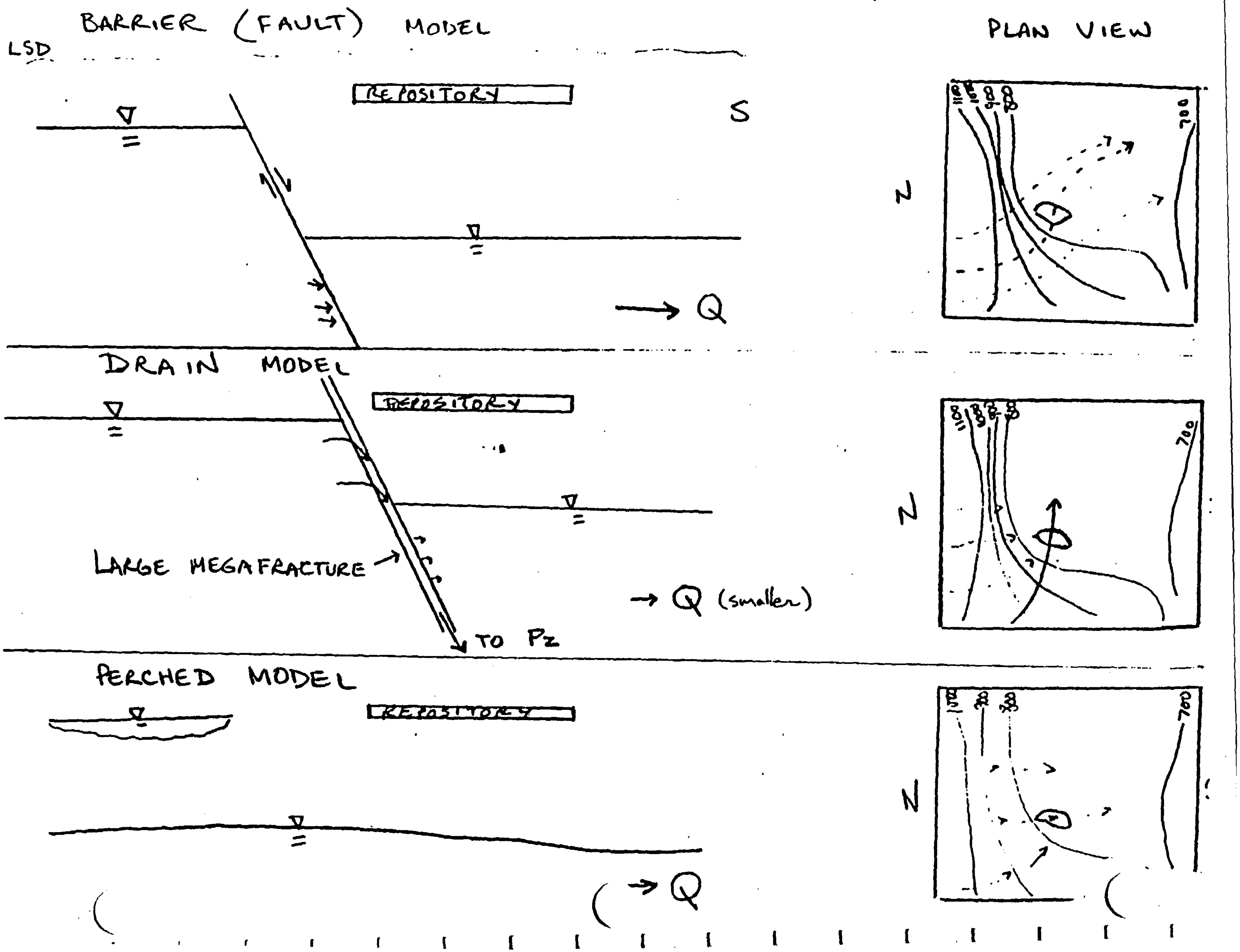
- faults that contain nontransmissive fault gouge or that juxtapose transmissive tuff against nontransmissive tuff

- the presence of a different type of lithology that is less subject to fracturing

- a change in the direction of the regional stress field and a resultant change in the intensity, interconnectedness, and orientation of open fractures on either side of the area with the large hydraulic gradient

- an apparent large gradient resulting from a disconnected, perched or semi-perched water body; or

- a highly permeable buried fault that drains water from tuff units into a deeper regional carbonate aquifer


BARRIER (FAULT) MODEL
LSD
PLAN VIEW
N
S
REPOSITORY
Q
700
DRAIN MODEL
REPOSITORY
LARGE MEGAFRACTURE
TO Pz
Q (smaller)
N
700
PERCHED MODEL
REPOSITORY
Q
N
700

Evidence for Perched Water in Borehole USW G-2

1. 12-m decline in the water level in G-2 over its hole history;

2. Water wet borehole walls and observed dripping water in the air filled part of the borehole above the basal vitrophyre of the Topopah Spring member

3. Decrease in the thermal gradient in the borehole with time

4. Observed downward flow in the water-filled part of the borehole from pulsed-heat flow surveying

5. Moderate hydraulic conductivity in the Calico Hills Formation

6. Less-than-full recovery (0.5 m) of the water level following hydraulic testing

7. Apparent partial saturation within the Calico Hills formation based on analyses of borehole geophysical logs, with a coincidental return to full saturation at an altitude of ~730 m (top of the Crater Flat tuff).

Issue: Resolution of the Cause of the Large Hydraulic Gradient

Proposal:

- Finish hydraulic testing and hydrochemical sampling in borehole USW G-2;

- Drill and test WT-24 (located between USW G-2 and UZ-14)

- Finish analysis of saturations in UZ-14 and compute saturations based on borehole geophysics data

- Drill other WT holes identified in Study Plan 8.3.1.2.1.3

- Prepare *complete* model analyses for each conceptual model of the large hydraulic gradient

THERMAL EVIDENCE FOR THE ROLES OF FAULTS AND THE LOWER CARBONATE AQUIFER IN THE PATTERN OF SATURATED-ZONE FLOW AT YUCCA MOUNTAIN

William W. Dudley, Jr.

U. S. Geological Survey

TSPA-VA Saturated Zone Flow and Transport Abstraction/Testing Workshop

April 1, 1997 Denver, Colorado

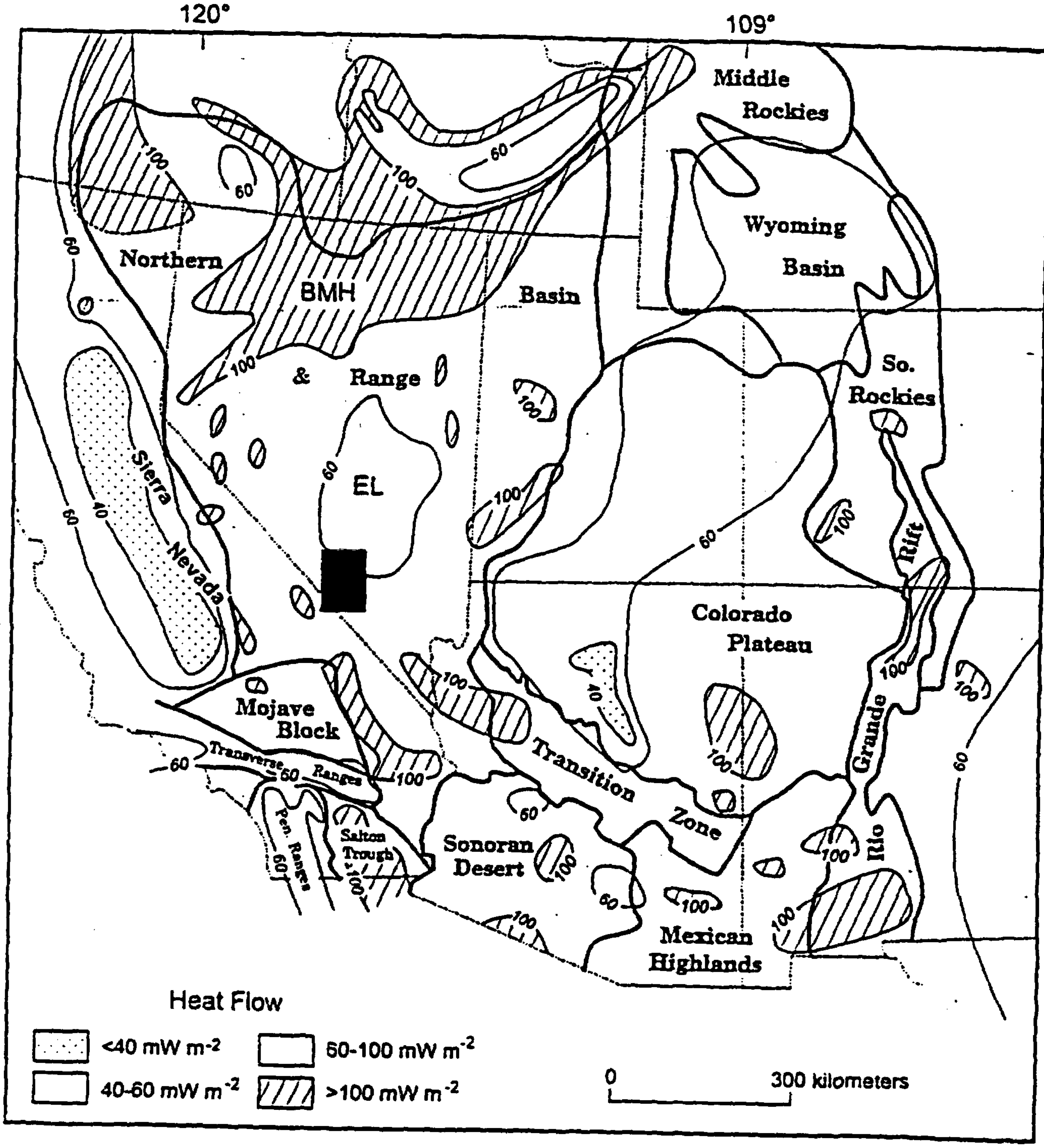


Figure 8.1. Distribution of heat flow in the western United States (modified from Sass and others, 1994). Abbreviations: BMH, Battle Mountain High; EL, Eureka Low. Black box at the south end of EL denotes location of figure 8.2.

From Sass and others, 1995

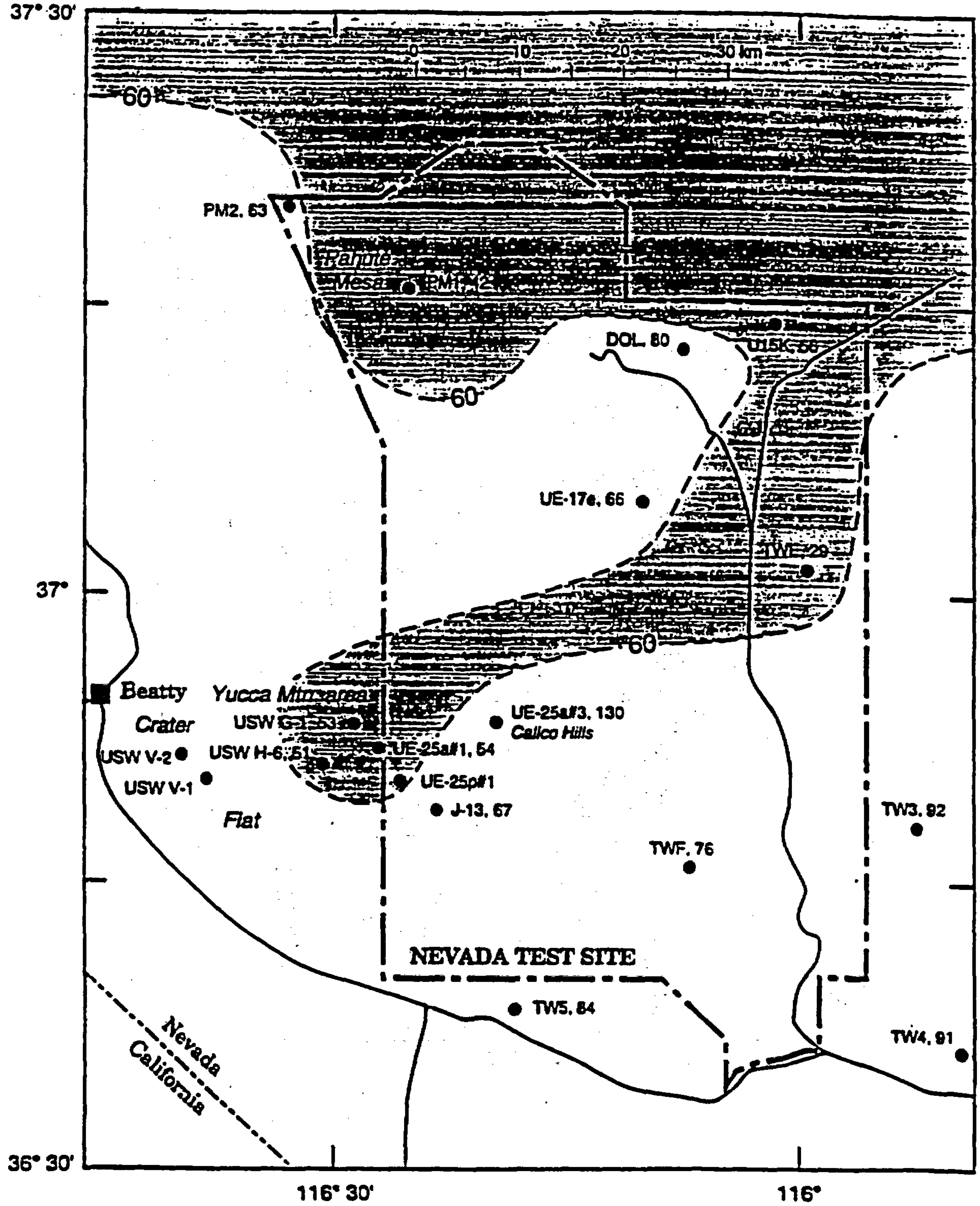
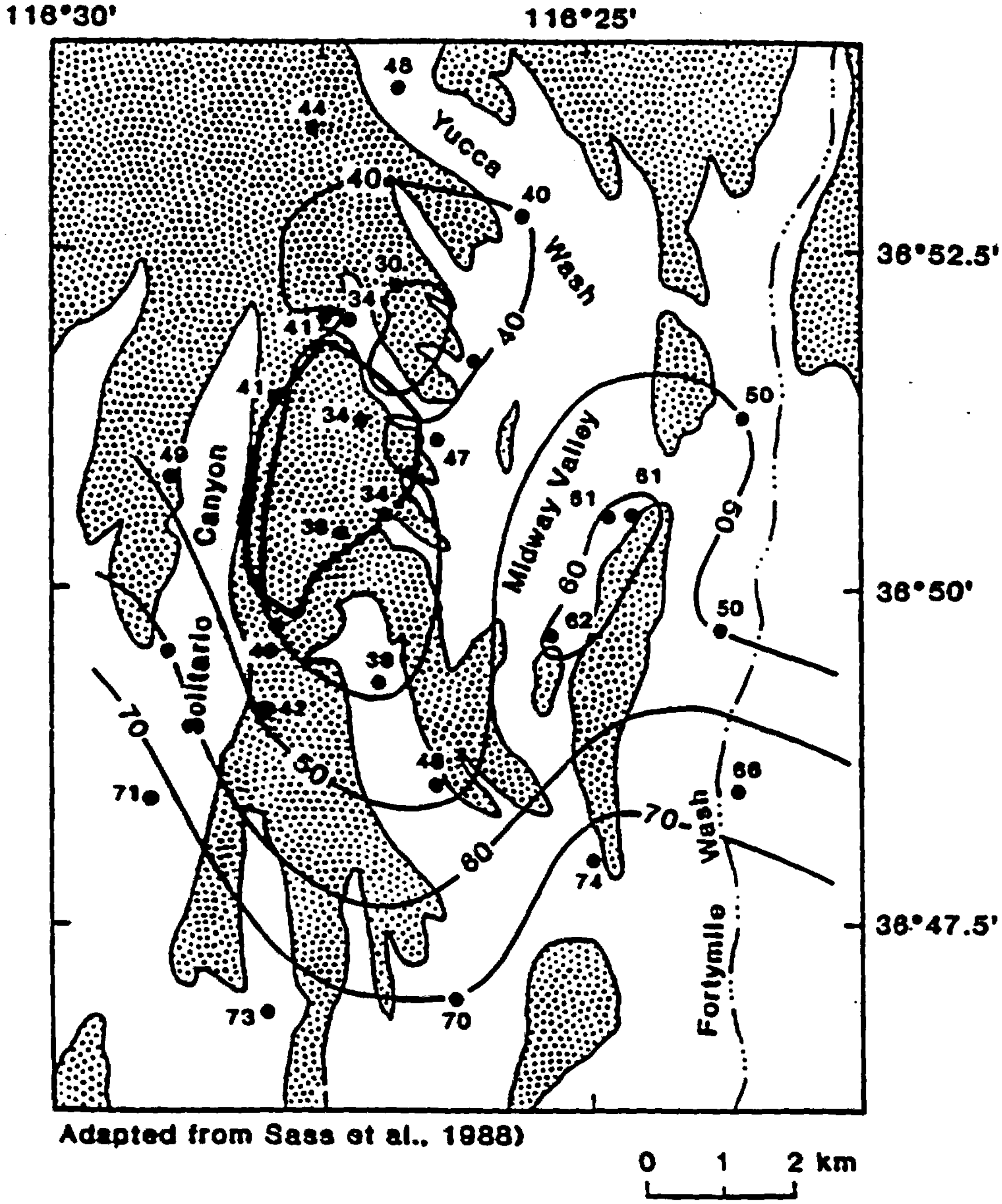


Figure 8.2. Configuration of 60 mW m^{-2} contour in the vicinity of the Nevada Test Site. Shaded area defines the southernmost part of the Eureka Low (see fig. 8.1). All heat flows shown were determined in the saturated zone (SZ). Where a heat flow could not be determined for the SZ (drill holes V-1, V-2, UE-25p#1), no value is plotted.

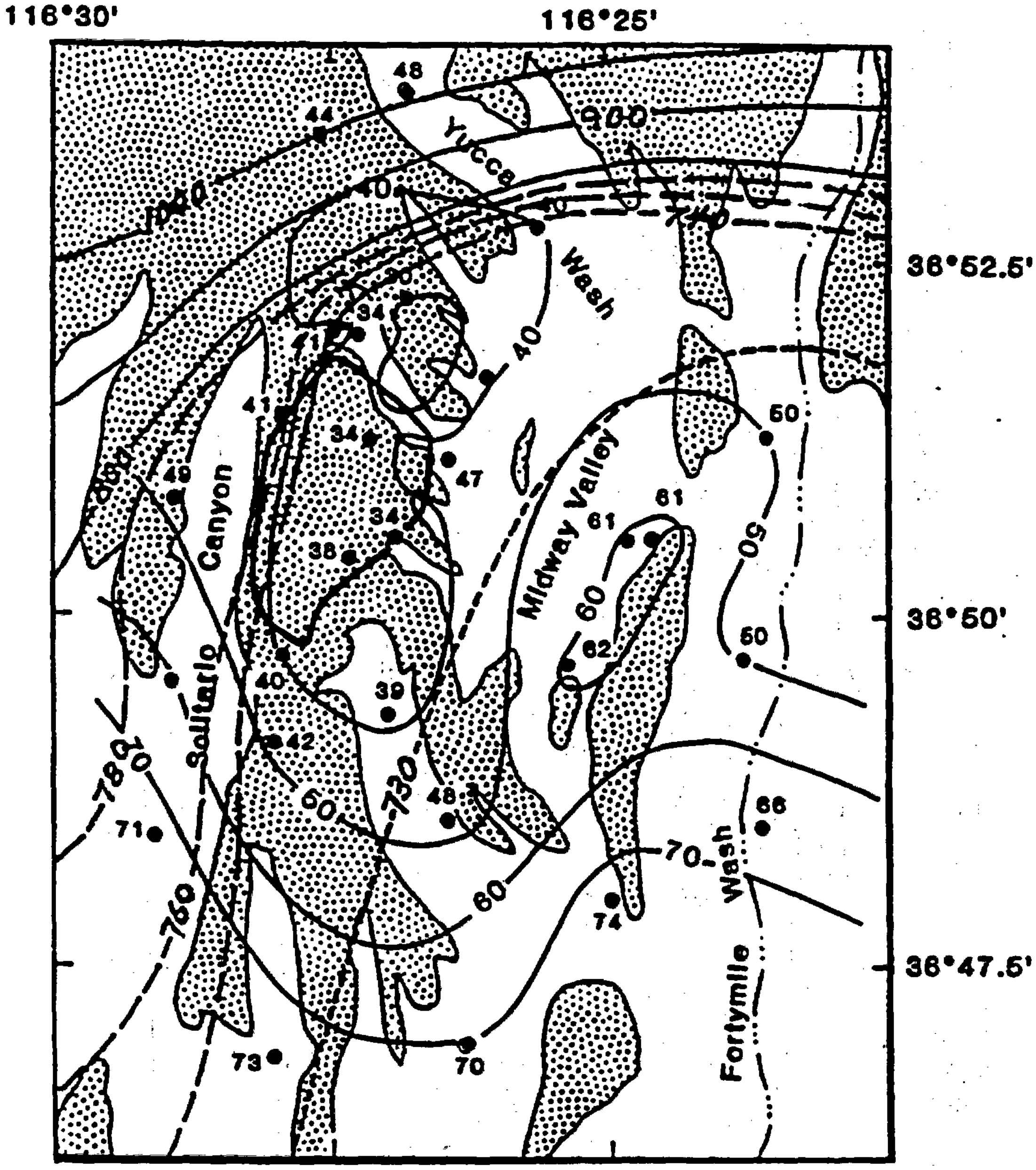
From Sass and others, 1995

HEAT FLOW IN UNSATURATED ZONE



Adapted from Sass et al., 1988)

HEAT FLOW IN UNSATURATED ZONE

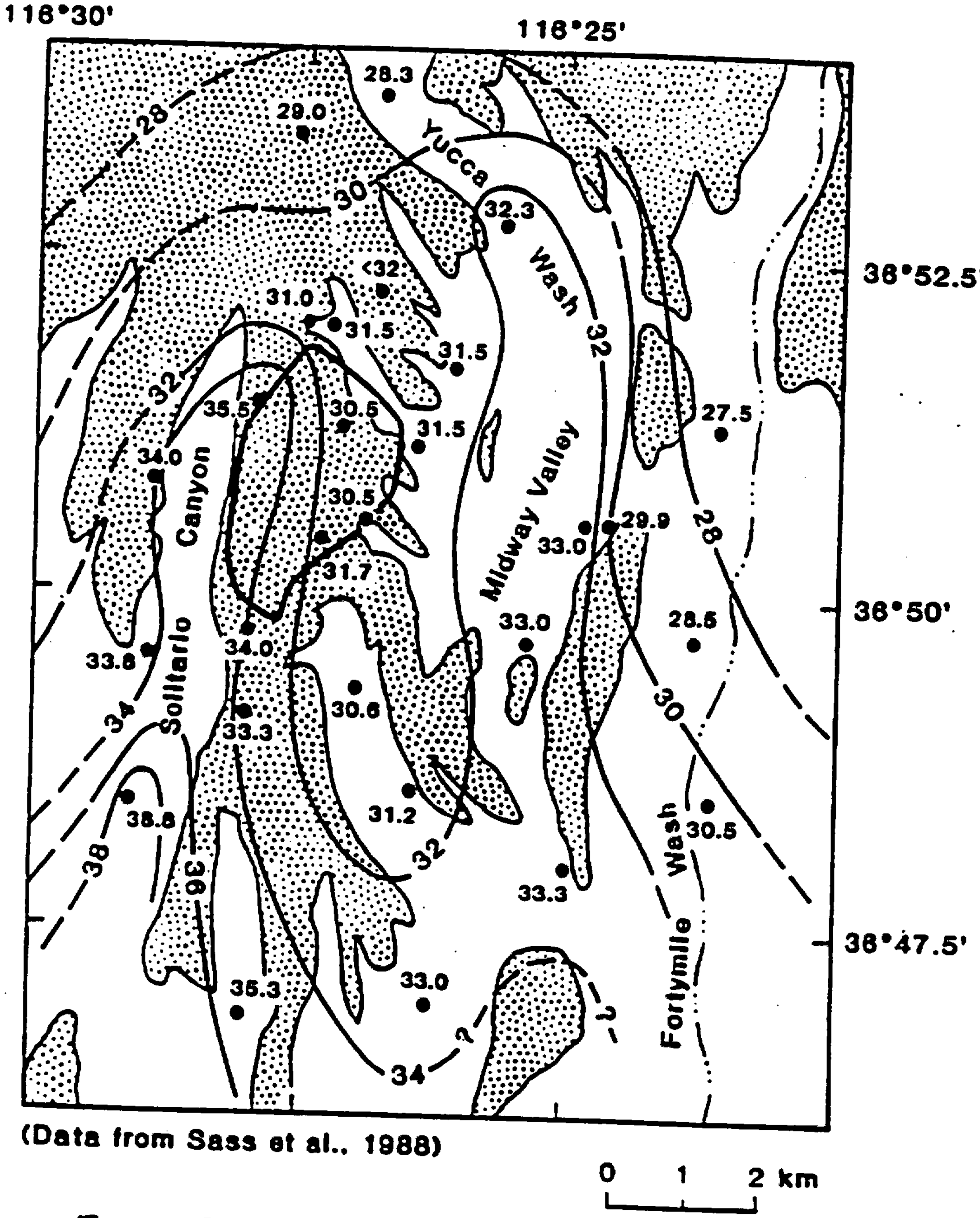


Adapted from Sass et al., 1988)

0 1 2 km

Water-table contours compiled from:
Robison, 1984
Dudley, 1990
Ervin and others, 1994

TEMPERATURE (°C) AT WATER TABLE



(Data from Sass et al., 1988)

From Sass and others, 1995

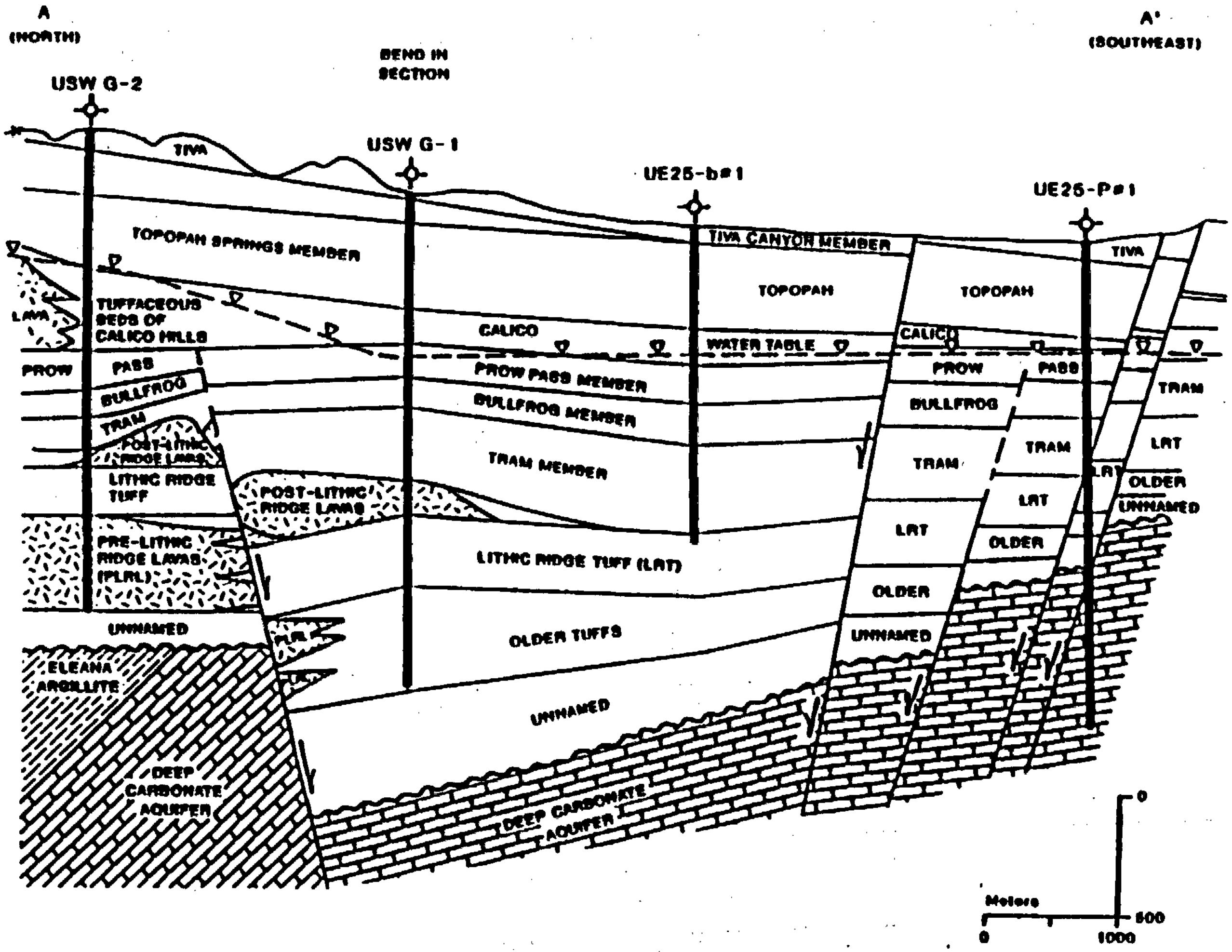
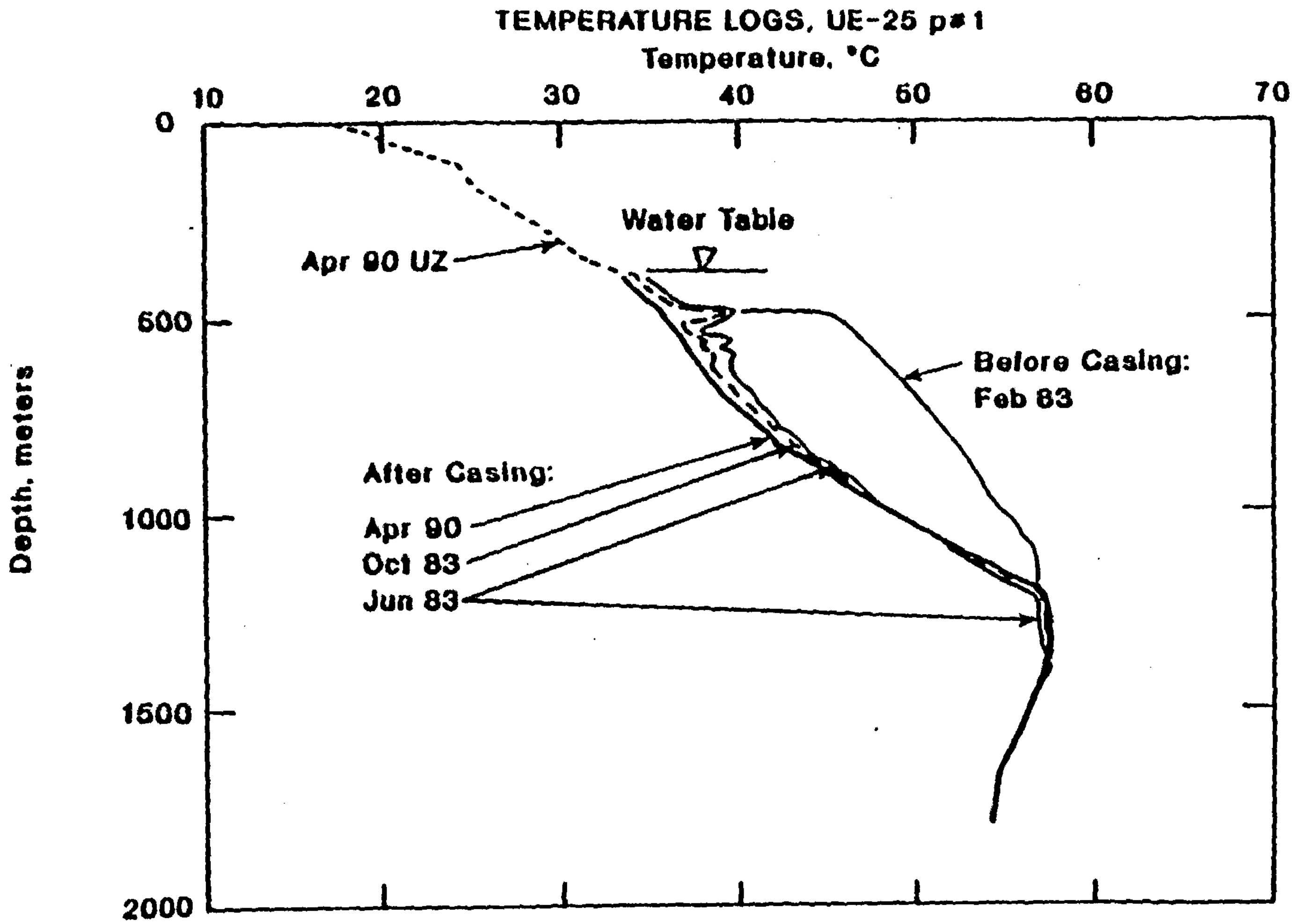
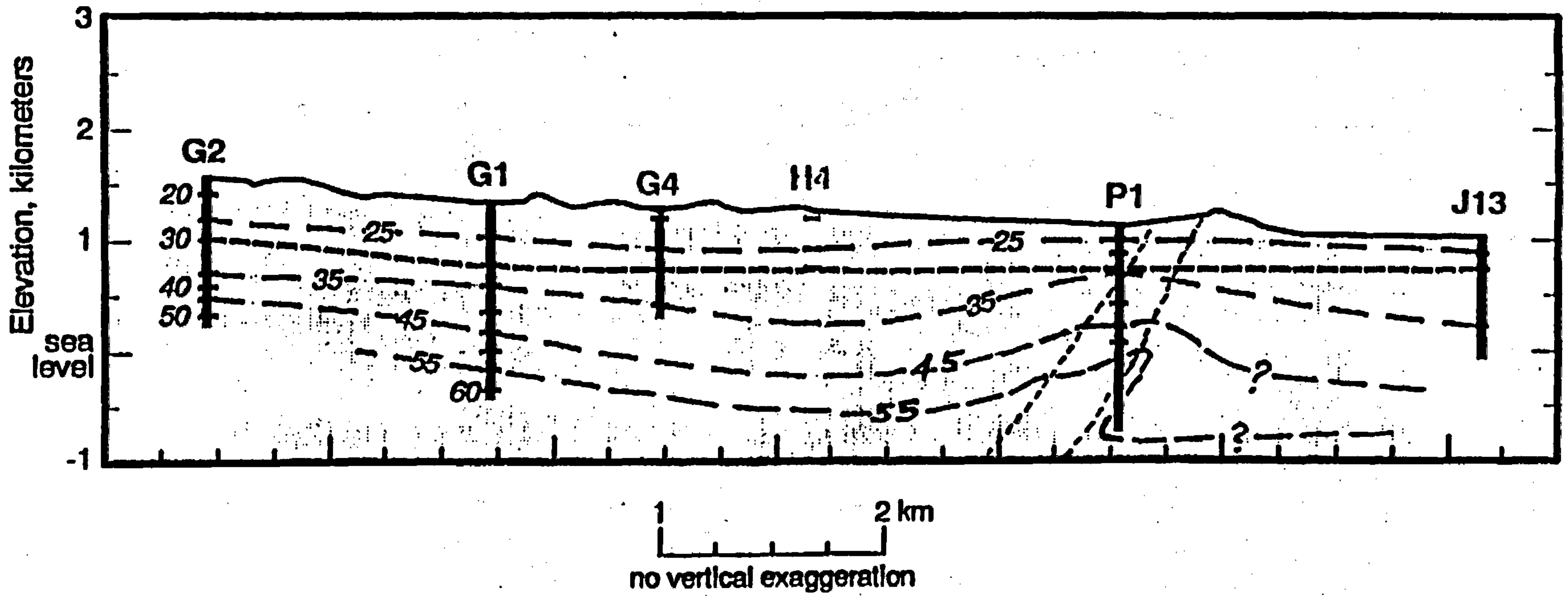


Fig. 11. North-to- southeast geologic section across Yucca Mountain showing the interpreted buried graben. Line of section shown in Fig. 5. Constructed using data from the full suite of lithology logs, cited in the caption of Fig. 4.

E-43

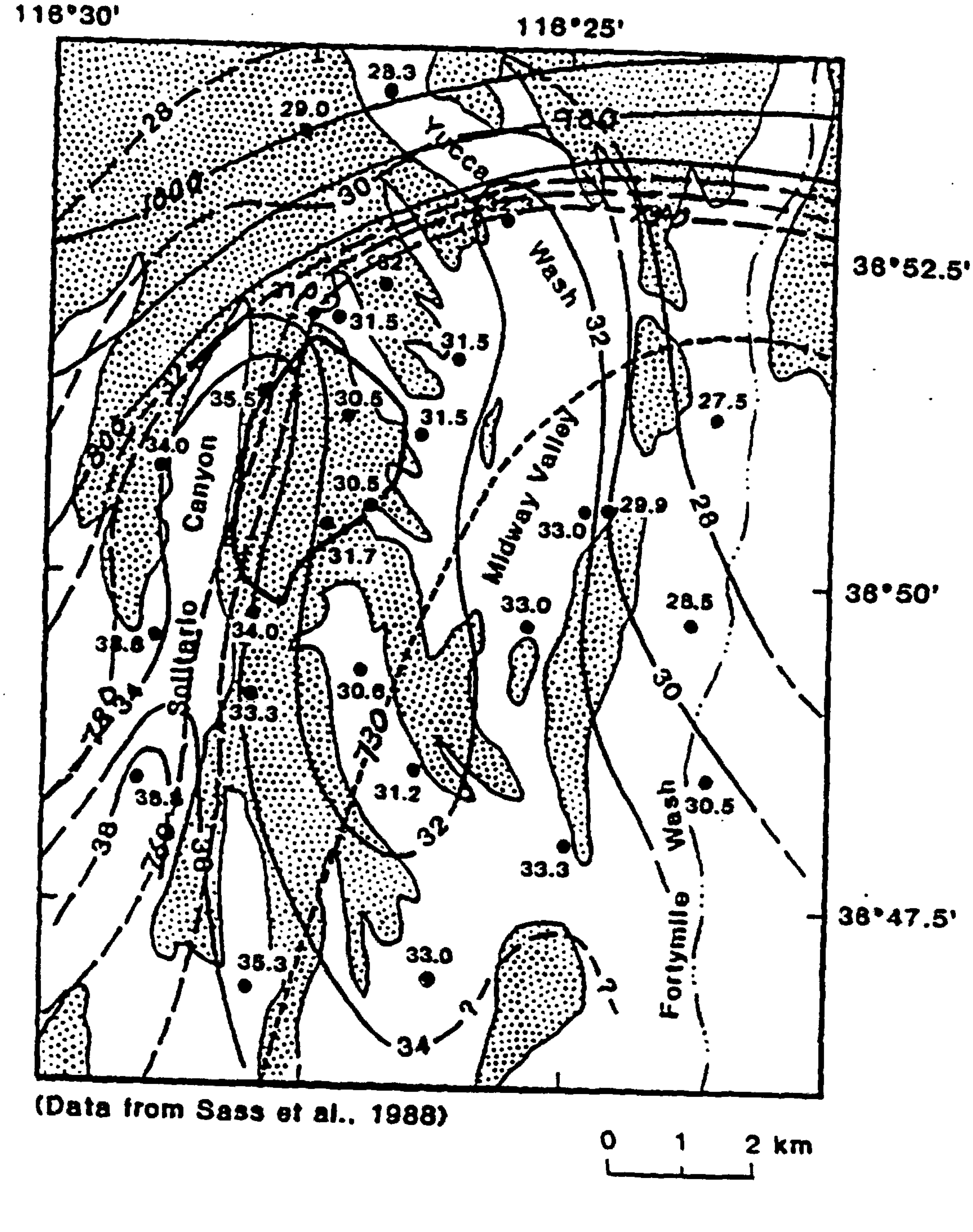


Compiled from: Craig and Robison, 1984
Sass and others, 1988
Sass and others, 1995



Modified from Sass and others, 1988

TEMPERATURE (°C) AT WATER TABLE



(Data from Sass et al., 1988)

REFERENCES

Craig, R. W., and J. H. Robison, 1984. Geohydrology of Rocks Penetrated by Well UE-25p#1, Yucca Mountain Area, Nye County, Nevada. U. S. Geological Survey, Water-Resources Investigations Report 84-4248

Dudley, W.W., Jr., 1990. Multidisciplinary hydrologic investigations at Yucca Mountain. High Level Radioactive Waste Management, International Topical Meeting Proceedings: American Nuclear Society and American Society of Civil Engineers, v. 1, p. 1-9

Ervin, E. M., R. R. Luckey, and D.J. Burkhardt, 1994. Revised Potentiometric-Surface Map, Yucca Mountain and Vicinity, Nevada. U. S. Geological Survey, Water-Resources Investigations Report 93-4000

Fridrich, C.J., Dudley, W.W., Jr., and Stuckless, J.S., 1994. Hydrogeologic analysis of the saturated-zone ground-water system under Yucca Mountain, Nevada. Journal of Hydrology, v. 154, p. 133-168

Robison, J. H., 1984. Ground-Water Level Data and Preliminary Potentiometric-Surface Maps, Yucca Mountain and Vicinity, Nye County, Nevada. U. S. Geological Survey, Water-Resources Investigations Report 84-4197

Sass, J. H., A. H. Lachenbruch, W. W. Dudley, Jr., S. S. Priest, R. J. Munroe, 1988. Temperature, thermal conductivity, and heat flow near Yucca Mountain, Nevada: Some tectonic and hydrologic implications. U.S. Geological Survey Open-File Report 87-649, 118 p.

Sass, J. H., W. W. Dudley, Jr., and A. H. Lachenbruch, 1995. Chapter 8, Regional thermal setting, *in* H. W. Oliver, D. A. Ponce, and W. C. Hunter (eds.), Major Results of Geophysical Investigations at Yucca Mountain and Vicinity, Southern Nevada. U.S. Geological Survey Open-File Report 95-74, p. 199-218

HYDRAULIC PROPERTIES of FAULTS

G.E.Barr, SNL

Head Change at Solitarion Canyon fault

Apparent Compartmentalizations

WT Temperature Data

Geologic Framework Model

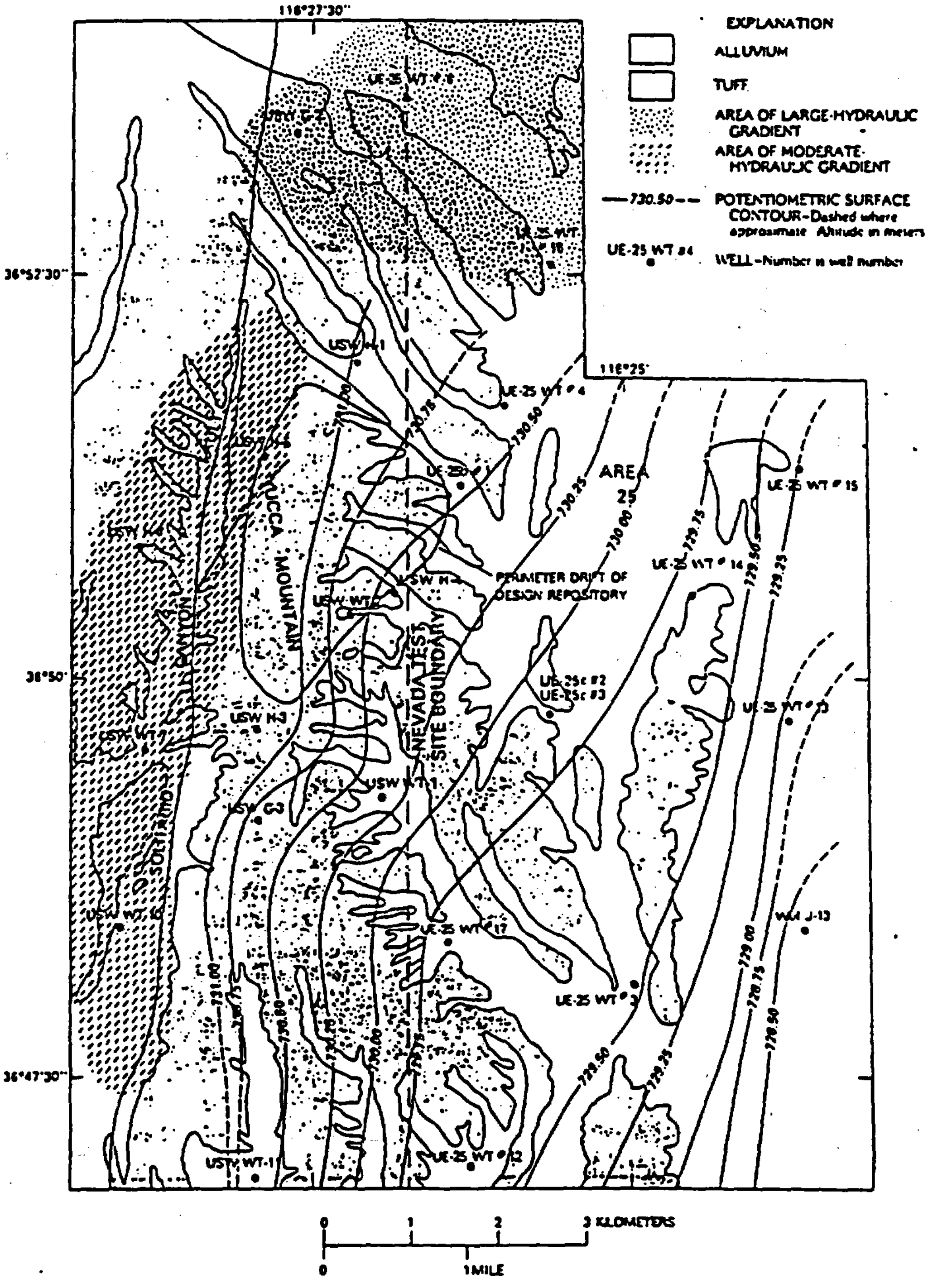
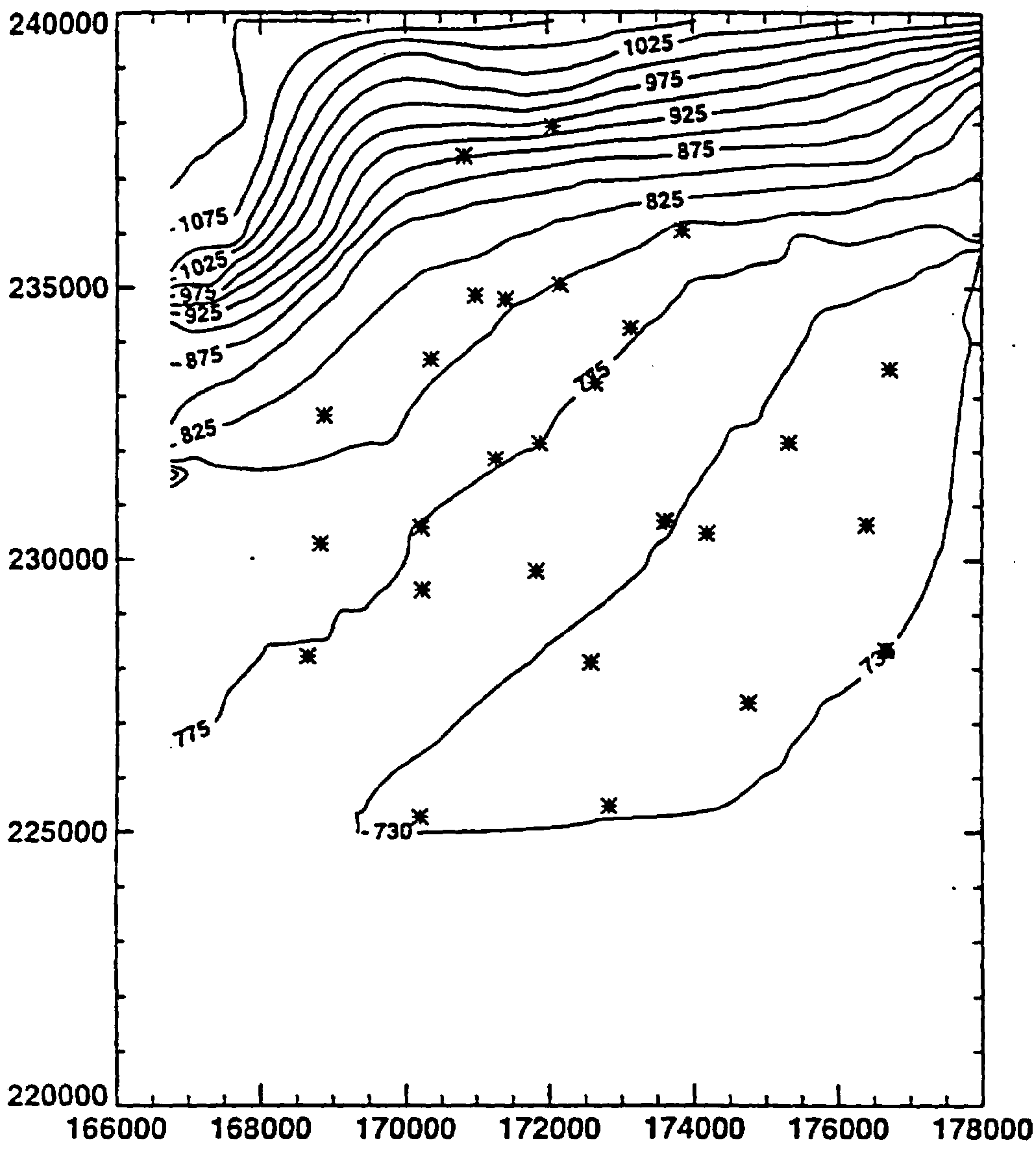


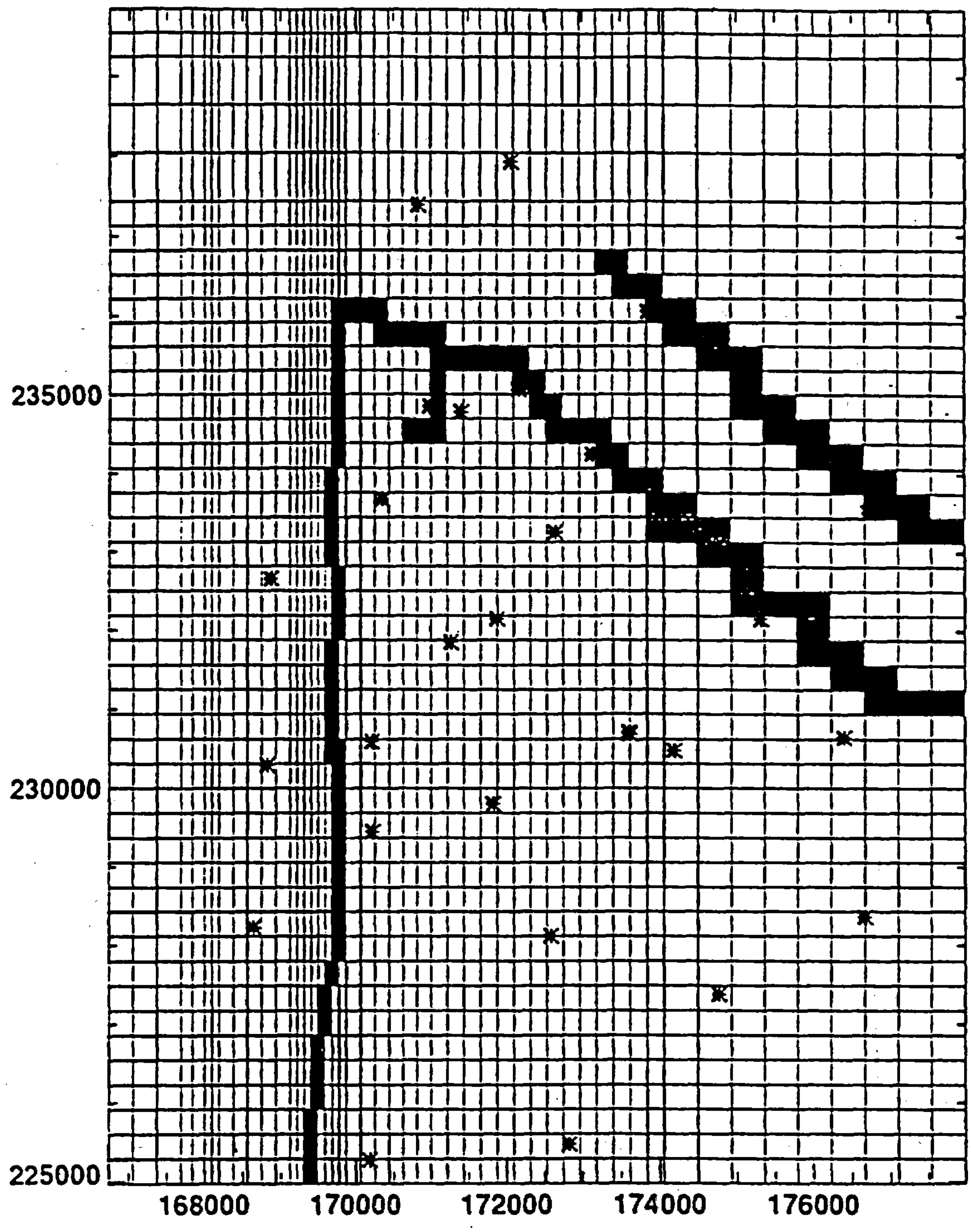
Figure 11-5. The revised potentiometric surface map from Ervin *et al.* (1993a).

zeld1.out
Level 5



No Faults

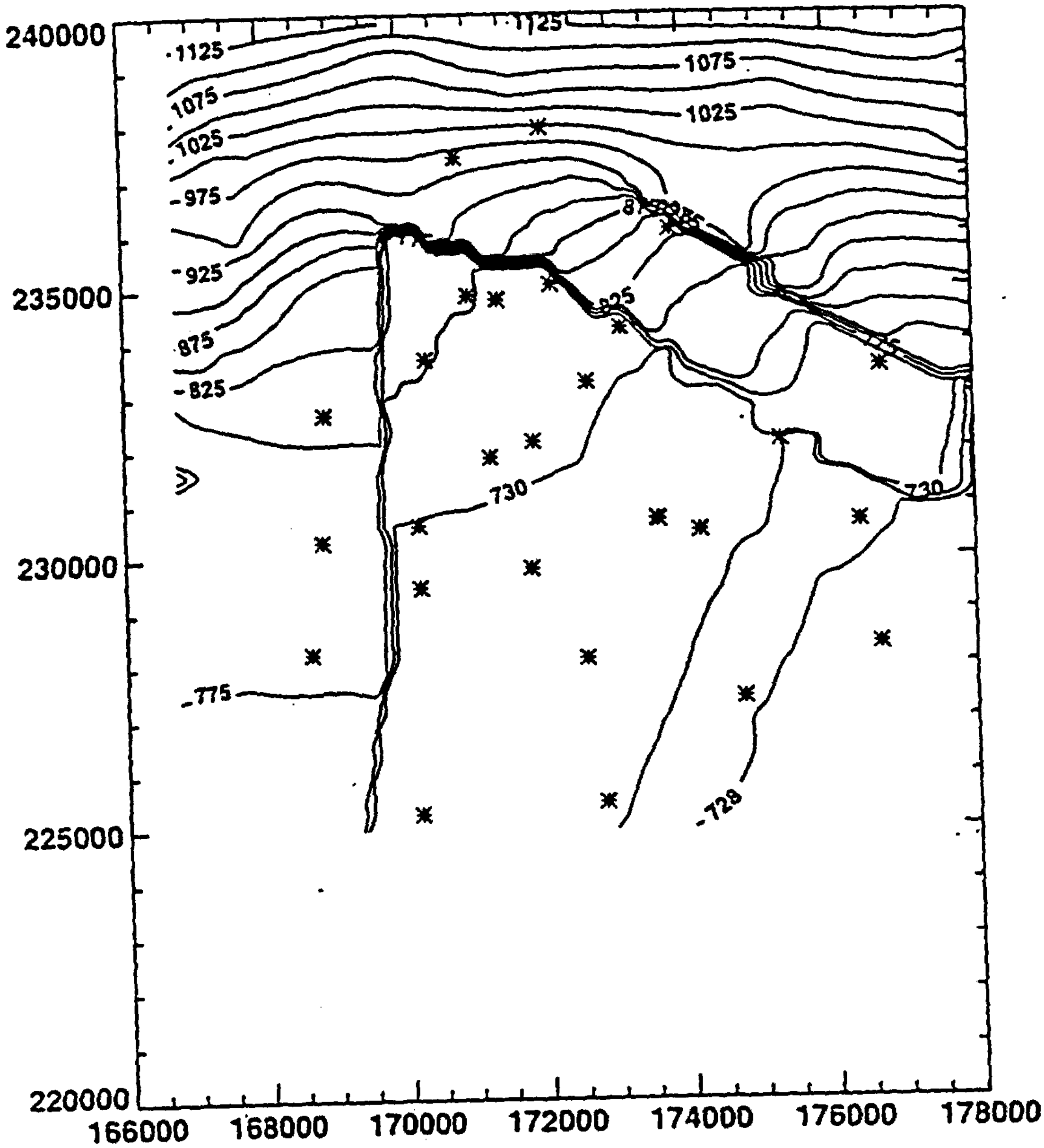
Faults 5.slw



Solitario Canyon Fault
Solitario Canyon Fault Extension (GAP)

H-5 Splay Extension (SplayX)
Drill Hole Wash
Yucca Fault

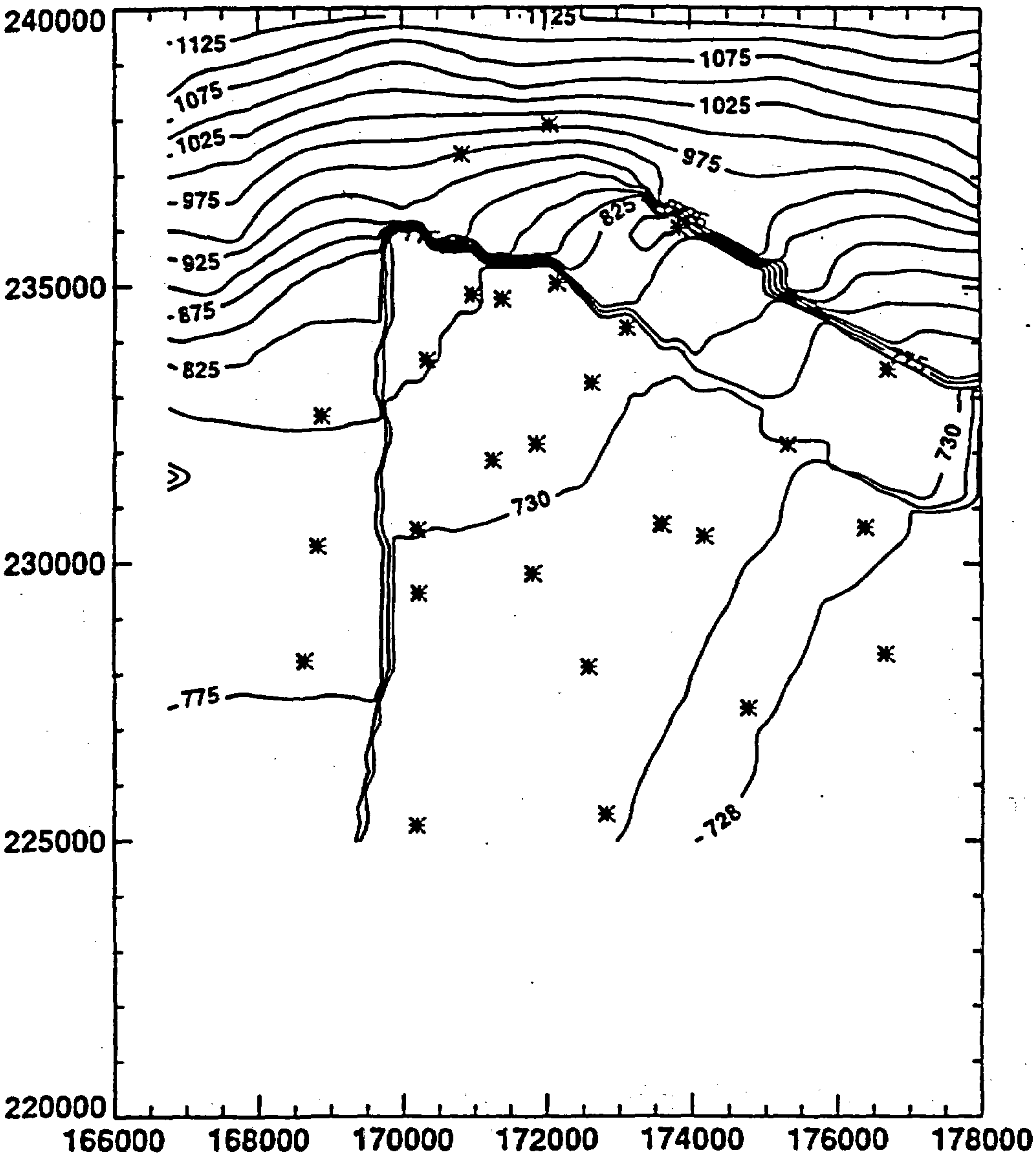
zelu1.out
Level 5



Bow Ridge fault absent

WT head at WT-16 = 801.15m

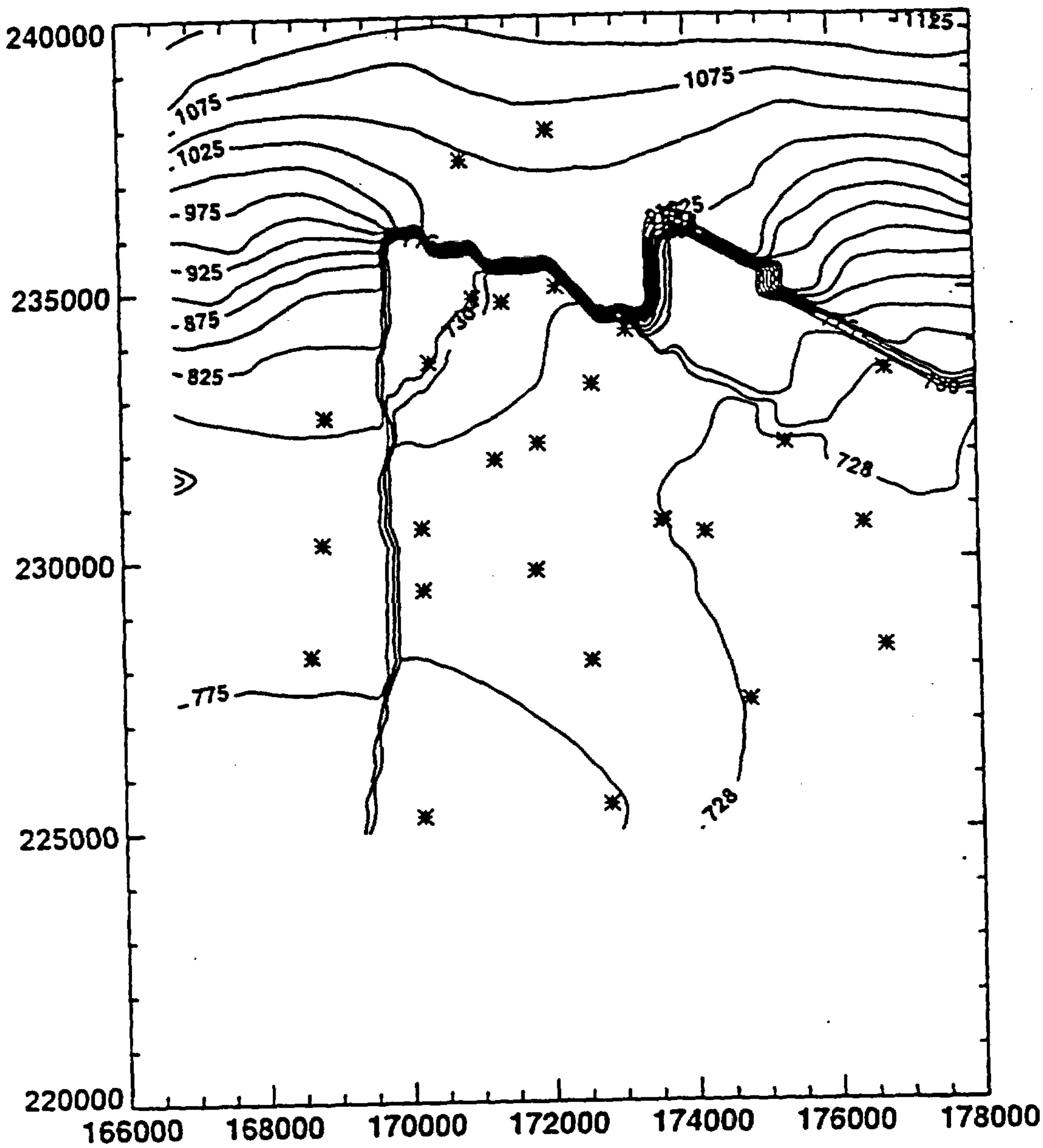
zeldra1.out
Level 5



Drain at WT-16

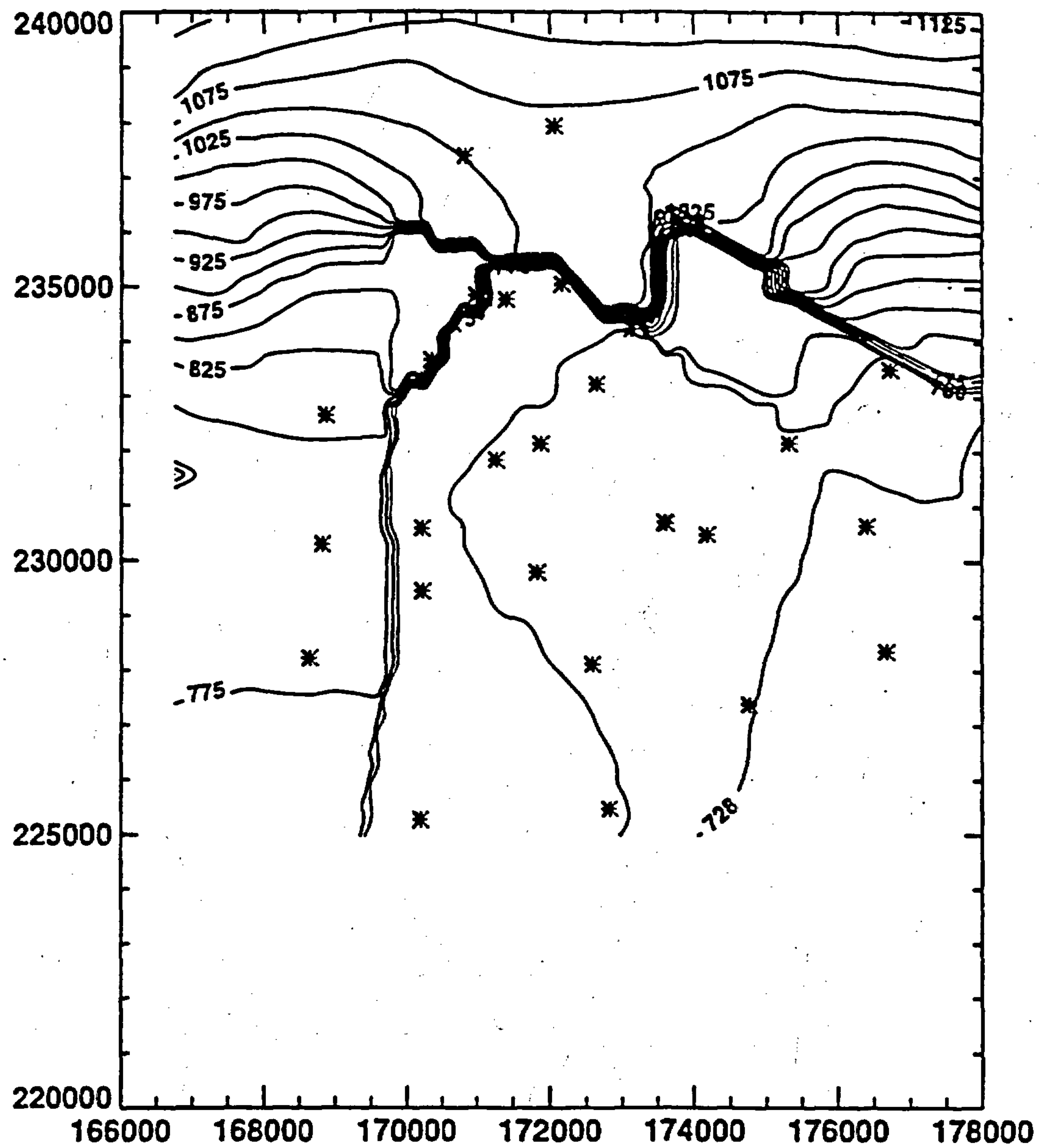
WT-16 = 827.72m

zelx1.out
Level 5

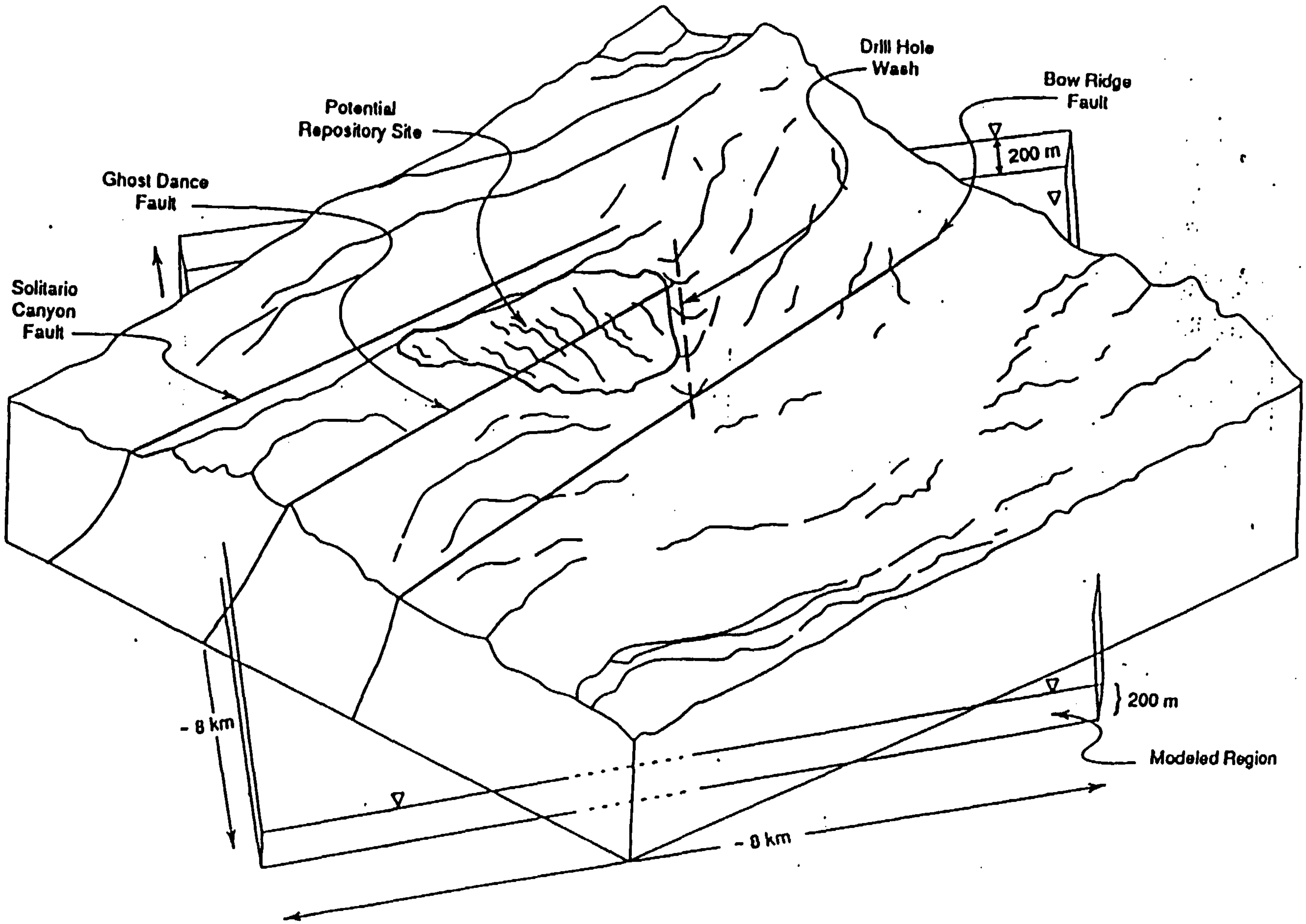


Bow Ridge fault, K = 5E-8m/s
WT-16 = 736.93m (738.32m)

zelz5.out
Level 5



SplayX = 5E-11 (5E-7)


Drill Hole
Wash
Bow Ridge
Fault
200 m
Potential
Repository Site
Ghost Dance
Fault
Solitario
Canyon
Fault
~ 8 km
200 m
Modeled Region
~ 8 km

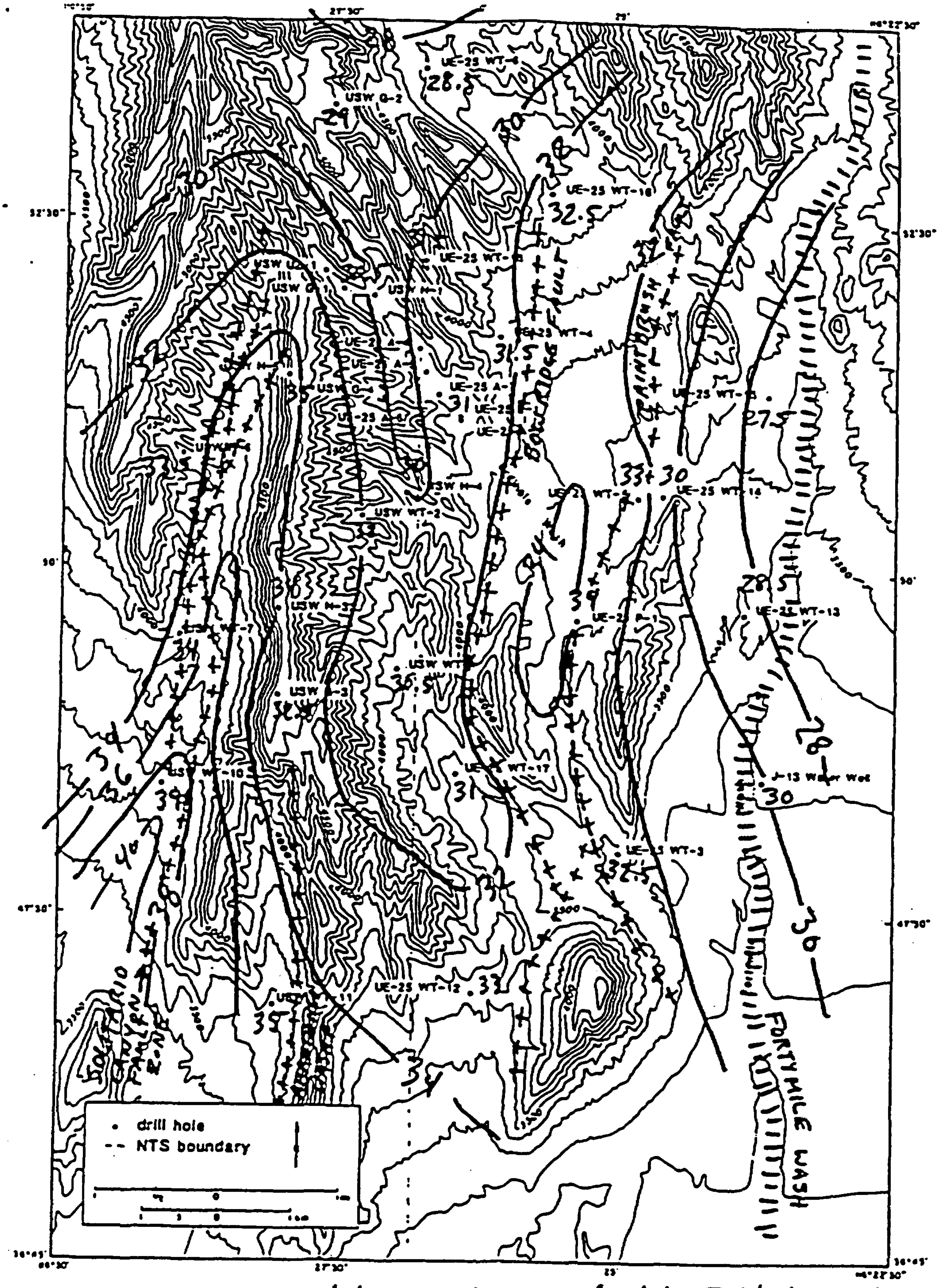


Figure 13: Contoured temperature at the Water Table (°C), showing also the 4 major normal faults cutting Yucca Mountain and Fortymile Wash. (Data from Sass, et al., 1987).

CARRIER and CONTAMINANT PLUMES

G.E.Barr, SNL

FAULT EFFECTS ON VERTICAL FLOW AND DISPERSION

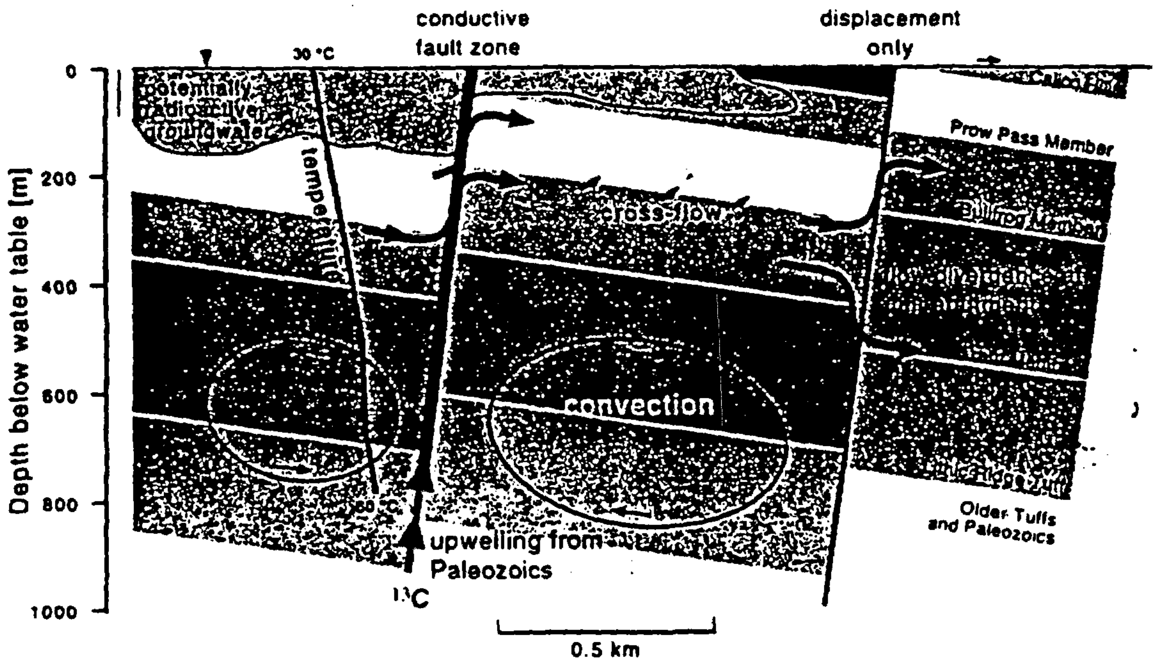
Issue:
1. Conceptual Models of SZ Flow
1.3 Vertical Flow

Andrew Cohen
LAWRENCE BERKELEY NATIONAL LABORATORY

SZ Flow and Transport Abstraction Workshop
Denver, CO
April 1, 1997

3-D SZ Flow Model at LBNL:
BERKELEY LAB
Curtis Oldenburg
Andrew Cohen
Ardyth Simmons

SZ Flow Conceptual Model

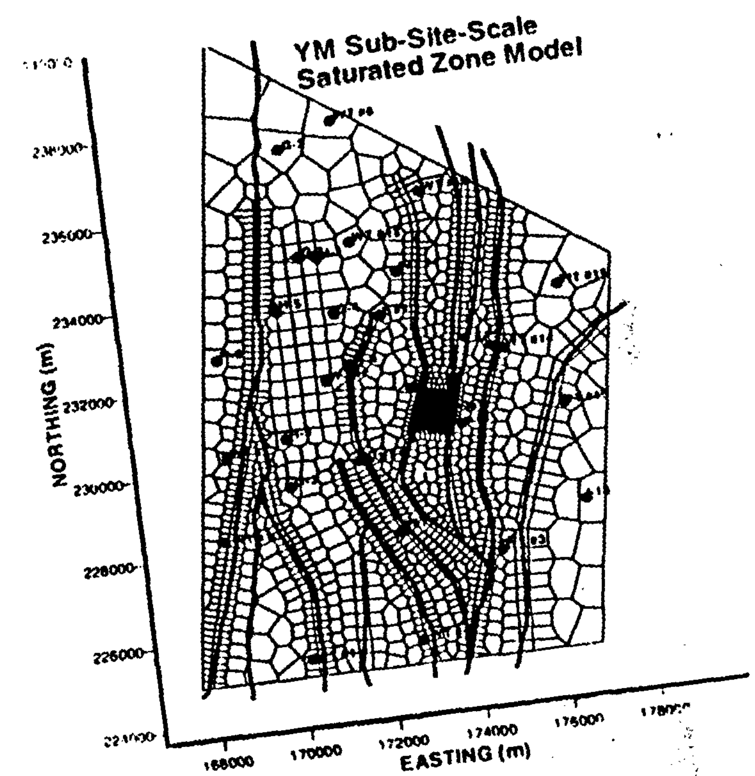


- Fault effects on vertical flow mainly hypothesized
- 3-D simulations are needed to :
  - provide new insights of fault effects on flow
  - determine the most important fault processes
  - construct an abstraction model properly
- Preliminary simulations show
  - fault zone upwelling can occur without paleozoic upwelling
  - cross-formational flow due to fault displacement only
  - water table temperature anomolies can occur without fluid upwelling

●A. Effects of Faults on Dispersion
- use 3-D Sub-Site-Scale SZ flow model
- consider fault zones and explicit fault offset
- model conforms to 3-D geologic framework model
- faults as barriers
- conductive fault zones
- displacement only faults
- hydraulic connection to Paleozoic formation
- thermal anomolies at water table
- utilize fault properties from UZ inverse model

●B. Importance of Thermal Convection
- scale analysis predictions for dilution
- extend to 3-D using Sub-Site-Scale SZ Model
- examine mixing effects from faults
- compare dilution from free convection to that from flow divergence at faults

●C. Hydrochemistry
- utilize UZ Model results of water table infiltration
- utilize SZ and UZ geochemical data
- use geochemical data to constrain simulation results



CLIMATE CHANGE - FUTURE WORK

- Future Work:
  - » Complete Regional Simulations
- Sensitivity:
  - » Determine controls resulting in unacceptable water-level rise
  - » Apply results to site model

CLIMATE CHANGE

Major Issue #4: Coupling to other components of TSPA

4.1 Climate Change

Frank A. D'Agnese

US Geological Survey

Tuesday, April 1, 1997

E-64

DISTRIBUTION OF REGIONAL DISCHARGE - FUTURE WORK

Directly Measure ET at:

- Franklin Lake Playa - Done
  - » 22,800 m^3/d +/-25%
- Ash Meadows/Peter's Playa/Carson Slough - Done
  - » 74,600 m^3/d +/-15%
- Death Valley Playa - NOT DONE
  - » 40,000 to 150,000 m^3/d
- Oasis Valley - NOT DONE
  - » 7000 to 17,000 m^3/d

DISTRIBUTION OF DISCHARGE

Major Issue #1: Conceptual Models of SZ Flow

1.5 Distribution of Regional Discharge

Frank A. D'Agnese

US Geological Survey

Tuesday, April 1, 1997

DISTRIBUTION OF REGIONAL RECHARGE - FUTURE WORK

- Practically impossible to measure regional recharge
- Need to improve discharge measurements
  - ET, springs, pumping
- Maybe increase number of recharge zones
- Sensitivity - use MODFLOWP confidence intervals
  - low - fixed
  - moderate - 3%; range 2-4%
  - high - 23%; range 20-25%

DISTRIBUTION OF RECHARGE

Major Issue #1: Conceptual Models of SZ Flow

1.4 Distribution of Regional Recharge

Frank A. D'Agnese

US Geological Survey

Tuesday, April 1, 1997

DISTRIBUTION OF SITE-SCALE RECHARGE

Conceptual Models of SZ Flow
(1.4 Distribution of Recharge)

Patrick Tucci
U.S. Geological Survey
April 1, 1997

PROBLEMS:

- Distribution and rates of recharge are not well known or understood;
- Models are very sensitive to this parameter;
- Needed to calculate source term for SZ transport models.

PREVIOUS WORK:

- No recharge *on* Yucca Mtn. (Fortymile Wash or inflow from North) (Czarnecki and Waddell, 1984, D'Agnese, et al., 9n press, Osterkamp, et al., 1994, Savard, in press);

  \- OR -

- Minor recharge *on* Yucca Mtn., uniformly or discretely distributed (Czarnecki, 1985; Flint, et al., in press).

PROPOSED WORK:

- Complete proposed Fortymile Wash infiltration studies;
- Continue w/ UZ infiltration studies and isotope sampling in ESF and selected wells;
- Obtain better estimates of regional discharge;
- Sensitivity analyses of regional & site models.

APPLICATION TO TSPA/VA:

- Reduce uncertainty in output from site flow and transport models (which will be used by PA)

1. Conceptual Models of SZ Flow

1.5 Regional discharge

John B. Czarnecki
U.S. Geological Survey

April 1, 1997

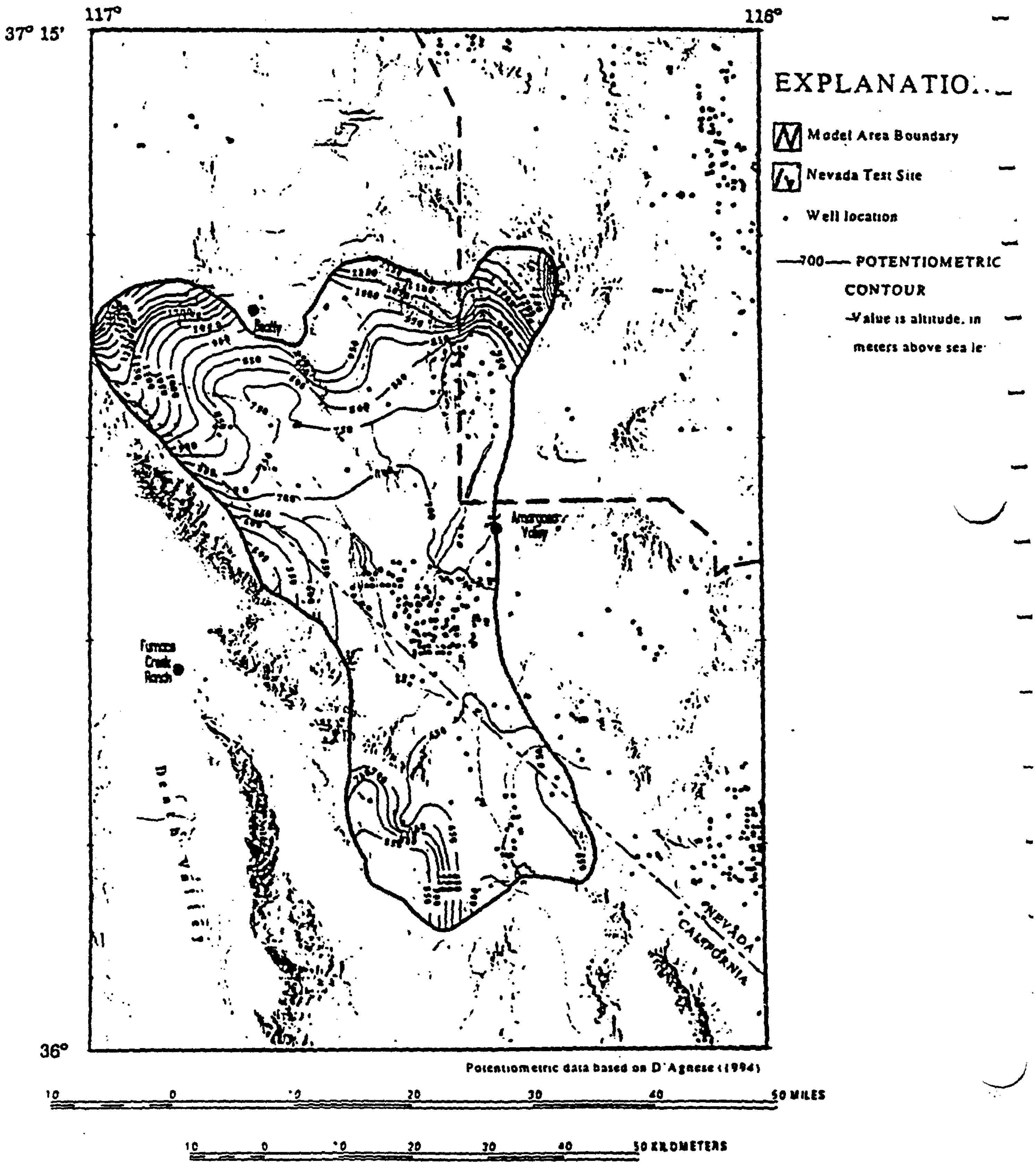


Figure 2. —Potentiometric surface.

Possible Sinks for Discharge for Water Leaving Yucca Mountain

- Franklin Lake playa (Alkali Flat): 23,000 m**3/d
- Furnace Creek Ranch (Death Valley): 19,000 m**3/d
- Pumping center in Amargosa Valley

Implications of Uncertainty in Discharge Conceptual Model

- Calibration discharge flux error
- Calibrated permeability values have proportionate error
- Ground-water travel time error is proportionate

DISCHARGE TO
SPRINGS AT FURNACE CR

[redacted]

SCALE 1: 700 000

10 0 10 20 30 40 50 MILES

10 0 10 20 30 40 50 KILOMETERS

Evidence Against Flow from Yucca Mountain Within Tertiary Rocks to Death Valley

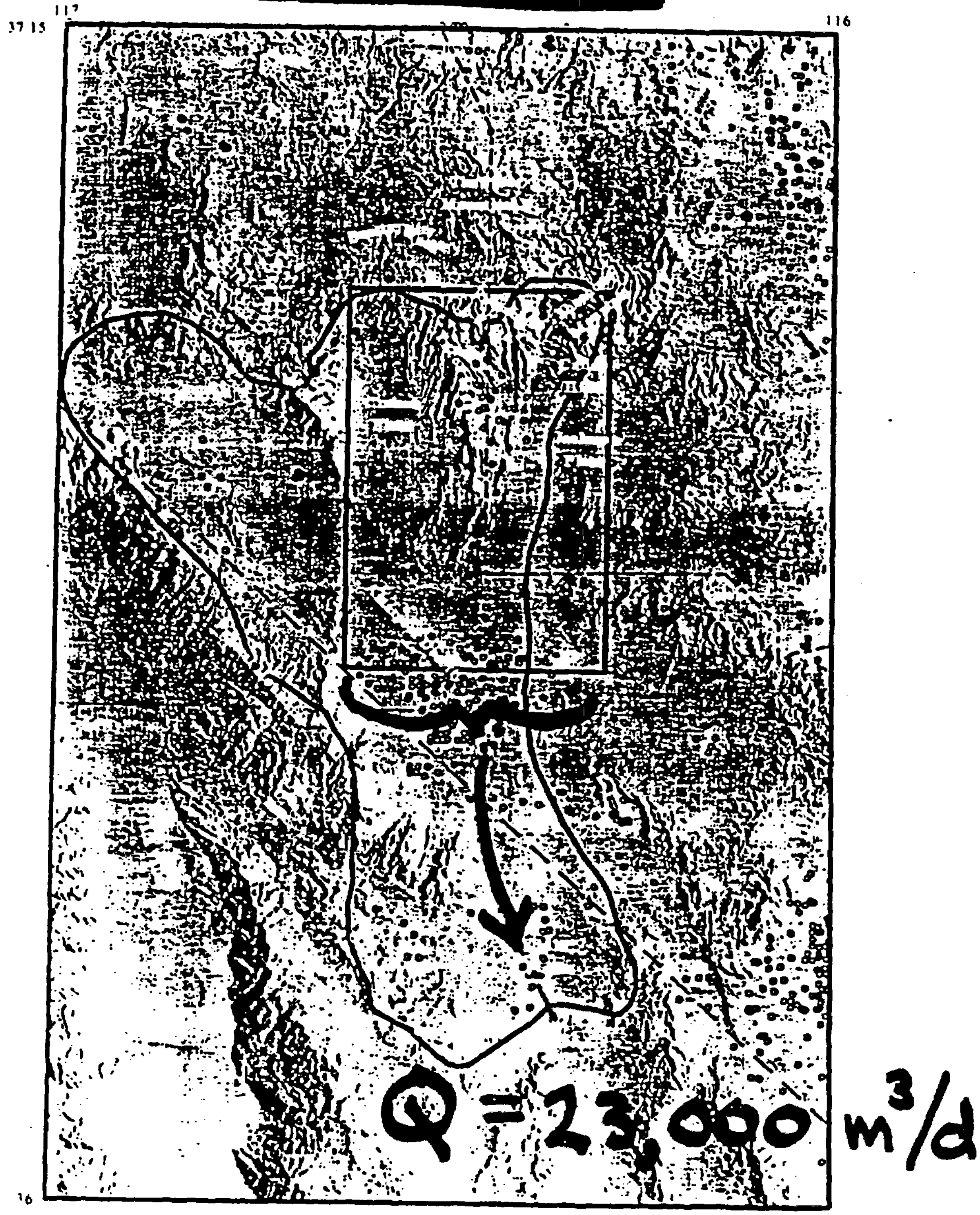
- Upward hydraulic gradient within Tertiary units and between Tertiary and Paleozoic units

- Dissimilar hydrochemistry between samples from Tertiary units and those from springs in Death Valley

- Ground-water divide under Greenwater Range which separates Tertiary systems in southern Amargosa Valley and Greenwater Valley

DISCHARGE TO FRANKLIN LAKE PLAYA

[redacted]



SCALE 1: 700 000

10 0 10 20 30 40 50 MILES

10 0 10 20 30 40 50 KILOMETERS

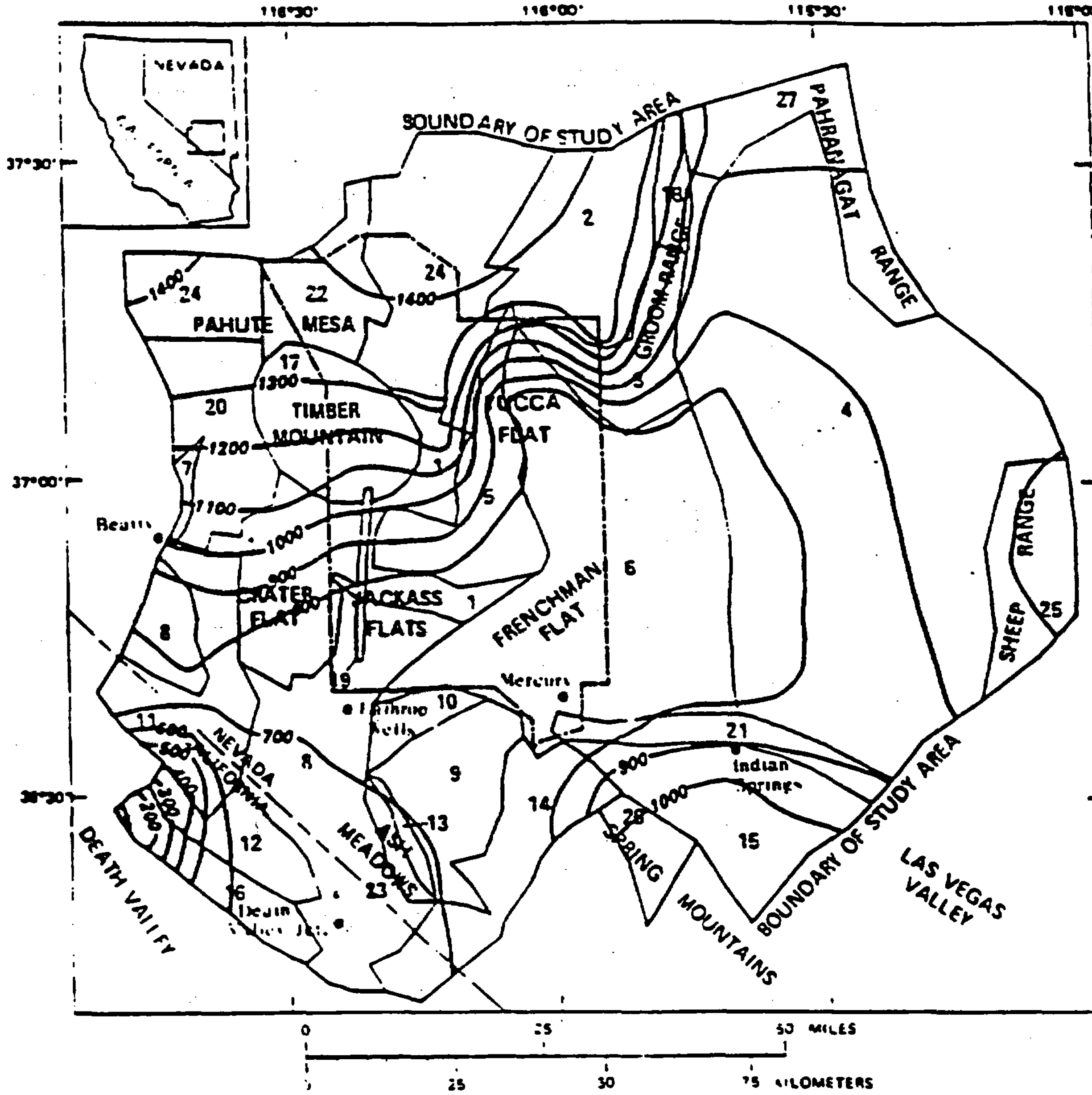
Issue: What is discharge out of Site Model southern boundary

Proposal:

- Hydrochemically sample borehole NT-1 on east side of Funeral Mountains

- Convert Felderhoff-Federal 25-1 to a multi-port observation well

- Refine upper layer of regional flow model so that flow in Tertiary section can be explicitely evaluated



EXPLANATION

—300— SIMULATED POTENTIOMETRIC CONTOUR—Shows altitude of simulated potentiometric surface. Contour interval 100 meters. Datum is sea level.

—28— ZONE NUMBER AND BOUNDARY

—·—·— BOUNDARY OF NEVADA TEST SITE

Figure 3.--Simulated hydraulic heads.

33

WADDELL '82

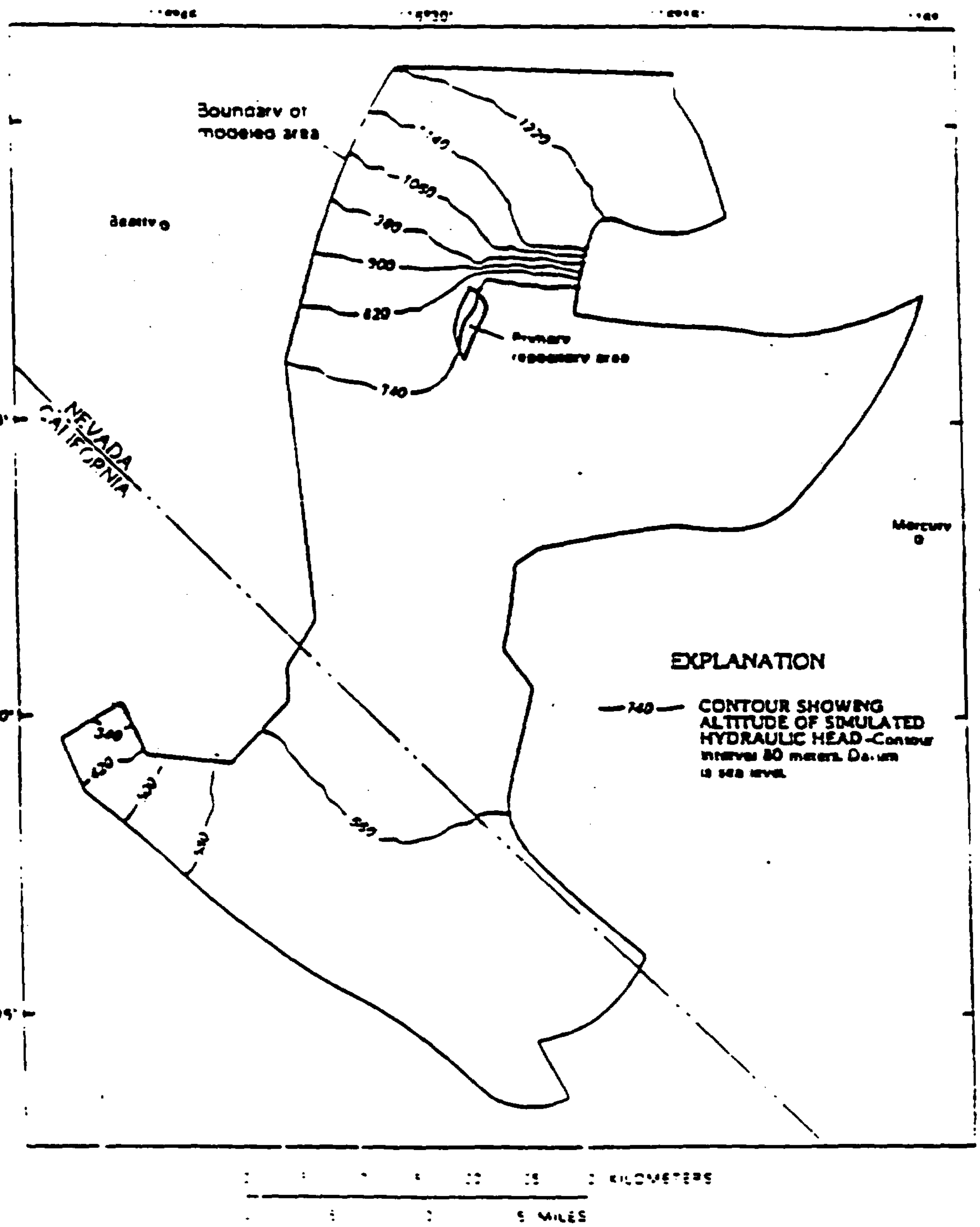


Figure [illegible].--Simulated hydraulic heads.

[illegible] & WADDELL '84

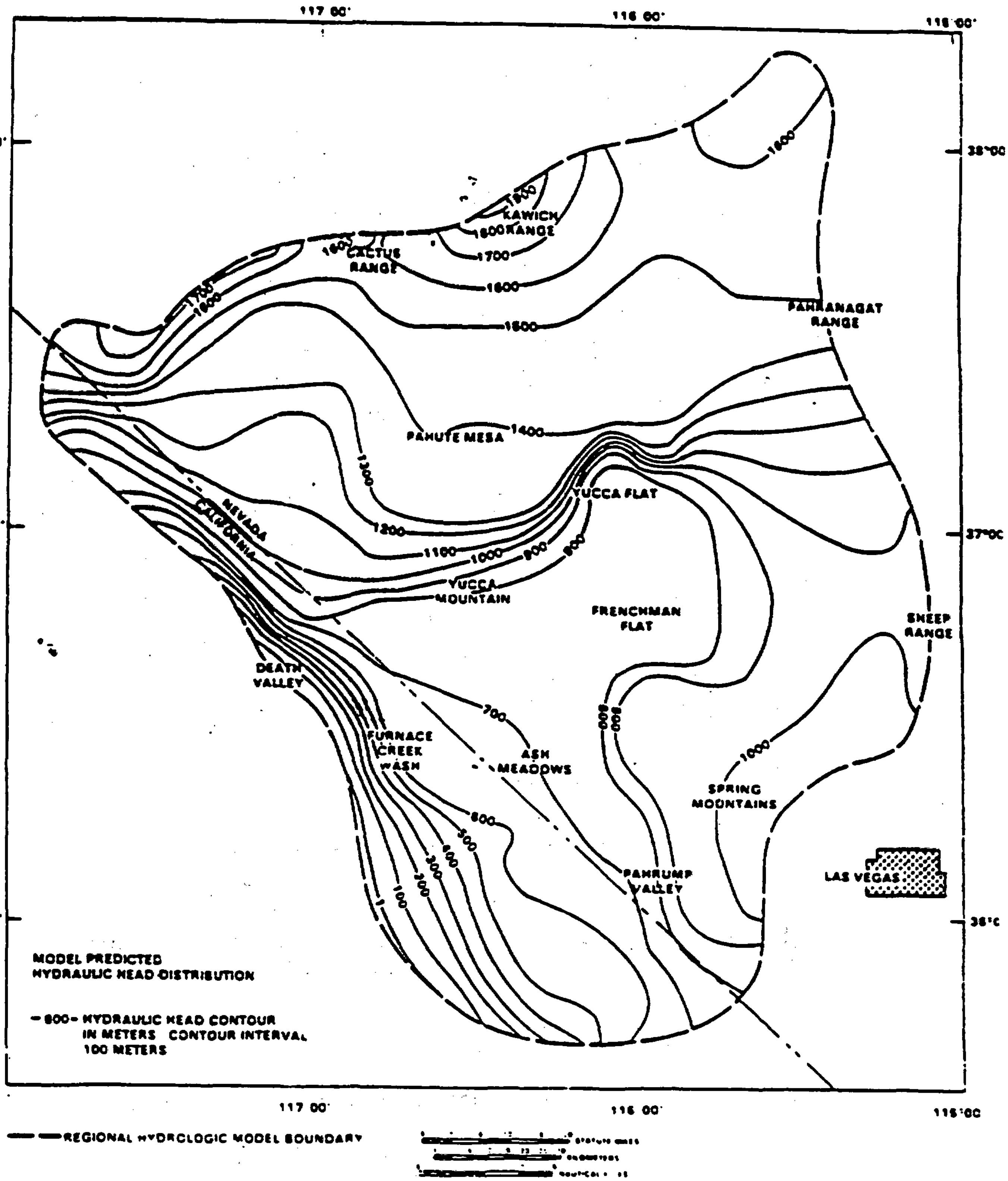
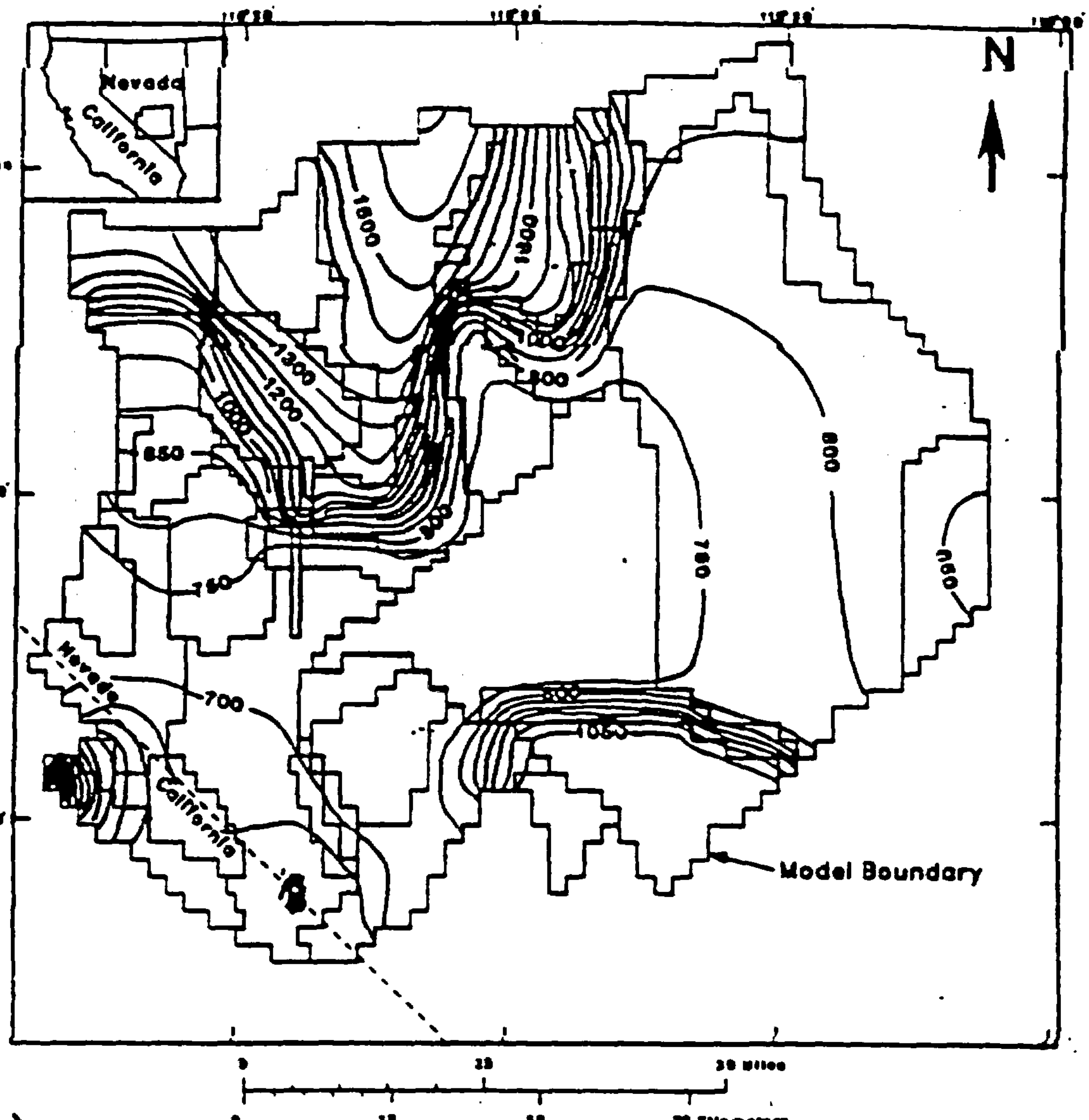


FIGURE 12. Model-Predicted Hydraulic Heads for Steady-State Confined Conditions (hydraulic heads in meters above MSL)

Rice '84



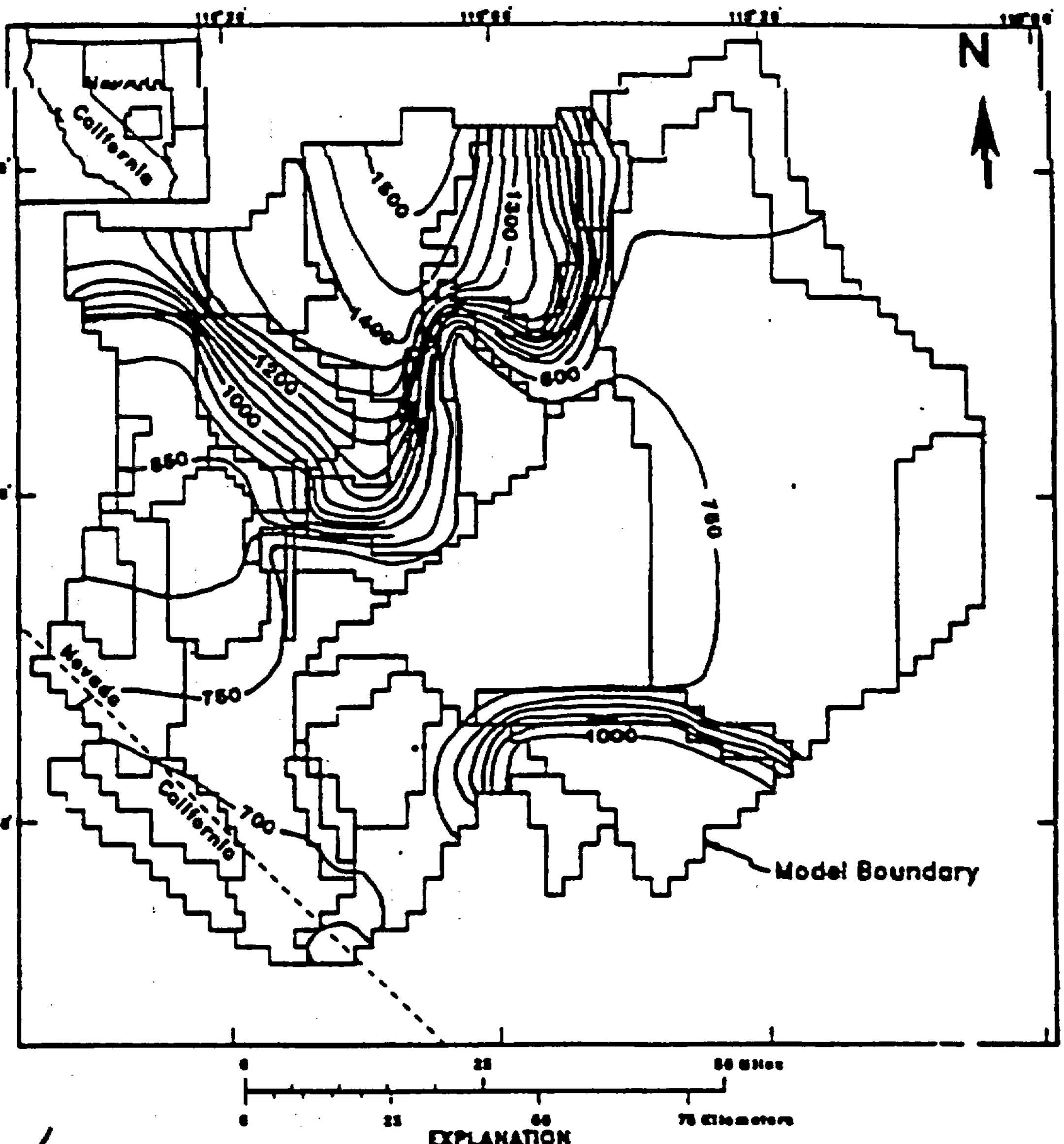
EXPLANATION

Simulated potentiometric surface, upper layer. Contour interval is 50 meters. Datum is sea level.

—— Model zone boundary
■ *Constant Head Node*

Figure 13a.--Simulated potentiometric surface for the upper model layer.

SINTON '87



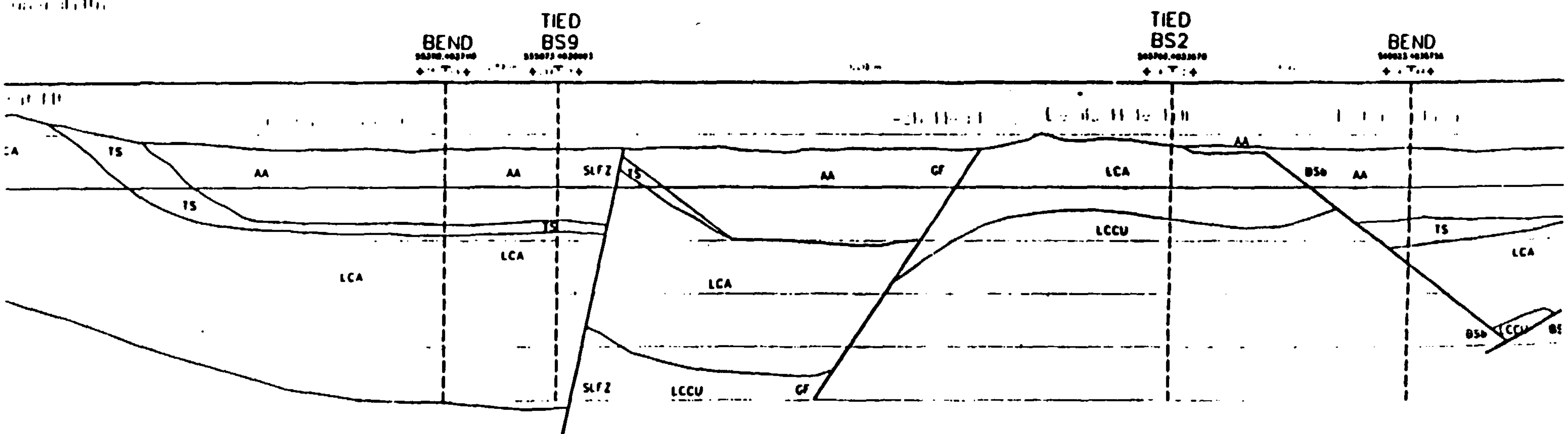
EXPLANATION

—900— Simulated potentiometric surface, lower layer. Contour interval is 50 meters. Datum is sea level.

—— Model zone boundary

Figure 13b.--Simulated potentiometric surface for the lower model layer.

SIMPLIFIED BRAD SCHIER MS3



PHIC CROSS SEC
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ATE

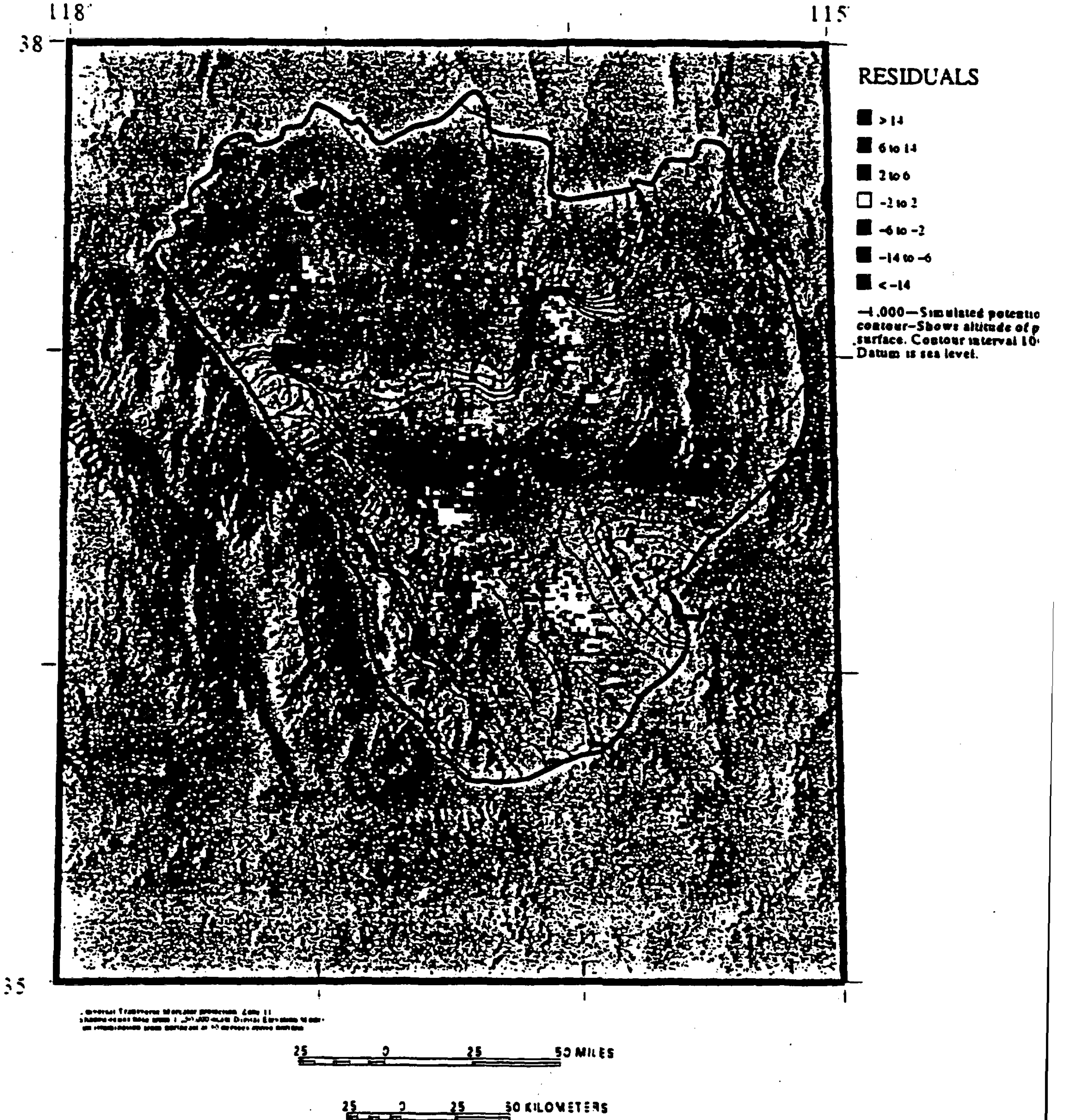
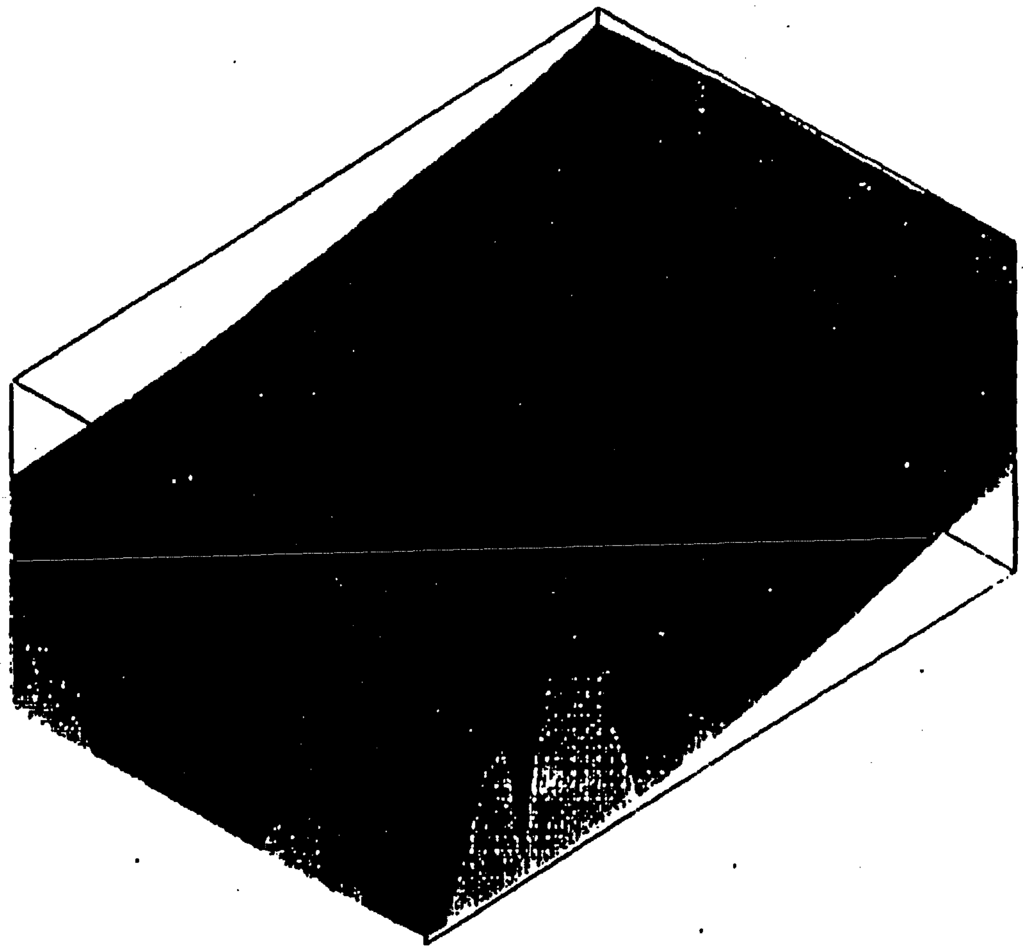
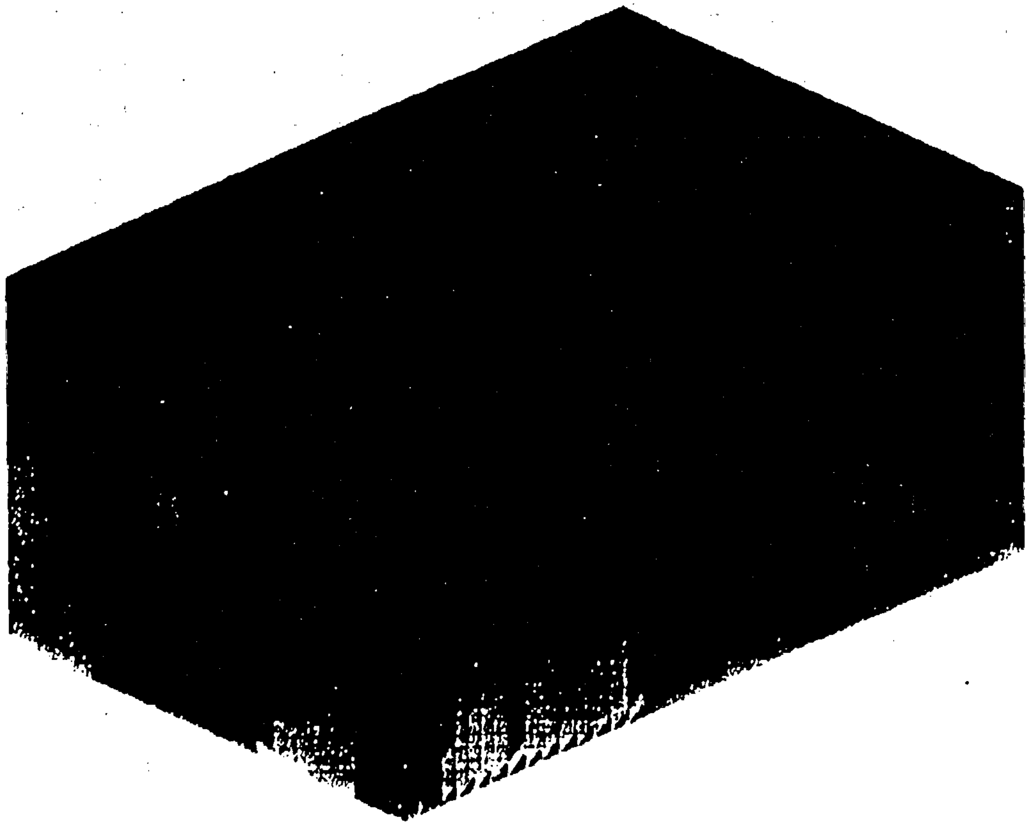


Figure 52 Hydraulic head weighted residuals (observed minus simulated) for model laye

Original Material Distribution



Structured Grid - Material Distribution



The grid details are shown in Table 5-2. For visual comparison with the stratigraphic model (Figure 26), the material distribution for grid 5 is shown in Figure 27..

Table 5-1. Permeabilities and Volumes of the Geologic Materials (original mesh)

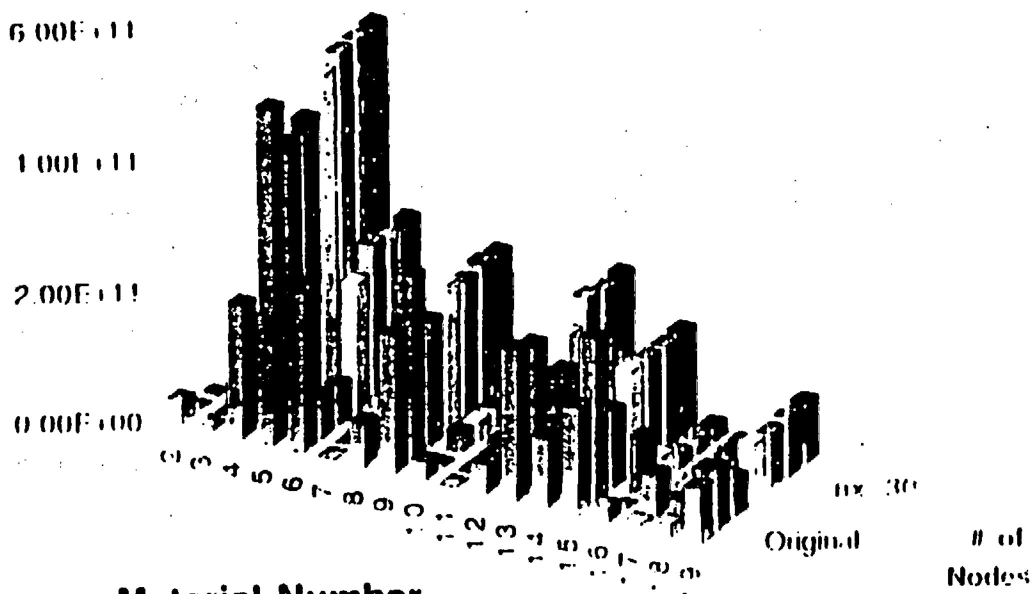
Material Number	Name	Permeability (m^2)	Volume (m^3)
1		1.e-17	0.000E+00
2		1.e-17	0.348E+11
3		1.e-17	0.636E+10
4	Lower Carbonate aquifer	2.e-12	0.203E+12
5	Eleana confining unit	2.e-13	0.512E+12
6	So. volcanics, amargosa	1.e-13	0.244E+12
7	Tertiary Limestones	9.e-14	0.884E+09
8	T sediments	8.e-14	0.647E+11
9	Lower volcanic confining unit	1.e-15	0.210E+12
10	Lower volcanic aquifer	3.e-13	0.274E+11
11	Middle volcanic confining unit	2.e-12	0.125E+10
12	Middle volcanic aquifer	2.e-11	0.456E+11
13	Upper volcanic confining unit	8.e-13	0.231E+12
14	Upper volcanic aquifer	2.e-13	0.105E+12
15	Basalts	6.e-14	0.164E+12
16	T limestone	9.e-14	0.222E+11
17	QTvc	1.e-14	0.878E+10
18		1.e-17	0.186E+11
19		1.e-17	0.846E+11
20 (outside original mesh)		1.e-17	

Table 5-2. Details of the numerical grids used

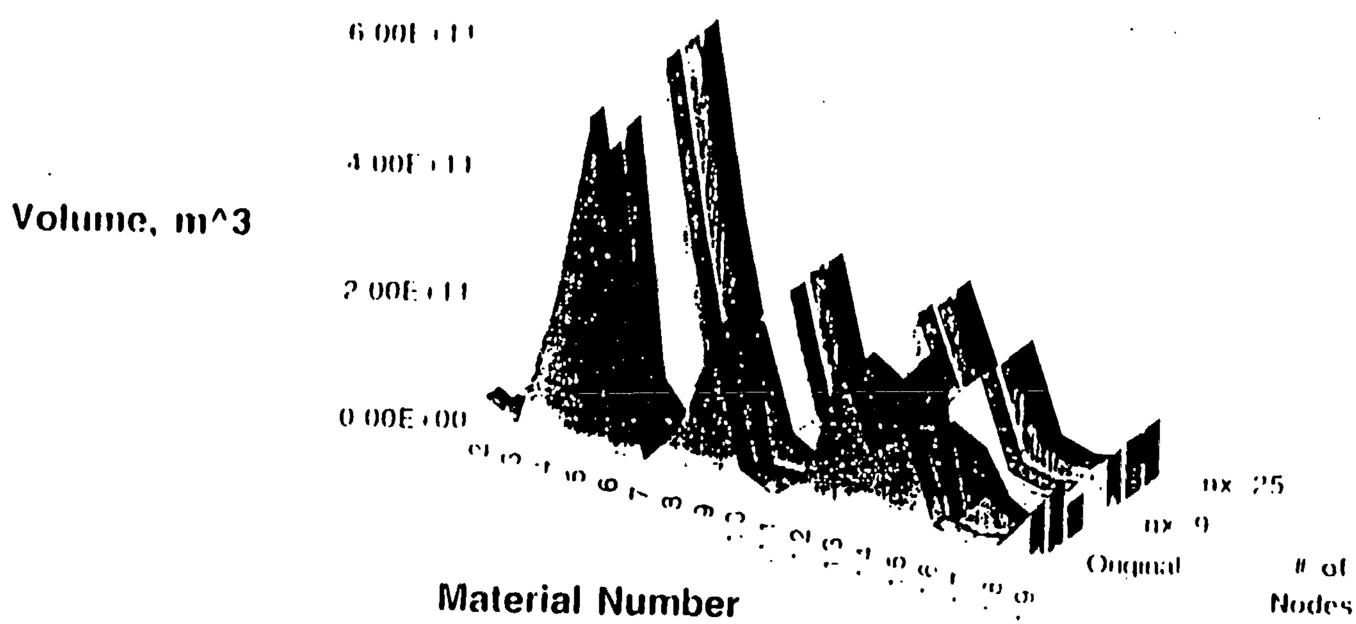
Grid Number	Total Number of Nodes	number of nodes in x and z direction	number of nodes in y-direction	spacing of nodes in x and y-direction (m)	spacing of nodes in z-direction (m)
1	96	4	6	3333	696
2	175	5	7	7500	521
3	1053	9	13	3750	260
4	7225	17	25	1875	130
5	23125	25	37	1250	87
6	40500	30	45	1000	70

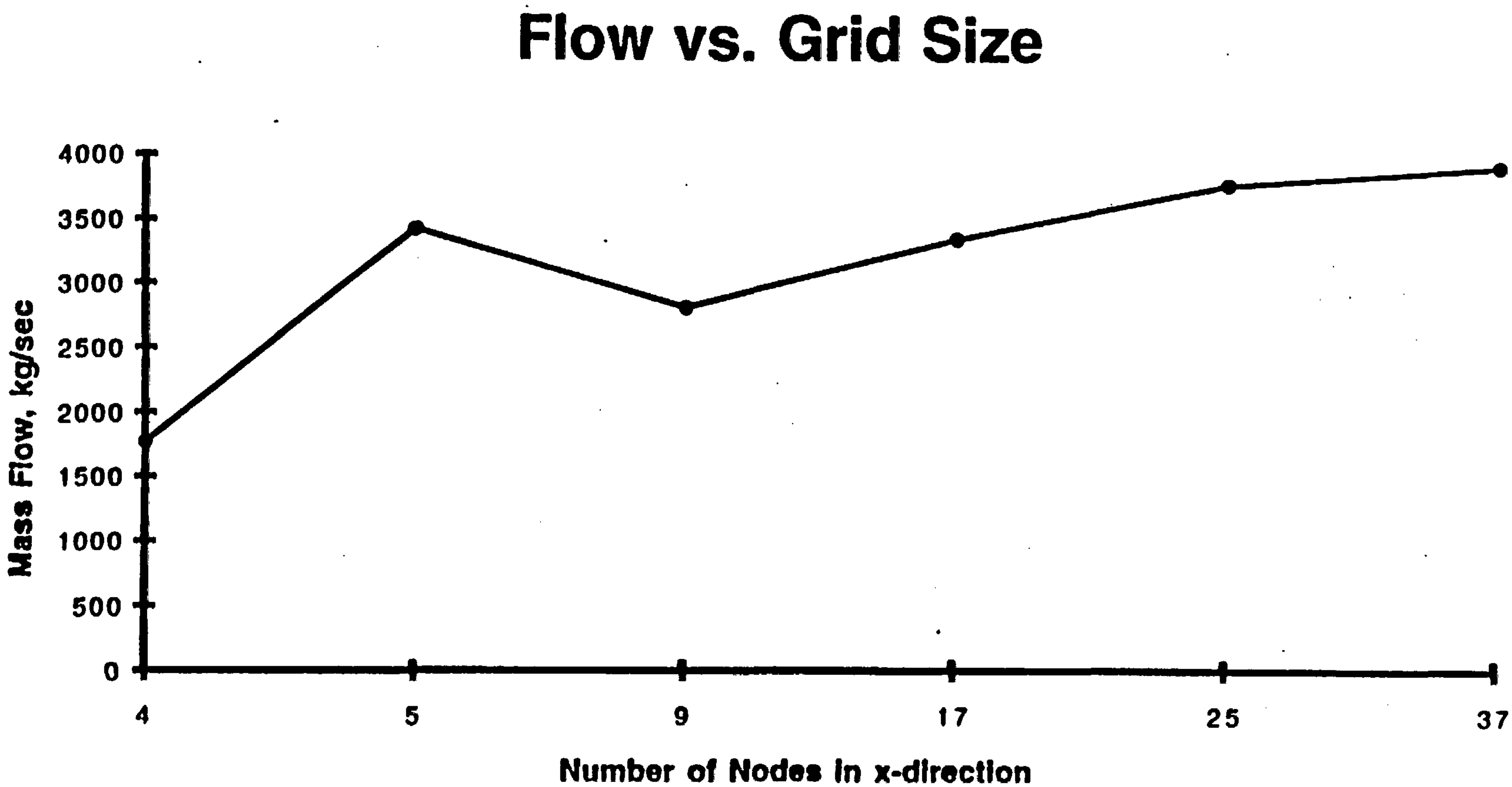
DRAFT

Material Volume



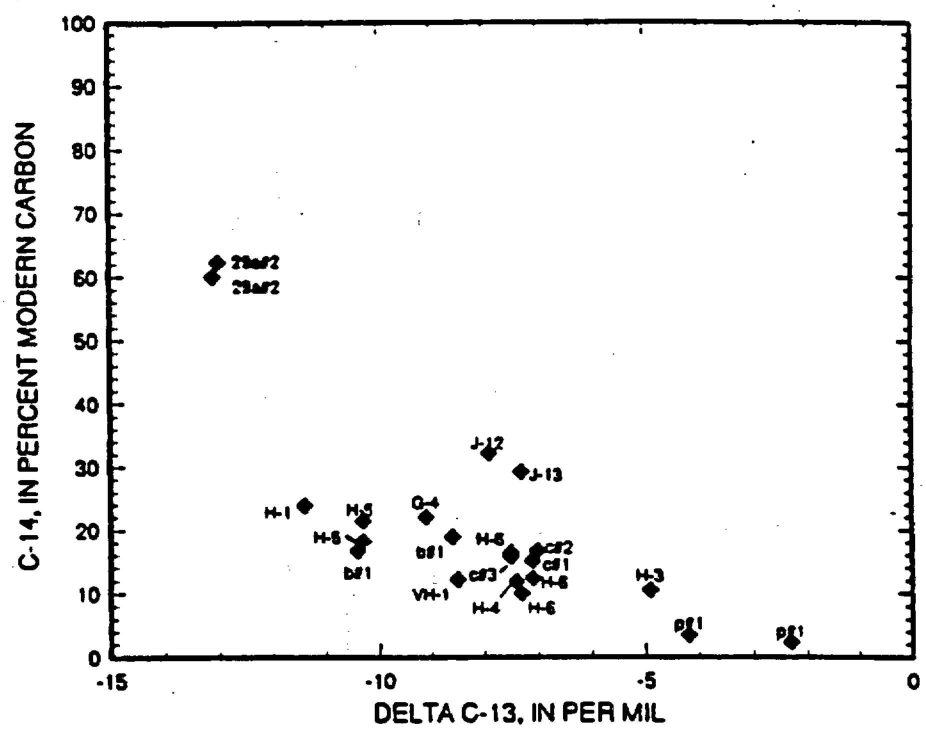
Material Volume

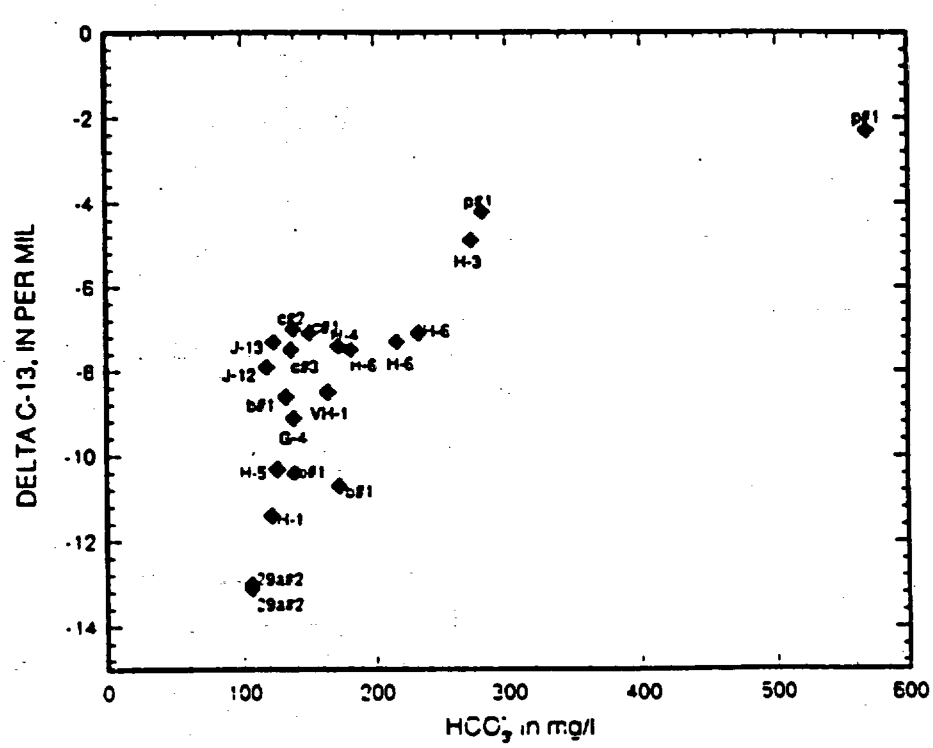


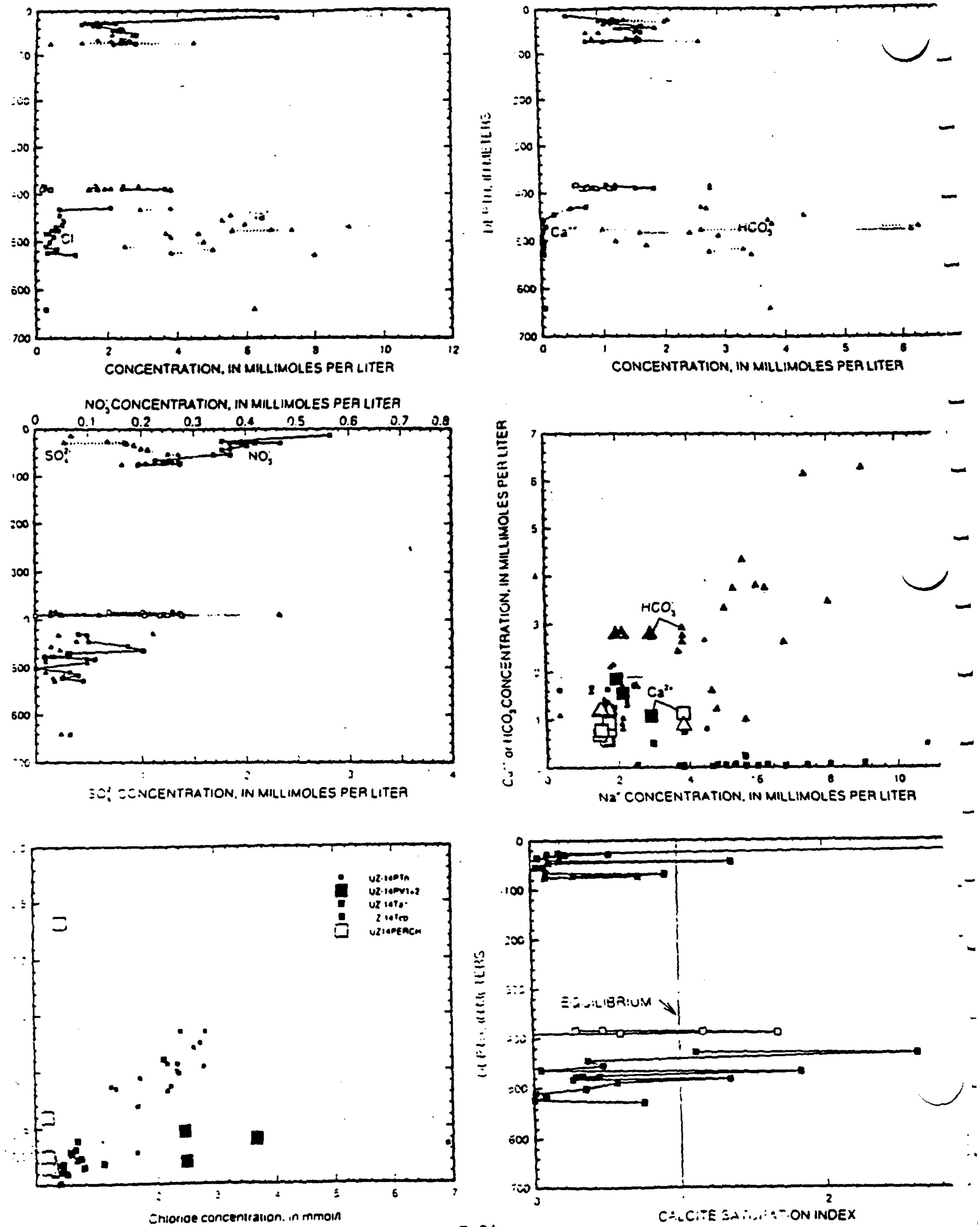

Flow vs. Grid Size
Mass Flow, kg/sec
4000
3500
3000
2500
2000
1500
1000
500
0
4
5
9
17
25
37
Number of Nodes in x-direction

Geochemistry and Isotopes

Edward Kwicklis


C-14, IN PERCENT MODERN CARBON
DELTA C-13, IN PER MIL
29af2
J-12
J-13
H-1
H-5
G-4
H-6
bf1
cf2
cf1
cf3
VH-1
H-4
H-3
pf1


DELTA C-13, IN PER MIL
HCO3, in mg/l
pf1
H-3
cf2
cf1
H-4
H-6
J-13
J-12
cf3
bf1
VH-1
G-4
H-5
H-1
29af2


CONCENTRATION, IN MILLIMOLES PER LITER
Cl
Na+
CONCENTRATION, IN MILLIMOLES PER LITER
Ca++
HCO3-
NO3- CONCENTRATION, IN MILLIMOLES PER LITER
SO4 2-
NO3
SO4 2- CONCENTRATION, IN MILLIMOLES PER LITER
Ca2+ or HCO3- CONCENTRATION, IN MILLIMOLES PER LITER
HCO3-
Ca2+
Na+ CONCENTRATION, IN MILLIMOLES PER LITER
UZ-14PTA
UZ-14PV1+2
UZ14PERCH
Chloride concentration, in mmol/l
EQUILIBRIUM
CALCITE SATURATION INDEX

Model:

$$m_{Cm} = m_{Ca} + m_{Mg} - m_{SO4} + 0.5\ (m_{Na} - m_{Cl})$$

$$m_{alk} = m_{Cm} + m_{Cb}$$

where Cm and Cb are carbon from minerals and of biogenic origin

$$(m_{alk})(^{14}C_{sample}) = (m_{Cm})(0pmc) + (m_{Cb})(x)$$

$$t = (5730yrs/ln2)\ ln(100/x)$$

$$(m_{alk})(\delta^{13}C_{sample}) = (m_{Cm})(y) + (m_{Cb})(-12\ permil)$$

borehole	uncorrected ^{14}C age (years)	corrected ^{14}C age (years)	$\delta^{13}C_m$ (permil)
p#1(deep)	30,300	24,236	+5.05
J-13	9,900	4,404	-2.65
H-3	18,100	12,941	+2.3
H-4	17,200	13,950	+0.73
c#3	14,900	9,317	-3.26
H-5	12,400	7,805	-8.8
G-4	12,160	5,063	-6.8
b#1(863-875m)	13,400	7,533	-5.58

TSPA Introduction to Issue 2:
Conceptual Models of SZ Geology

Jack Gauthier
SZ Abstraction/Testing Workshop
1–3 April 1997

Subissue 2.1
Flow Channelization

- Should channelization be incorporated in models (At what scale is a continuum representation valid)*
  - flow
  - transport
- Is channelization primarily in known faults
- What are the distributions of channel properties (spacing, effective aperture, etc.)

Subissue 2.2
Spatial Distribution of Hydraulic Conductivity

- Are producing zones related to hydrostratigraphic units* (Are producing zones connected)

Subissue 2.3
Geologic and Mineralogic Framework

- What is the appropriate resolution
  - near YM
  - down gradient
  - near a well
- How consistent must the regional-scale and site-scale models be

* Being considered for TSPA-VA

2.1 Flow Channelization

Chris Potter, USGS

- We have no specific constraints on the presence or absence of fault-controlled channelization of flow in the UZ, within the "5-km-fence."

- Based on surface geologic mapping, and to some degree on geophysical data, we know that there is a highly faulted graben down-gradient from the potential repository. This graben is about 1 km wide, with much complex internal faulting, and occupies the low ground in and west of Dune Wash. Between the potential repository area and the Dune Wash Graben is a transitional area that is locally riddled with minor faults and brecciation.

- How do we get a handle on the hydraulic conductivity of this broad fault zone?
  - compare its detailed (micro-and mesoscale) structural characteristics with those of the Mine Mtn- Spotted Ranged structural zone, which is inferred to be a regional-scale pathway.
  - compare its detailed (micro-and mesoscale) structural characteristics with those of known "fast pathways" in the UZ zone, as seen in the ESF.

- Similarly, we need to understand the detailed structural characteristics of the Solitario Canyon Fault Zone as they may (or may not) relate to flow channelization, in comparison with Dune Wash Graben.

- Related issue: "Subregional" hydrologic discharge at south end of Yucca Mountain near Lathrop Wells: to what extent does the highly faulted southern part of Yucca Mountain play a role in flow channelization? Need further structural studies linking the potential repository area with southern part of the mountain.

Other issues related to Site Structural Geology:

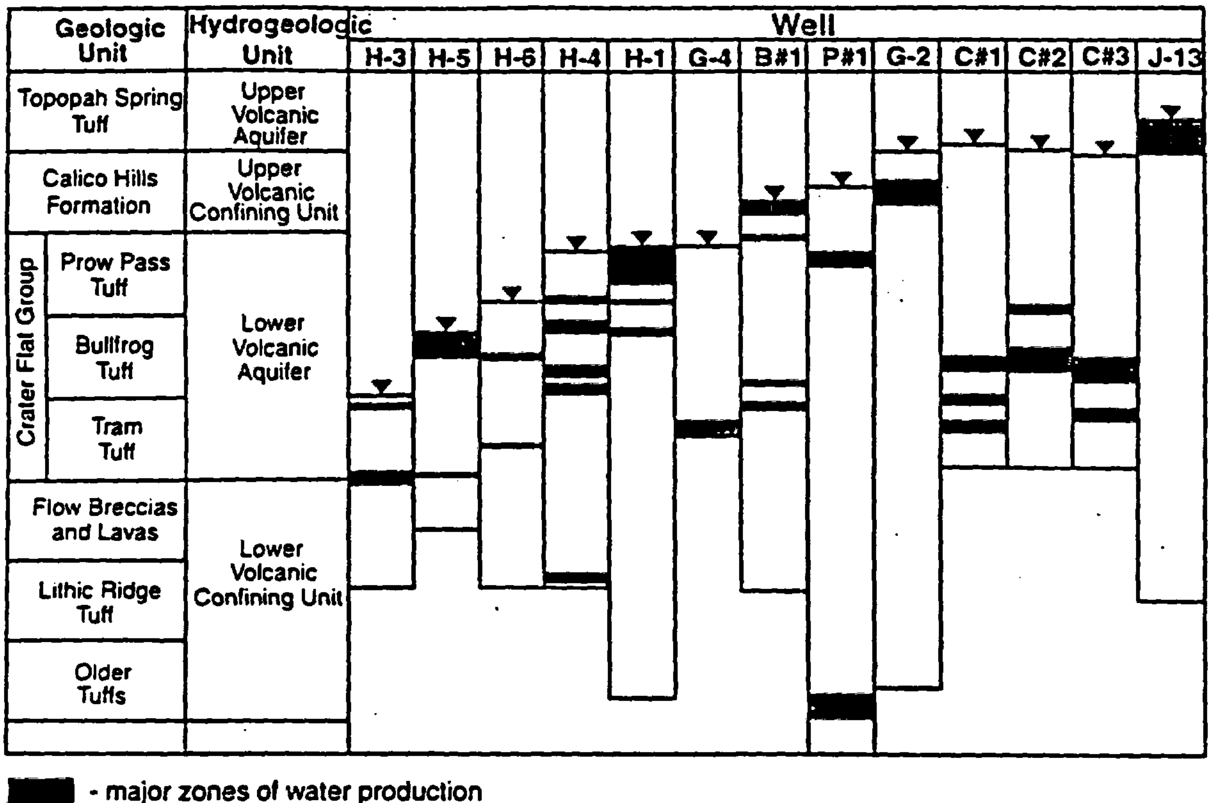
- **1.1 Alternative conceptual models: discrete fractures *vs.* continuum.** At what length scale do individual fractures become discrete flow channels, separate form the bulk permeability of the rock (a continuum " property related to the "background" fracture network)? This question may be addressed through the fractured-rock-mass studies that have been carried out at YM, including fast-pathway studies in the ESF.

- **2.3 Geologic and mineralogic framework**
- To ensure that structural controls are represented consistently at different scales, a geologic evaluation of the degree of consistency between site-scale and sub-regional models should be undertaken.
- The straw man proposal raises concern that the sub-regional model may not have sufficient spatial resolution to accurately represent flow in the SZ to a nearby well. We (USGS-YMP Structural studies group) would guess that none of the models has sufficient spatial resolution for this, including the site-scale model. For example. one of them captures the Dune Wash graben in a meaningful way. Need to incorporate more structural detail into the site scale model.

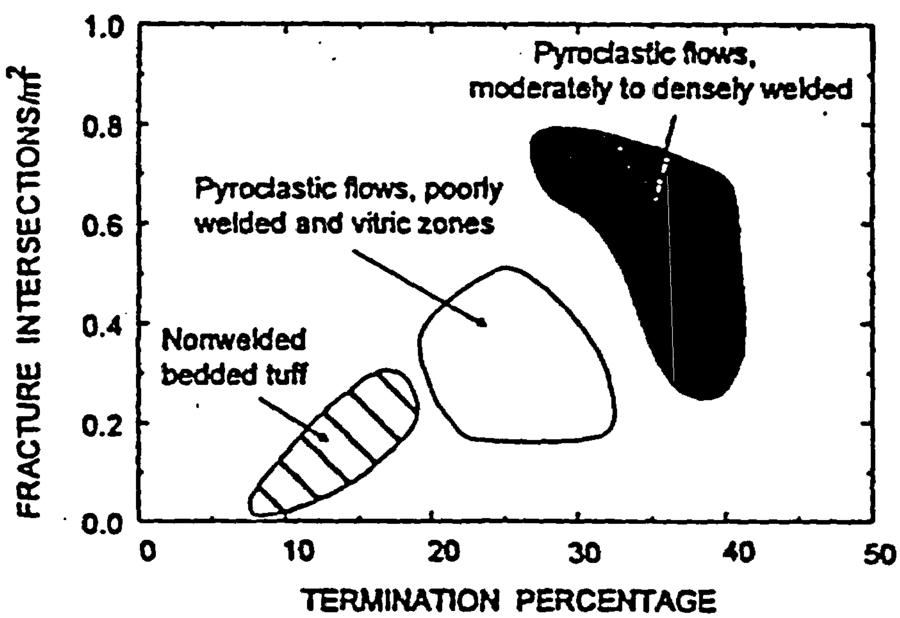
Sandia National Laboratories

Conceptual Models of SZ Geology (Flow Channelization) Issue 2.1

BILL W. ARNOLD
SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NM
April 1, 1997



from Geldon (1993), Luckey et al. (1996), Benson et al. (1983)



from Sweetkind and Williams-Stroud (1996)

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- Flow channelization probably occurs over a number of scales in the SZ, range-ing from individual fractures, to more transmissive hydrostratigraphic intervals, to large-scale, discrete structural features.

- At the scale of hydrostratigraphic units, degree of welding is the best predictor of fracture hydraulic conductivity and can be used as an indication of flow channelization along stratigraphic units.

- Studies of fracture connectivity indicate that fracture networks can be subdi-vided into three populations based on degree of welding (non-welded and bedded tuffs, poorly welded and vitric tuffs, and moderately to densely welded tuffs). These subdivisions can serve as a method of classification of hydrostratigraphic units to define potential flow channelization due to stratigraphic variations.

F-100

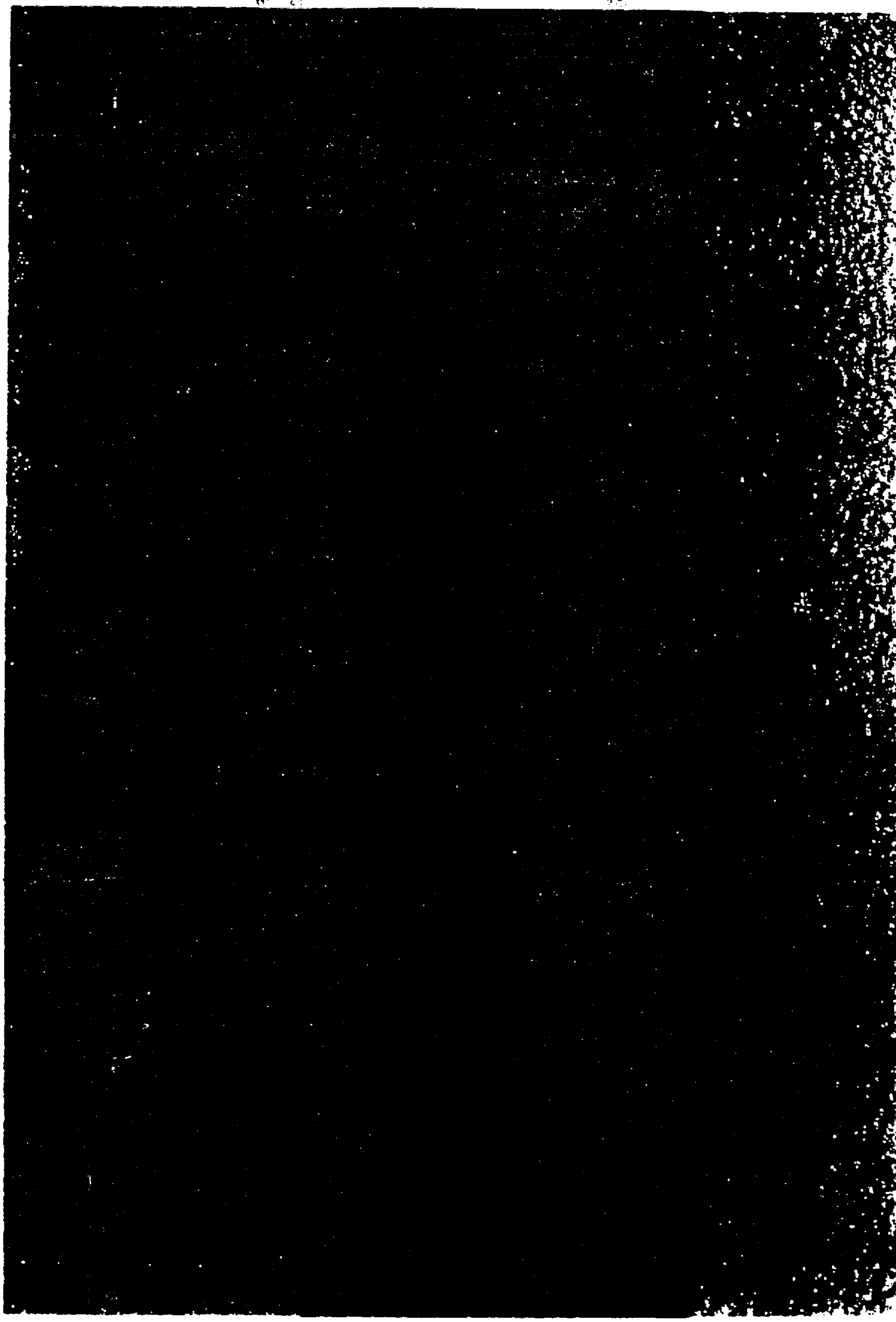
Issue 2: Conceptual Models of SZ Geology
Subtopic 2.1: Flow channelization

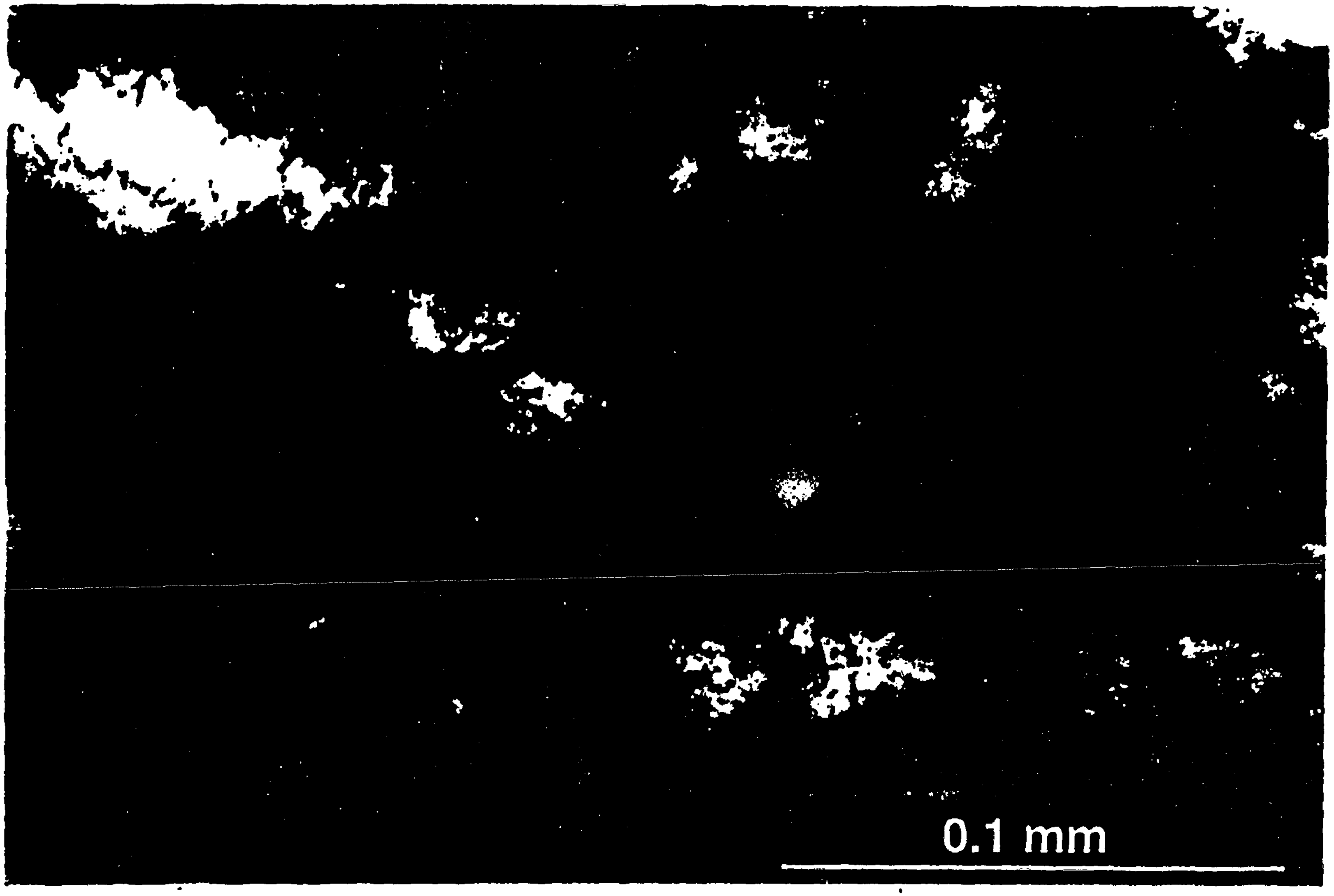
Observation: Several fractured intervals in the SZ are characterized by mineralization and Liesegang structures indicative of long-term flow and transport. In several instances these altered fractures correspond to depths where packer tests indicate high flow. Current fracture-flow experiments indicate particularly high retardation of some problem radionuclides, particularly Np, along such transmissive fractures.

Question: Do these fracture features reliably indicate channels of present transmission, and can they be modeled as such?

Resolution: For TSPA-VA, preliminary data connecting sorption (including microautoradiography results), flow volumes/rates, and mineralogy from pre-QA core may be available in a form amenable to simplified abstraction. In the longer term, for performance confirmation, a more complete variety of transmissive fractures must be considered and the question of vertical linkage between transmissive intervals should be considered.

Dave Vaniman/LANL

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Examination of the Effects of Intra-unit Heterogeneity on Saturated Zone Flow Paths, Yucca Mountain

Major Issue

2. Conceptual Models of Saturated Zone Geology

Sub Issue:

2.1 Spatial Distribution of Hydraulic Conductivity

Sean A. McKenna

Sandia National Laboratories

4/1/97

E-104

QUESTIONS:

- Does spatial heterogeneity of K within units cause a significant difference to PA versus using mean values in units?
- Does currently available fine-scale resolution of lithologic units within geologic framework model matter to PA calculations

METHODS:

Use Clayton et al., Geologic Framework Model as basis for modeling investigation

Classify units as non-welded, moderately welded, or densely welded (following Sweetkind and Williams-Stroud, 1996) and assign mean K values to each

non-welded	-14.0 (log10 m^2)
moderately welded	-13.0 (log10 m^2)
densely welded	-11.5 (log10 m^2)

Geostatistically simulate spatially variable K within each unit

Vary the level of heterogeneity within units (log10 std. dev. = 0.0, 0.25, 0.5, etc.)

Vary spatial correlation parameters within units

Vary degree of lithologic unit resolution

Compare pathline locations and travel times across various levels of heterogeneity

Simple model of Saturated Zone to 300 feet below water table

INITIAL OBSERVATIONS:

Spatially variable K within units makes a difference in travel times and in path locations.

Are the difference significant?

PROPOSED WORK:

Incorporate faulting into models to integrate with flow focusing study.

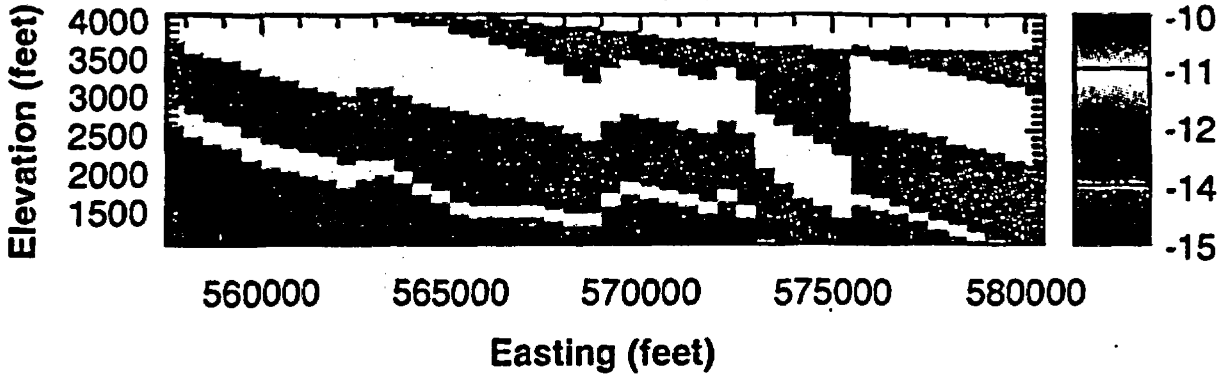
Use fine scale model to get idea of the magnitude of dispersivity values.

Expand current model (better treatment of boundary conditions, more layers)

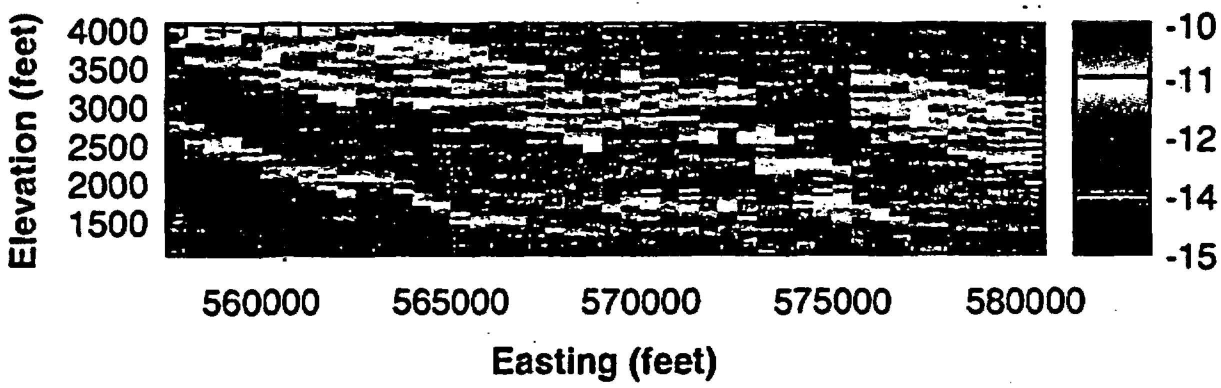
Abstract results to TSPA in terms of defining dispersivities and mixing/channeling

East-West Section at 763,500 feet (232,700 meters)

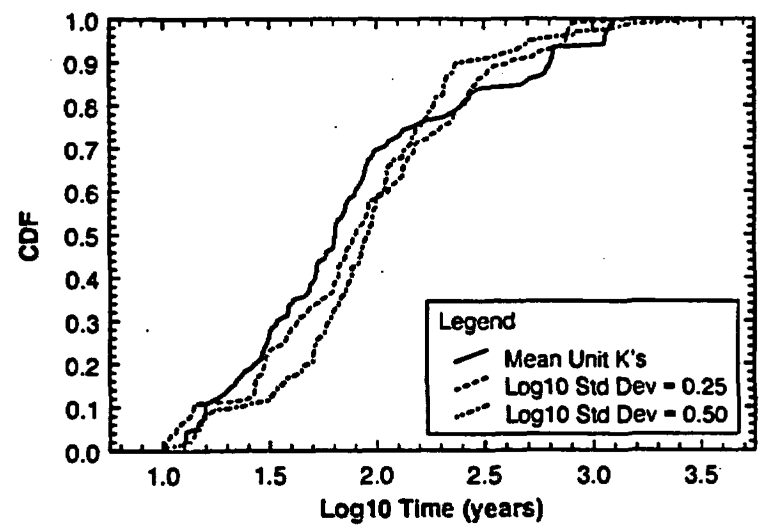
Mean Permeabilities (log10 m^2)



Heterogeneous Permeabilities (std. dev. = 0.5)



Travel Time cdfs (log10 years)



ISSUE: SPATIAL DISTRIBUTION OF HYDRAULIC CONDUCTIVITY

Art Geldon, *U.S. Geological Survey, Denver*

Pumping tests conducted in the C-holes in March 1984, May 1984, November 1984, May 1995, June 1995, February 1996, and May 8, 1996 to March 26, 1997 (a period of 322 days) have constrained values of transmissivity and storativity in the Calico Hills Formation and Crater Flat Group at the C-holes complex and as far away as USW H-4 (7,366 feet from UE-25 c#3). Hydraulic conductivity can be calculated from the known thickness of transmissive intervals within a test interval, the entire thickness of the test interval, or an assumed thickness of transmissive rock between boreholes. Consequently, computation of hydraulic conductivity is less certain than other hydraulic properties. Nevertheless, hydraulic conductivity has been calculated in C-hole pumping tests by assuming that the known thickness of transmissive rock in a test interval is the effective thickness.

Tuffaceous rocks in the saturated zone of the C-holes are about 1,600 feet thick. Pumping tests consistently have shown the composite transmissivity to be about 20,000 feet squared per day, the composite horizontal hydraulic conductivity to be 20-60 ft/d, vertical to horizontal anisotropy to be 0.1, and the storativity to be 0.001-0.004. Specific yield values range from 0.01 to 0.2 in pumping tests, but modeling in transient mode required a value of 0.007.

Hydrologic properties are distributed heterogeneously within the C-hole complex. For example, hydraulic conductivity between c#2 and c#3 is 1-5 ft/d in the Calico Hills interval, 5-10 ft/d in the Prow Pass interval, 8-10 ft/d in the upper Bullfrog interval, about 200 ft/d in the lower Bullfrog interval, and 70 ft/d in the upper Tram interval (table 1). Hydraulic conductivity values between c#1 and c#3 typically are about half of those between c#2 and c#3 for the upper Bullfrog, lower Bullfrog, and upper Tram intervals (this result, though, is highly dependent on the assumed effective thickness used in calculating hydraulic conductivity values). Despite appearances, hydraulic conductivity in the C-holes is not stratabound; variations result from the proximity of hydrogeologic intervals to a northerly stiking fault (the Midway Valley or Paintbrush Canyon Fault) and a cross-cutting, northwesterly trending fault zone that extends from Bow Ridge to Antler Wash.

Pumping tests conducted in May 1995 and May 1996 to March 1997 have shown that interconnected fractures that allow all hydrogeologic intervals to respond to pumping in the C-holes, regardless of which interval is being pumped, have to extend from the C-holes to ONC-1, 2,765 feet northwest of UE-25 c#3, because drawdown occurs in the Prow Pass in ONC-1 when the lower Bullfrog is being pumped in c#3. Moreover, hydrologic properties computed for ONC-1 during these tests are about the same as for the composite saturated-zone section in the C-holes. Similar ground-water hydraulics and hydrologic properties in the C-holes and ONC-1 indicate that the tuffaceous rocks between the two sites have a relatively uniform hydrologic character.

Pumping UE-25 c#3 for more than 109 days indicates that the cone of depression spreads alternately to areas less conductive or as conductive as rock in the C-holes. The rock in USW H-4 might be typical of some of the less conductive rock within the volume of aquifer stressed by pumping c#3. Drawdown in H-4 after 72,000 minutes of pumping c#3, indicated a transmissivity of about 7,000 feet squared per day, a hydraulic conductivity of 8 ft/d, and a storativity of 0.002 for the Crater Flat Group and upper Lithic Ridge Tuff in H-4.

The May 1995 pumping test in the C-holes demonstrated (1) that transmissivity in the vicinity of the C-holes is largest along a northwesterly trending axis aligned with the Bow Ridge-Antler Wash fault zone mapped by Day and others (in press) and smallest in an orthogonal direction; (2) a well-defined relation exists between drawdown and distance along the northwesterly trending axis; and (3) northerly trending faults at local scales, such as the C-hole complex, can influence drawdown and transmissivity more than the northwesterly trending faults.

Little is known about hydrologic properties of the Paleozoic carbonate rocks that underlie Miocene tuffaceous rocks in the Yucca Mountain area, but Leap and Belmonte (1992) determined transmissivity values between 52,000 and 120,000 feet squared per day and a storativity value of 0.0005 from a cross-hole pumping test in the Amargosa Desert about 24 miles from the C-holes. Unpublished numerical modeling by Art Geldon (USGS) indicated a hydraulic conductivity of 160 ft/d for the Paleozoic rocks in the vicinity of the C-hole complex.

Methods of abstracting pumping test results

1) Assume that interval hydraulic conductivity values in the C-holes have the same spatial relationship to faults at the surface as they do in the boreholes, and estimate a surface distribution of hydraulic conductivity based on the distance of areas at the surface from fault traces.

2) Hydraulic conductivity values determined for outlying observation wells, such as USW H-4, during C-hole pumping tests can be assumed to represent hydraulic conductivity in the area of the observation well.

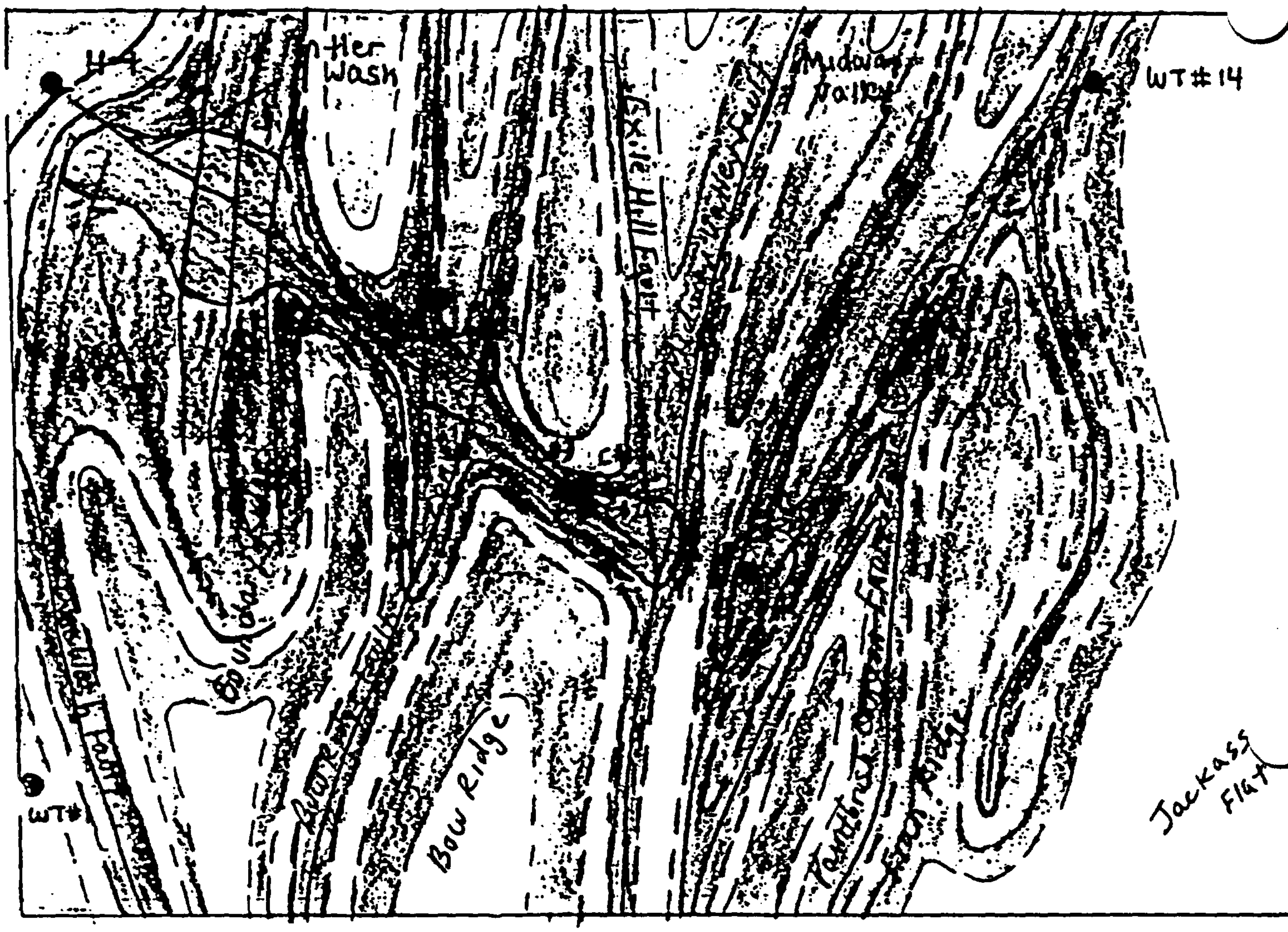
3) Analyses of drawdown in the pumping well at the C-hole complex consistently indicate values of transmissivity and hydraulic conductivity two orders of magnitude smaller than determined using observation well drawdown or recovery. As a rule of thumb, multiply values of hydraulic conductivity determined in single-well pumping tests at Yucca Mountain by 100 to get a realistic site-scale hydraulic conductivity for the area in which the test was conducted.

4) Use distance-drawdown relationships determined in the May 1995 C-hole pumping test to estimate drawdown as a function of distance and direction from c#3. Estimate transmissivity and hydraulic conductivity from drawdown by an approximation of the Theis equation or from hydraulic gradient by Darcy's Law.

5) As shown in the accompanying figure, pumping tests in UE-25 c#3 in 1995-1997 can be interpreted to indicate that hydraulic conductivity decreases from about 200 ft/d in the most complexly faulted areas to about 5 ft/d in the least faulted areas.

5) Construct a numerical model to confirm the estimated hydraulic conductivity distribution.

TABLE 1 - SUMMARY OF C-HOLE PUMPING TEST RESULTS 1984-96				
HYDROGEOLOGIC UNIT	EFFECTIVE THICKNESS (FEET)	TRANSMISSIVITY (FT SQ/D)	HYDRAULIC CONDUCTIVITY (FT/D)	STORATIVITY
CALICO HILLS				
C#1	198	100	0.5	NO DATA
C#2	149	100-800	1-5	0.0005-.004
PROW PASS				
C#1	62	400-800	7-10	.00004-.003
C#2	78	400-600	5-8	.001-.006
UPPER BULLFROG				
C#1	151	400-500	2-3	.00008-.002
C#2	79	600-900	8-10	.00002-.00005
LOWER BULLFROG				
C#1	206	18000-19000	90	.0002
C#2	96	17000-20000	170-210	.001
UPPER TRAM				
C#1	163	8000	40	.0001
C#2	70	6000	70	.001
COMPOSITE				
C#1	780-826	18000-27000	20-30	.001-.004
C#2	474-541	23000-28000	50-60	.003-.004
ONC-1	NO DATA	19000-31000	NO DATA	.002-.003
H-4	907	7000-35000	8-40	.002



EXPLANATION

HYDRAULIC CONDUCTIVITY, IN FEET PER DAY

200	10
100	5
50	

Issue 2: Conceptual Models of SZ Geology
Subtopic: 2.3: Geologic and mineralogic framework

Observation: There are two fundamental problems in the geologic and mineralogic framework of flow and transport in the SZ.:

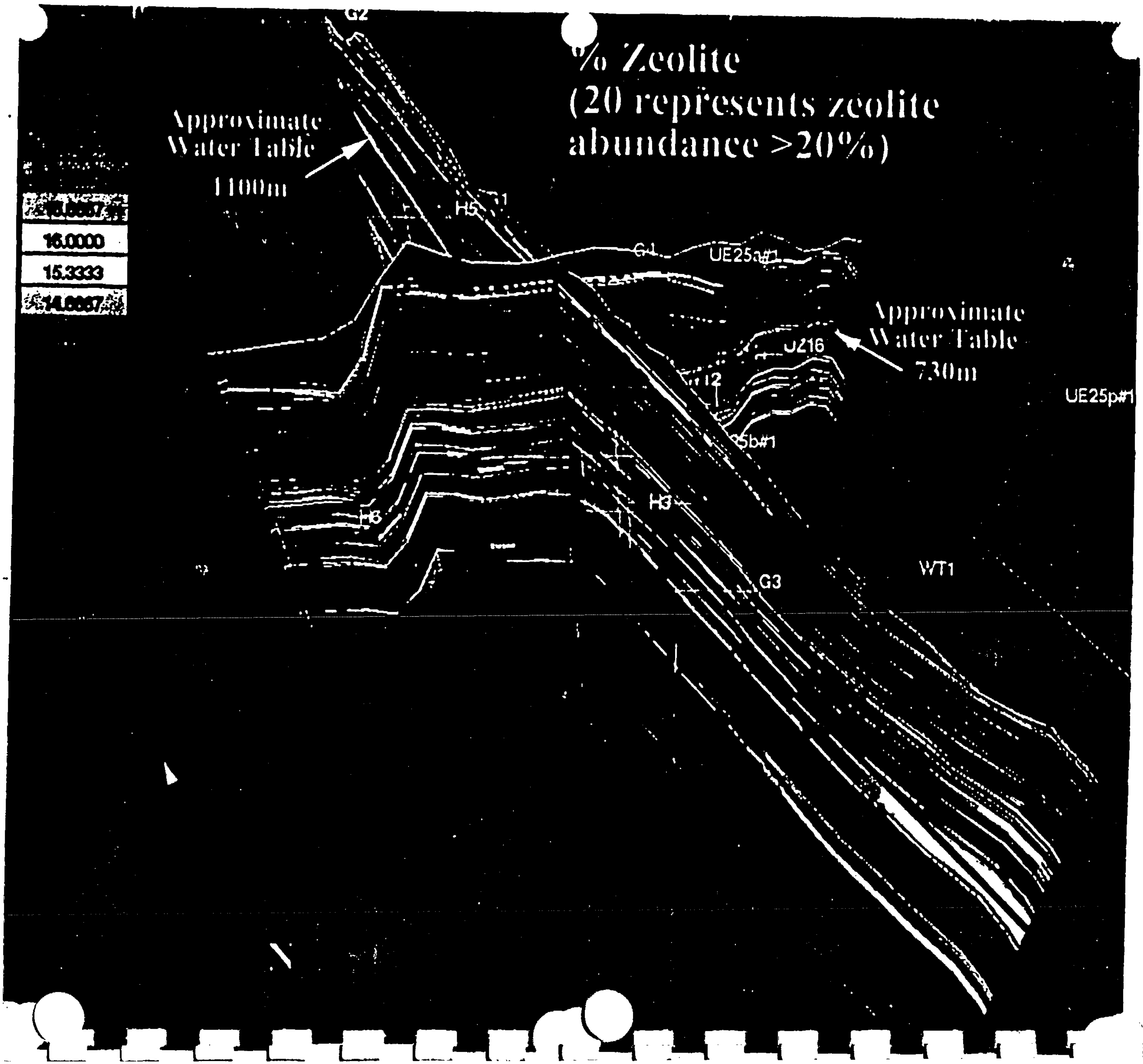
1) QA samples are available from the upper SZ beneath the exploration block from 5 recent holes (UZ-16, UZ-14, SD-7, 9, and 12) but characterization of the deeper SZ (below the Bullfrog Tuff) is largely restricted to pre-QA core and cuttings.

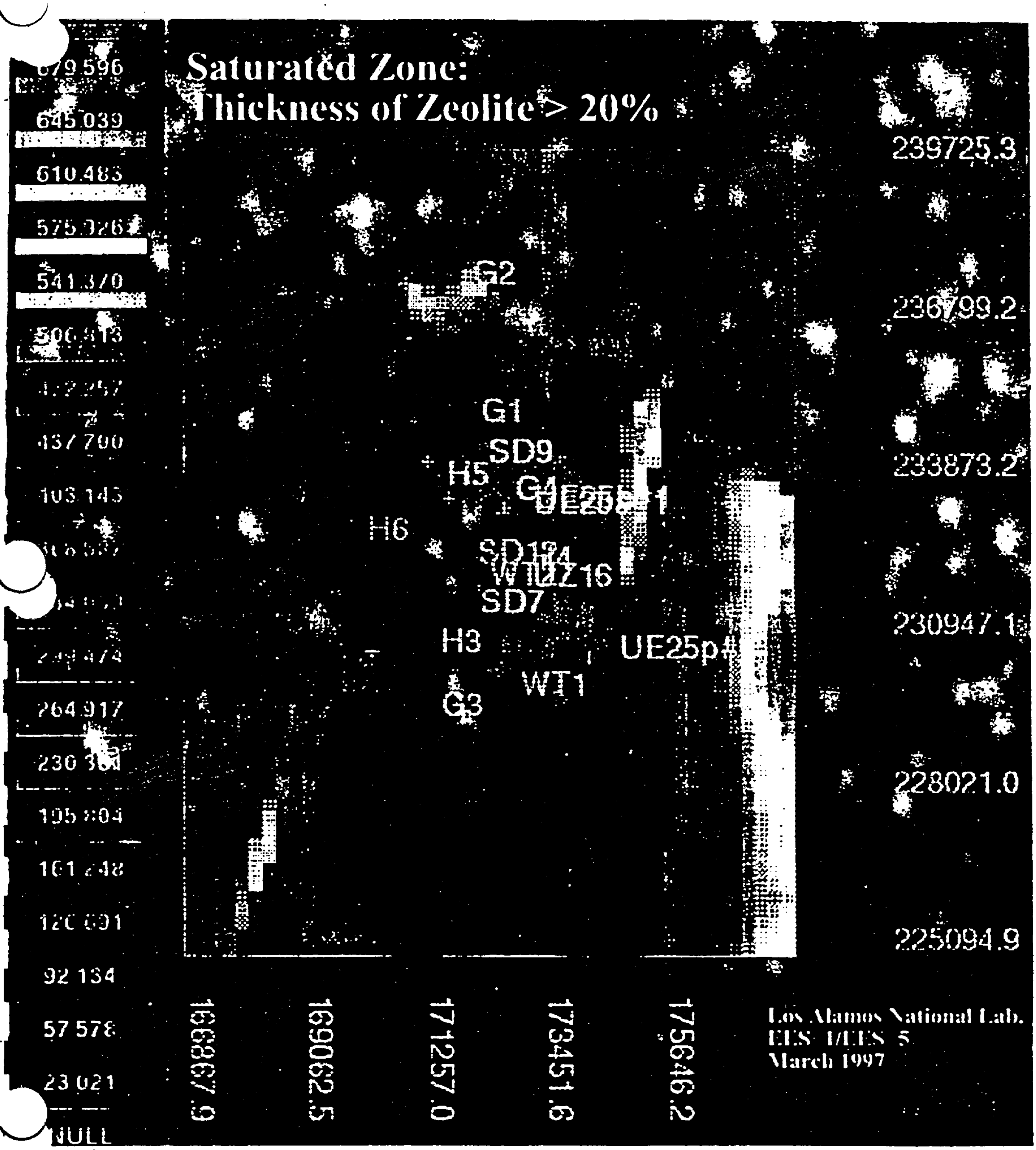
2) Comparisons between transmissive intervals and mineralogic zones are presently limited to pack-and-pump data from pre-QA cores.

Question: For TSPA-VA, are the mineralogic and geologic models sufficiently detailed to consider SZ transport in three dimensions?

Resolution: It should be possible to link SZ transmission models from several of the newer drill holes with quantitative mineralogy results. In the future, beyond TSPA-VA and into confirmation testing, more comparisons between transmissive zones, non-transmissive zones, and XRD-measured mineral abundances are needed.

Dave Vaniman/LANL


% Zeolite
(20 represents zeolite abundance >20%)
Approximate Water Table 1100m
Approximate Water Table 730m
16.0000
15.3333
G2
H5
G1
UE25a#1
UZ16
UE25p#1
H3
G3
WT1


Saturated Zone:
Thickness of Zeolite > 20%
645.039
610.483
575.926
541.370
437.700
403.145
264.917
195.804
161.248
92.134
57.578
23.021
NULL
G2
G1
SD9
H5
H6
SD7
H3
UE25p#1
WT1
G3
239725.3
236799.2
233873.2
230947.1
228021.0
225094.9
166867.9
169062.5
171257.0
173451.6
175646.2
Los Alamos National Lab.
EES-1/EES-5
March 1997

TSPA Introduction to Issue 3: Transport Processes and Parameters

Jack Gauthier
SZ Abstraction/Testing Workshop
1–3 April 1997

Subissue 3.1 Dispersivity

- What dispersivity values should be used*
  - longitudinal
  - transverse
- How would channelization reduce dispersivity
- Should upstream dispersion be constrained

* Being considered for TSPA-VA

Subissue 3.2 Matrix Diffusion (Effective Porosity)

- What diffusion coefficients should be used*
- Can an effective porosity be used*
  - what are the length and time scales
- Are the C-well and laboratory values representative of the natural system

Subissue 3.3 Sorption

- What is the distribution of K_ds*
  - fracture
  - matrix
- Are the C-well and laboratory values representative of the natural system

Subissue 3.4 Colloid Transport

- Should colloidal transport be considered (And for what radionuclides—Pu, Np?)
- What parameters are important to the problem (e.g., K_d, colloid conc., filtration/sedimentation)
- Are measured colloid concentrations (J-13) indicative of maximums in the natural system
- What do the C-wells microspheres tell us

Bruce A. Robinson
Los Alamos National Laboratory

Title: Dispersivity

Issue 3, Talk #1

Synopsis

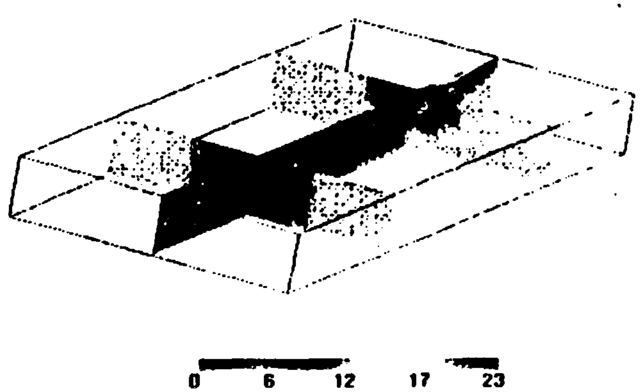
Dispersivity controls the extent of spreading of a solute plume, and hence will control concentration at the accessible environment. The key parameter is actually the transverse dispersivity, a parameter we have very little information about.

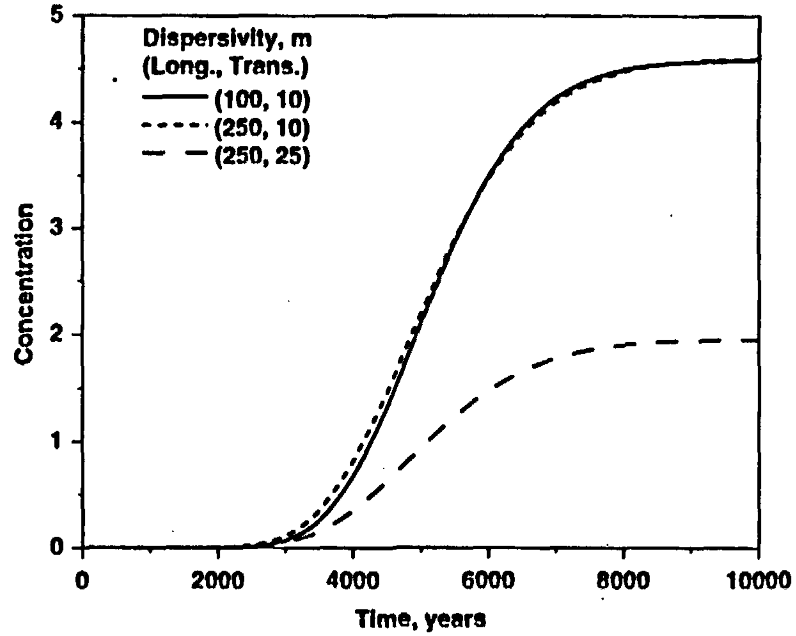
Proposal (no modeling, for once)

- **Literature Review**
  - Comprehensive review of the literature in this field
  - Focus on measurements of transverse dispersivity
  - Focus on results in fractured media
  - Don't forget scaling issues
- **C-Wells Experiments**
  - Extract dispersivity values from experiments
  - Propose tests to determine transverse dispersivity, if possible (maybe available by LA)
  - Estimate uncertainty
- **Deliver results to PA**

Influence of Longitudinal and Transverse Dispersivity

E-117





uz_vg2-3

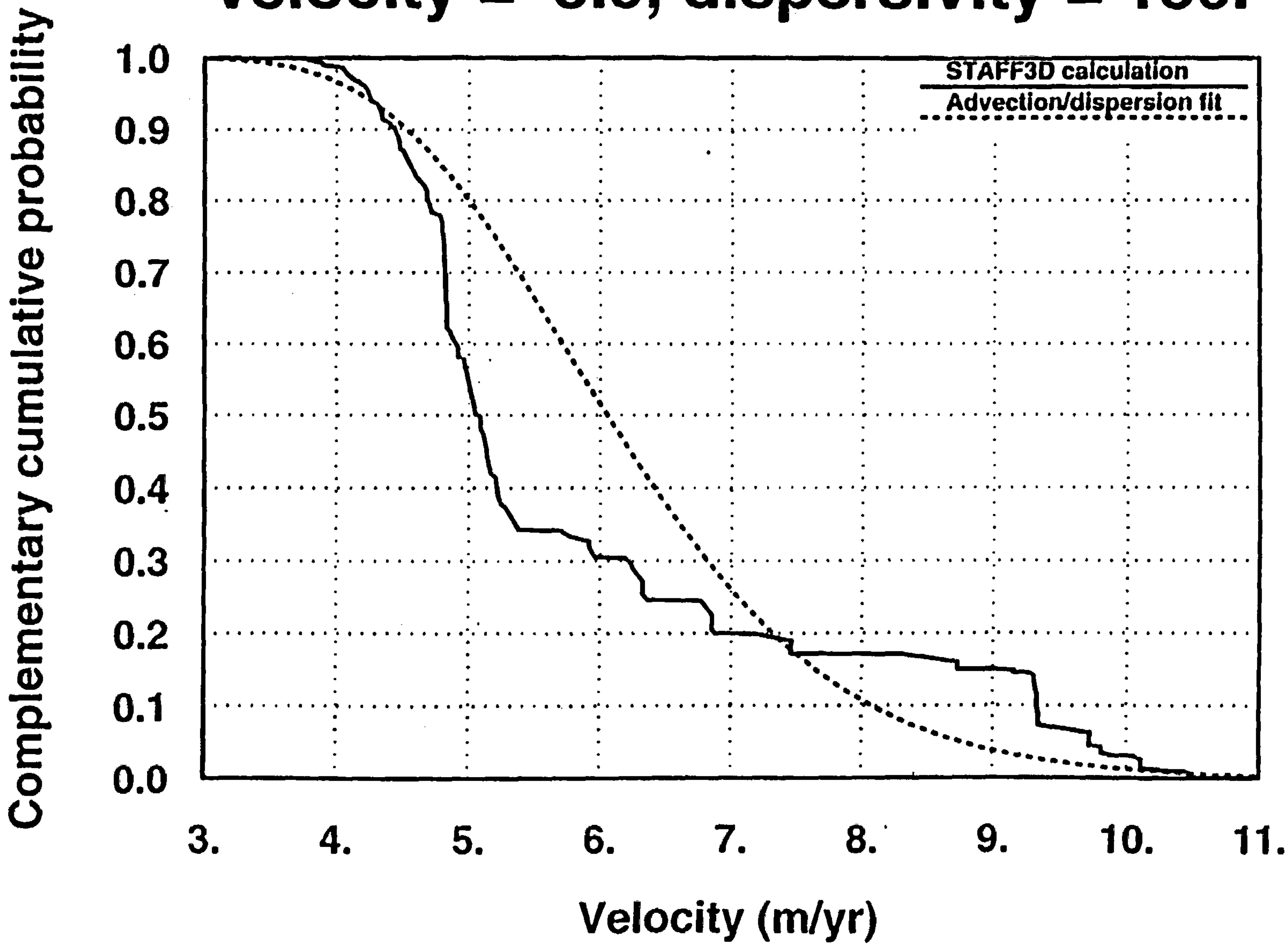
Geoanalysis Group, Los Alamos

Dispersivity is used to compensate for structure that is left out of the model

- Sub-grid-block structure
- Unknown or omitted features
- Flow channelization

E-118

Example from TSPA-1993
Prow Pass source, no drain
velocity = 5.9, dispersivity = 130.



3. Transport Process and Parameters

3.1 Dispersivity

Chunhong Li, INTERA

Uncertainty is the core
April 1, 1997

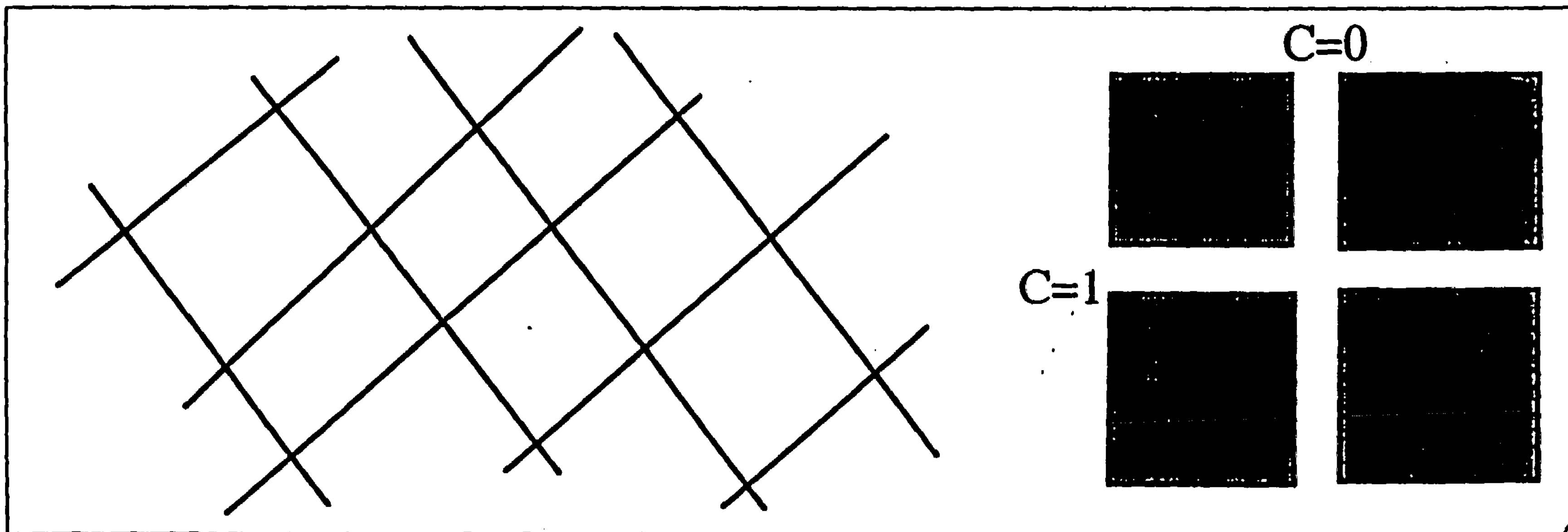
Dispersion/Dispersivity depends on

Flow models/conditions:

Discrete, DK, ECM

Dispersivity is directly related to

Fracture connectivity & junction Pe



Physical/chemical processes:

Adsorption and m.diffusion

TSPA point of view:

Source term from UZ

Less of field data/Large uncertainty

Problems need to be addressed:

The importance of dispersion in SZ (relates to UZ)

What range of dispersivity to use (scale dependent, fractal)

The combined effects of dispersion and other processes

3. Transport Processes and Parameters
3.2 Matrix Diffusion

Matrix Diffusion:
Results and Implications of the C-Wells Bullfrog Tuff Test

Jake Turin (turin@lanl.gov)

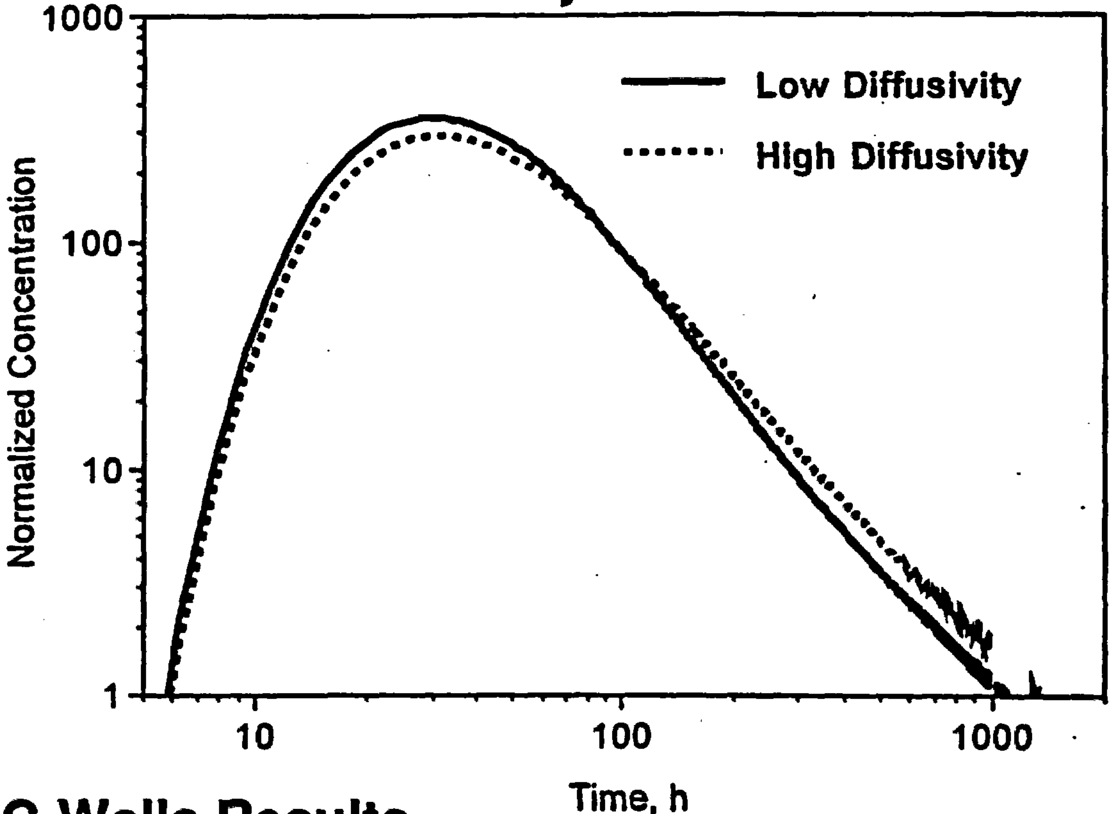
Los Alamos National Laboratory

TSPA - SZ Workshop

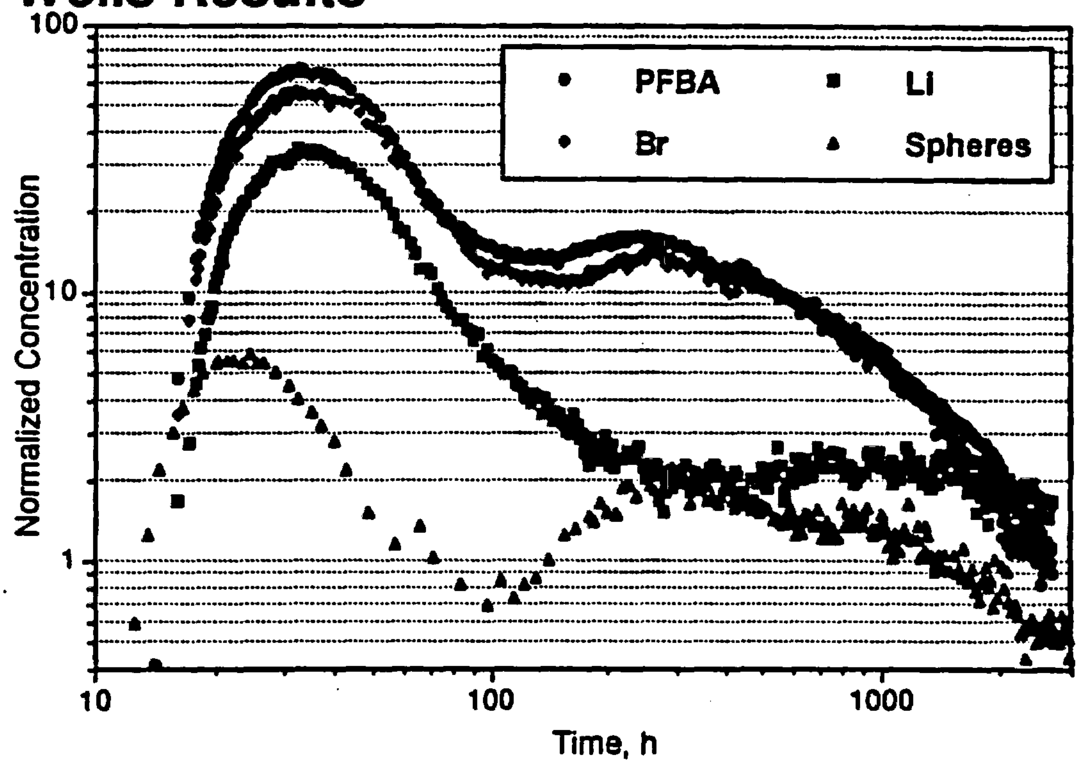
April 1, 1997

E-123

Matrix Diffusion: Theory



C-Wells Results



Earth and Environmental Sciences **Los Alamos**

Matrix Diffusion

- C-Wells conservative tracer results provide clear indication of matrix diffusion in Bullfrog Tuff.
- Further analysis is necessary to establish best estimates, confidence limits, and bounds for parameters.
- Hand-off to TSPA will be documented evidence of field-scale matrix diffusion, parameter estimates, and confidence limits.
- Planned FY98 Prow Pass Tuff test will yield similar information for different unit, provide data on stratigraphic dependence of matrix diffusion parameters.

Bruce A. Robinson
Los Alamos National Laboratory
Title: Matrix Diffusion (Effective Porosity)
Issue 3, Talk #5

Synopsis

Theoretical results and C-Wells experiments suggest that matrix diffusion occurs in the SZ. This means that the effective porosity should be greater than the fracture porosity, perhaps approaching the matrix porosity. Effective continuum models can be assumed if this is true.

Proposal

- For the SZ Flow and Transport base case:
  - Evaluate the matrix diffusion time scale at each location in the model
  - Compare to type curve, obtain an effective porossity
  - If the matrix porosity is obtained along the transport pathways, we are done. If not:
- Compare continuum to Dual Porosity Model
  - Compute effective porosity from type curve at every node
  - Compute transport of key radionuclide
  - Do the same for dual porosity model, compare results

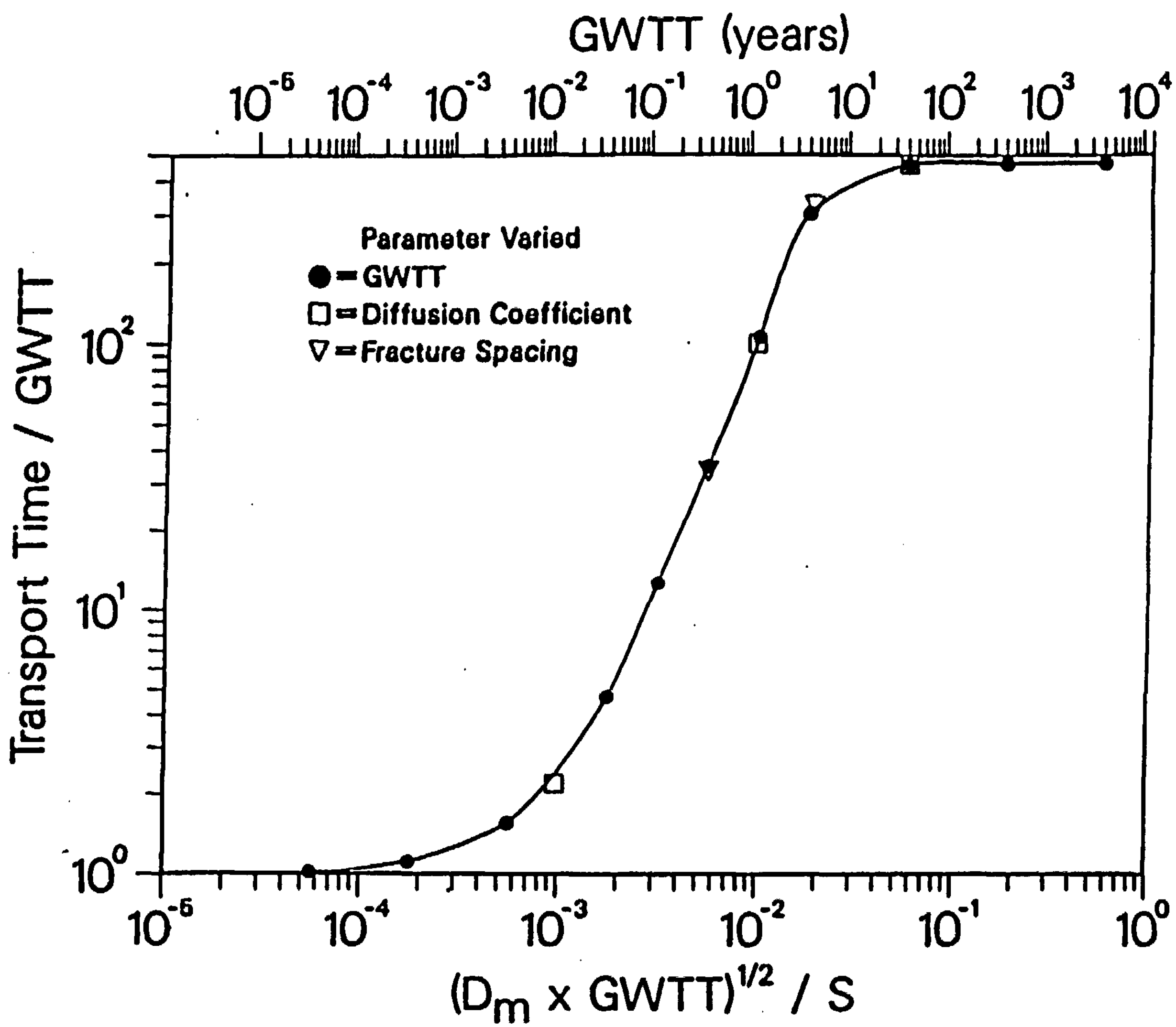


FIGURE 3 Simulation results for transport time for the matrix diffusion model. The upper x-axis applies only for the base case conditions of $D_m = 10^{-9}\ m^2/s$ and $S = 10\ m$.

Redox Potential Effect on Sorption

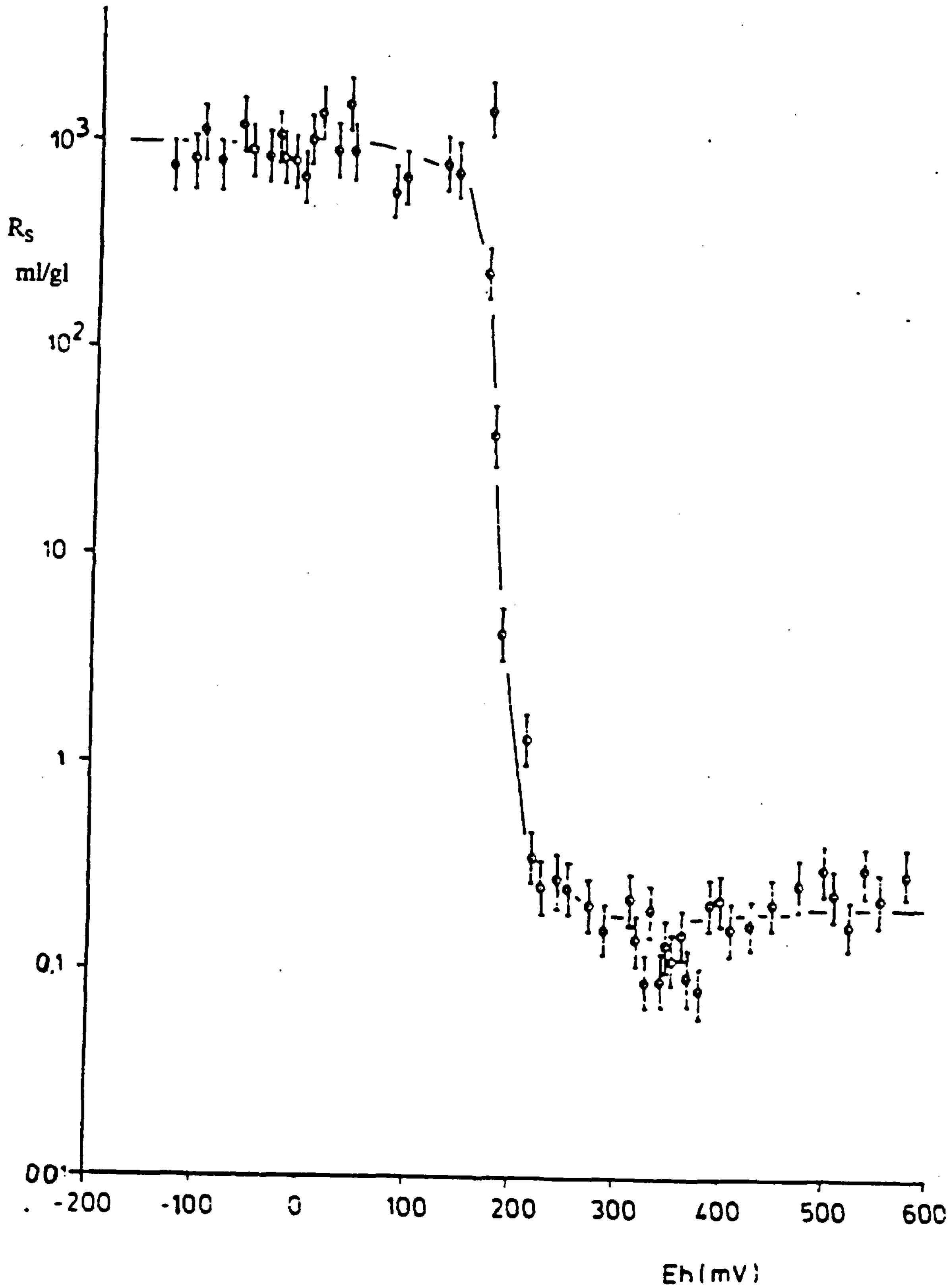
Ines Triay
LANL

ISSUE 3

E-129

K_d, m^3/kg

	Bentonite				Granite				Crystalline Rock	
	Oxidizing best estimate	min - max	Reducing best estimate	min - max	Oxidizing best estimate	min - max	Reducing best estimate	min - max	Oxidizing best estimate	Reducing best estimate
Am	2	0.25 - 10	2	0.25 - 10	5	0.5 - 80	5	0.5 - 80	0.05	3
Np	0.1	0.05 - 0.12	1	0.1 - 5	0.01	0.001 - 10	5	0.1 - 10	0.002	0.2
Pu	1	0.1 - 3.5	1.5	0.1 - 5	3	1 - 80	5	0.5 - 80	0.03	0.3
Th	1	0.002 - 6	1	0.002 - 6	5	0.1 - 10	5	0.1 - 10	0.2	0.2
U	0.02	0 - 0.1	0.2	0.1 - 1	0.01	0.002 - 1	5	0.01 - 10	0.002	0.2



R_S
ml/gl
10^3
10^2
10
1
0,1
0.01
-200
-100
0
100
200
300
400
500
600
Eh(mV)

E-132

3. Transport Processes and Parameters
3.3 Sorption

Sorption:
Results and Implications of the C-Wells Bullfrog Tuff Test

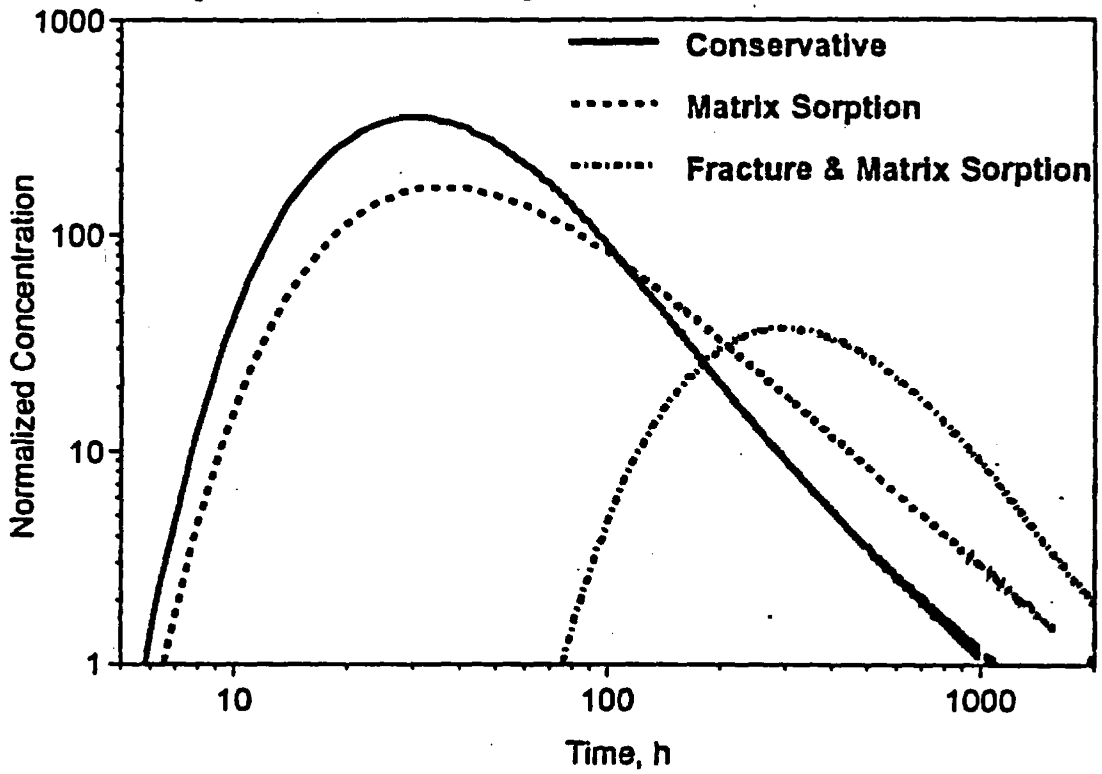
Jake Turin (turin@lanl.gov)

Los Alamos National Laboratory

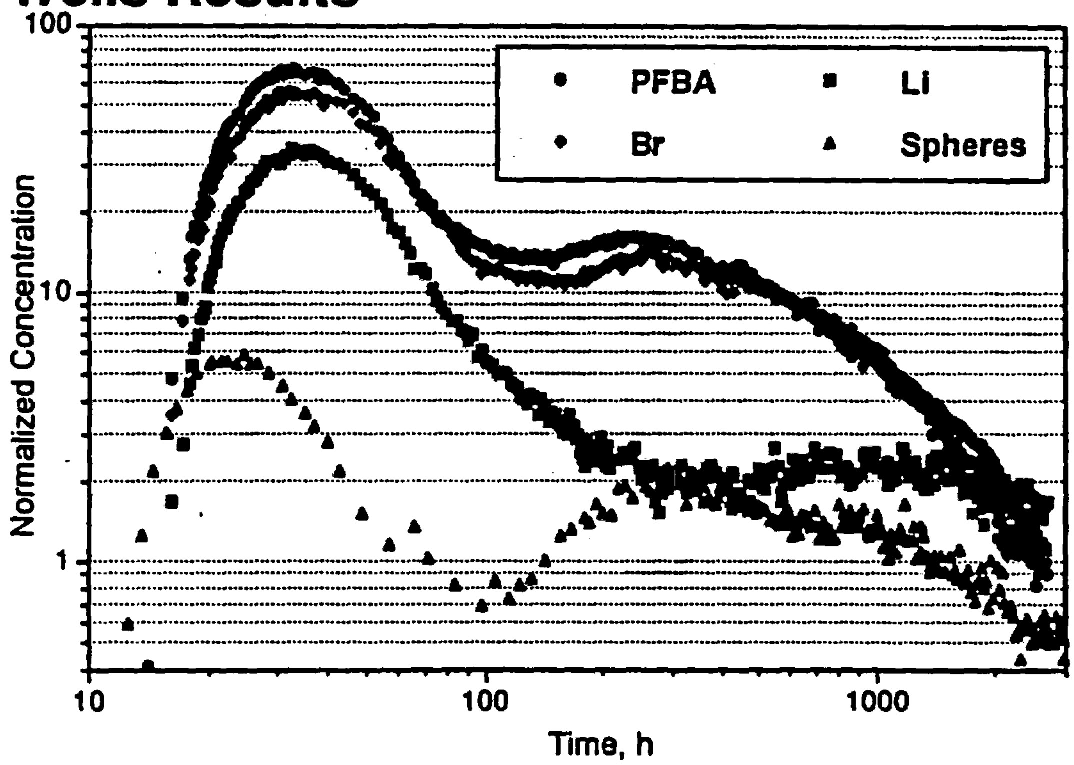
TSPA - SZ Workshop

April 1, 1997

Solute Sorption: Theory



C-Wells Results



Sorption

- C-Wells lithium breakthrough curves provide concrete evidence of field-scale sorption. Preliminary analysis suggests good agreement with laboratory results.
- Further analysis of data will better differentiate fracture / matrix sorption, establish confidence limits and provide bounding estimates of field sorption parameters.
- Hand-off to TSPA will be recommendations for deriving field-scale sorption parameters for radionuclides from laboratory data.
- Planned FY98 Prow Pass test will include multiple sorbing tracers to better differentiate sorption processes.

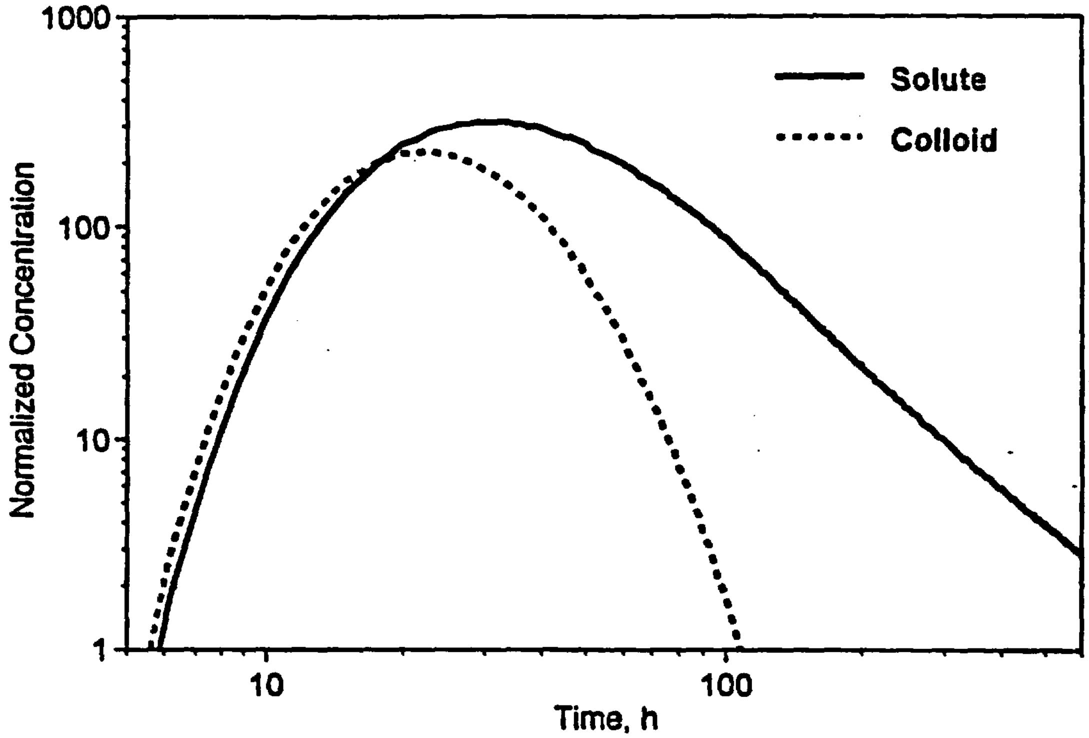
Colloid Transport:
Results and Implications of the C-Wells Bullfrog Tuff Test

Jake Turin (turin@lanl.gov)
Los Alamos National Laboratory

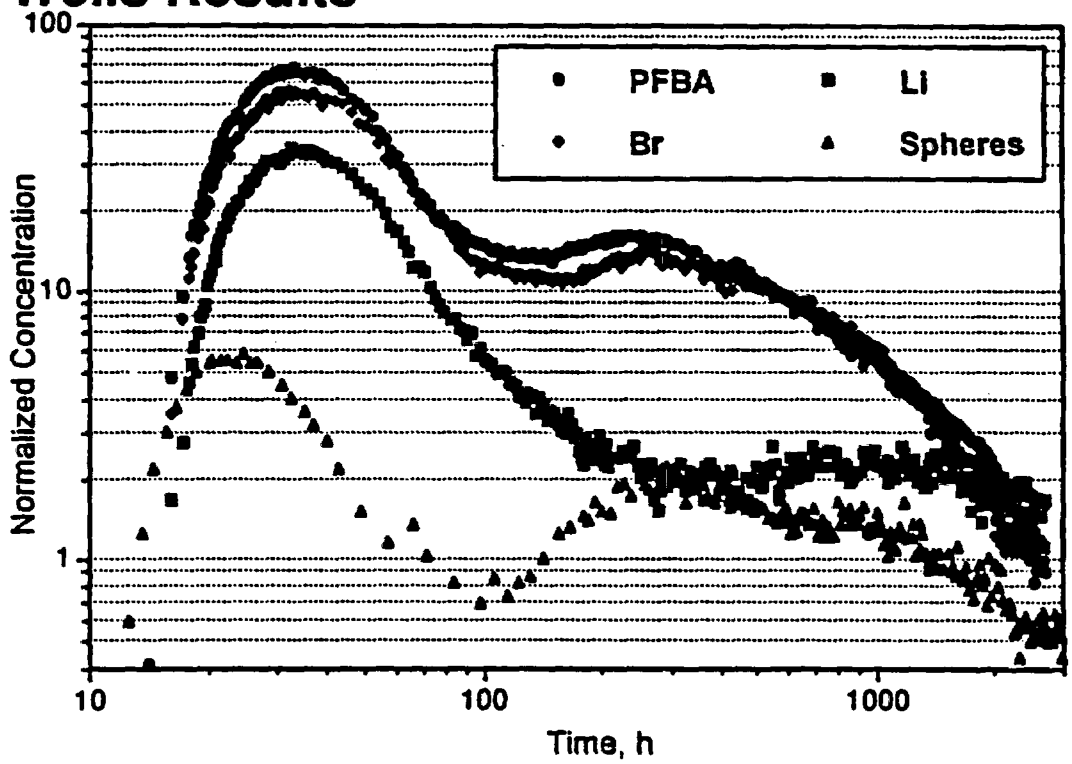
TSPA - SZ Workshop

April 1, 1997

Colloid Transport: Theory



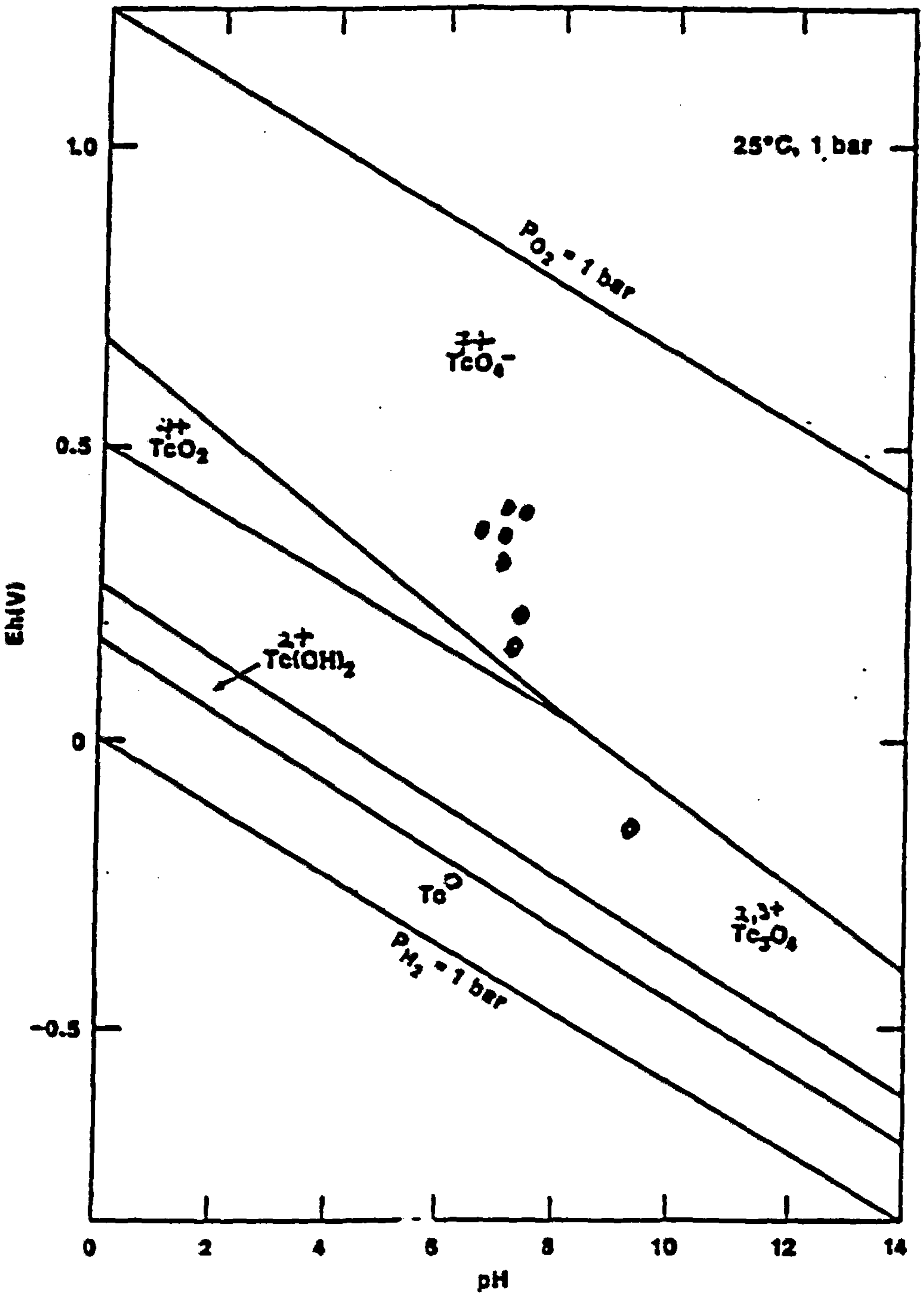
C-Wells Results



REDOX POTENTIAL (Eh) AND TRANSPORT

Arend Meijer
LANL/GCX
(505) 256-3769

E-138

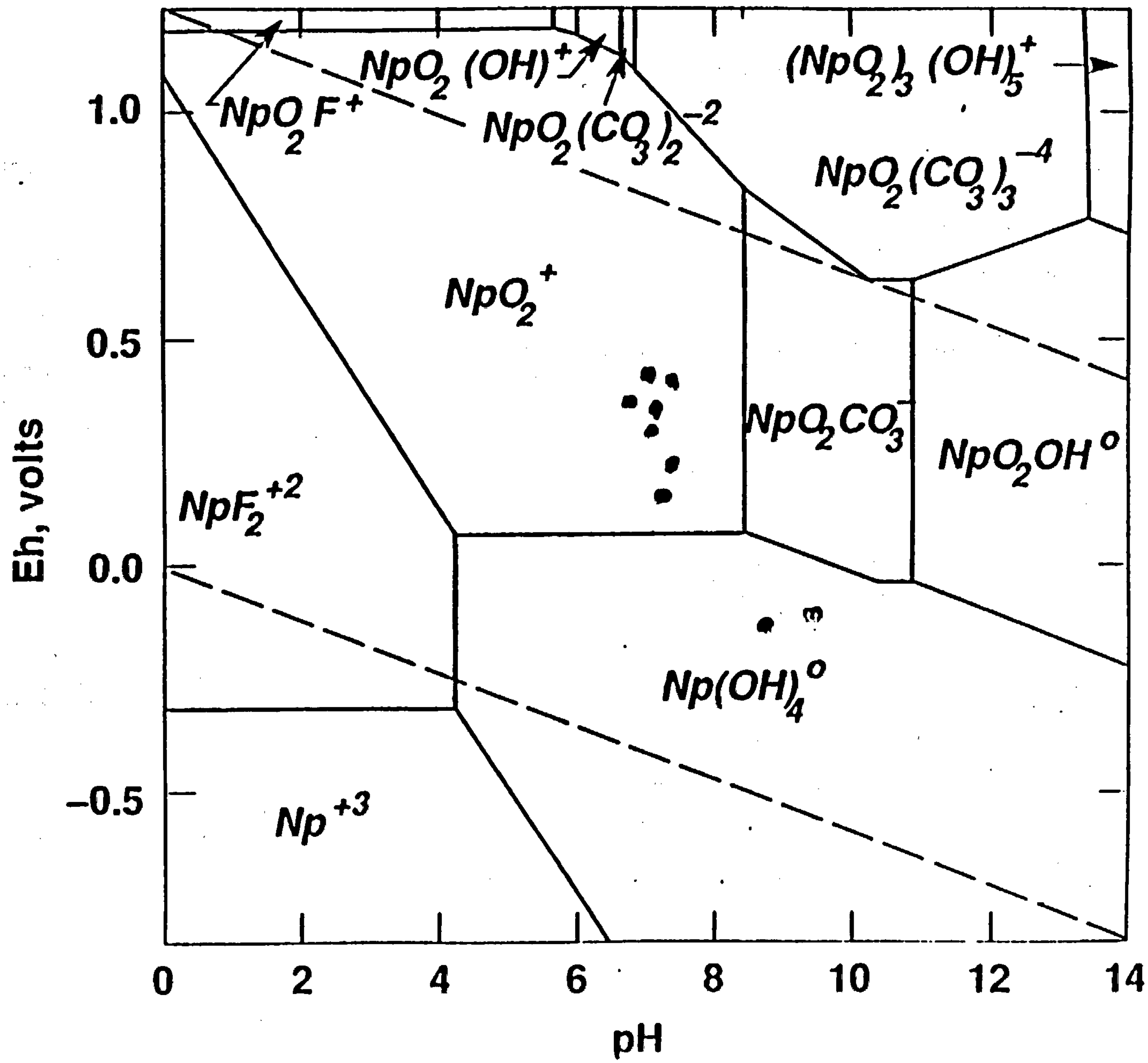


Brookins (1988)

Colloid Transport

- C-Wells microsphere results provide unequivocal evidence of colloid transport through 30 m of fractured Bullfrog Tuff. Low microsphere recovery (relative to solutes) indicates some attenuation process (filtration or retardation).
- Further analysis of results will permit quantification of colloid transport parameters, with (large) associated uncertainty estimates.
- Hand-off to TSPA will include clear evidence of colloid transport, some estimate of colloid transport parameters (with caveats).
- Planned Prow Pass test will use multiple size spheres to better differentiate processes.

Np aqueous speciation / J-13 water — 25°C



E-140

TSPA Introduction to Issue 4: Coupling to Other Components of TSPA

Jack Gauthier
SZ Abstraction/Testing Workshop
1–3 April 1997

Subissue 4.1 Climate Change

- Water-table levels*
- Boundary conditions
  - recharge
  - outflows
- Changes in flow paths
  - transport parameters

* Being considered for TSPA-VA

Subissue 4.2 Thermal and Chemical Plume

- Will heat from an 80+ MTU/acre repository significantly affect the SZ
- Will dissolution/precipitation reactions be significant
- What alterations will be permanent

Subissue 4.3 Well Withdrawal Scenarios

- What are representative withdrawal parameters*
  - location
  - rate
  - depth
  - other
- What influence would the withdrawal have on SZ flow
- Should well withdrawal be incorporated in models
- Should channelization be incorporated in models

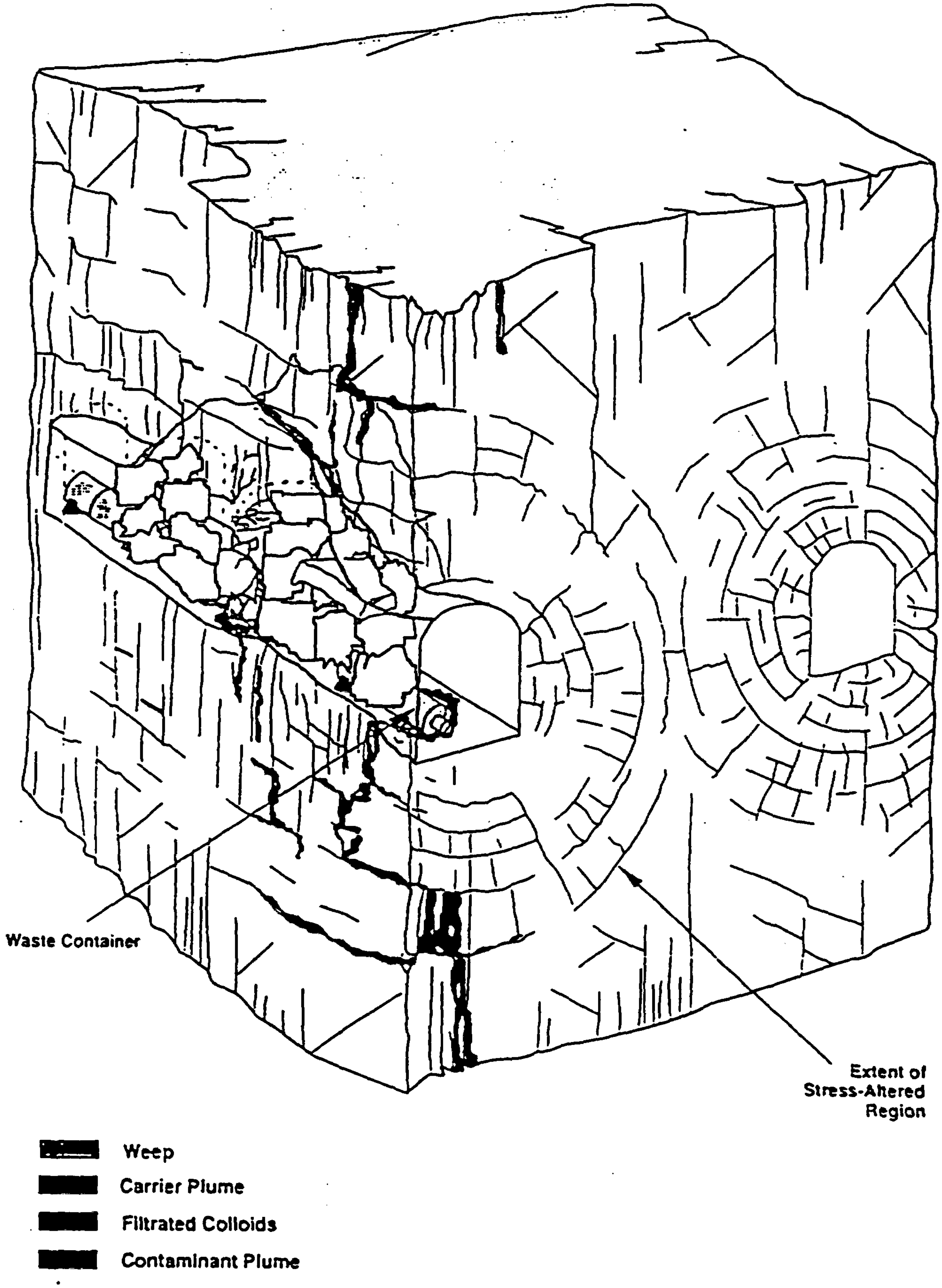
Subissue 4.4 Coupling with UZ Transport

- How should UZ and SZ be coupled
  - are transport pathways connected
- Would water-table rise be rapid enough to affect radionuclide concentrations in the SZ
- What part does the perched water play

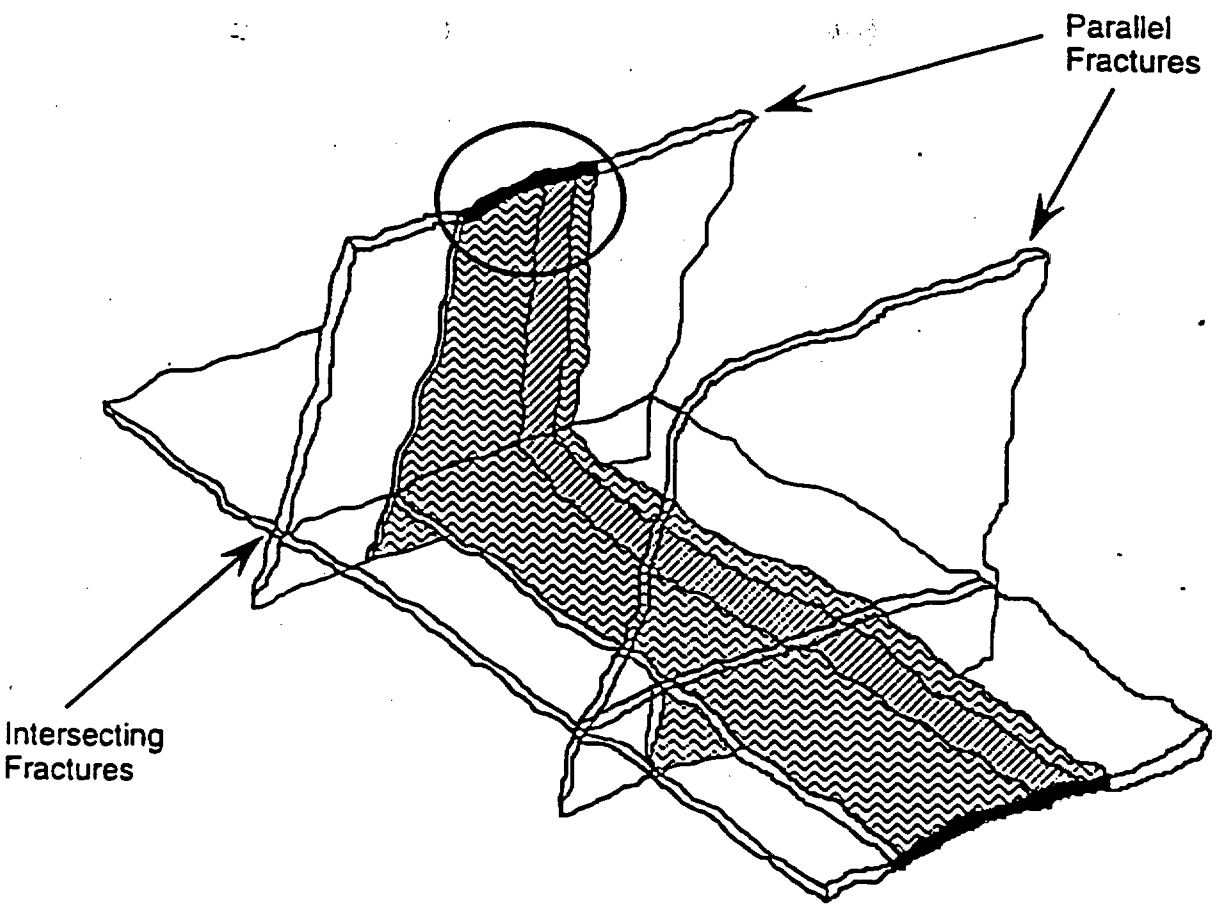
BASIC ISSUES

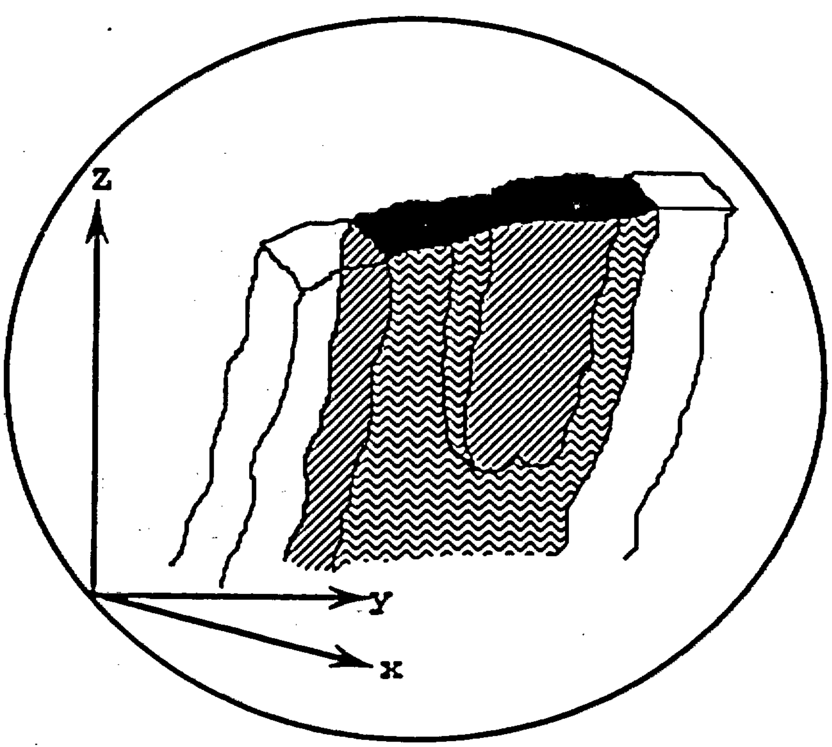
How Fluids Reach the WT

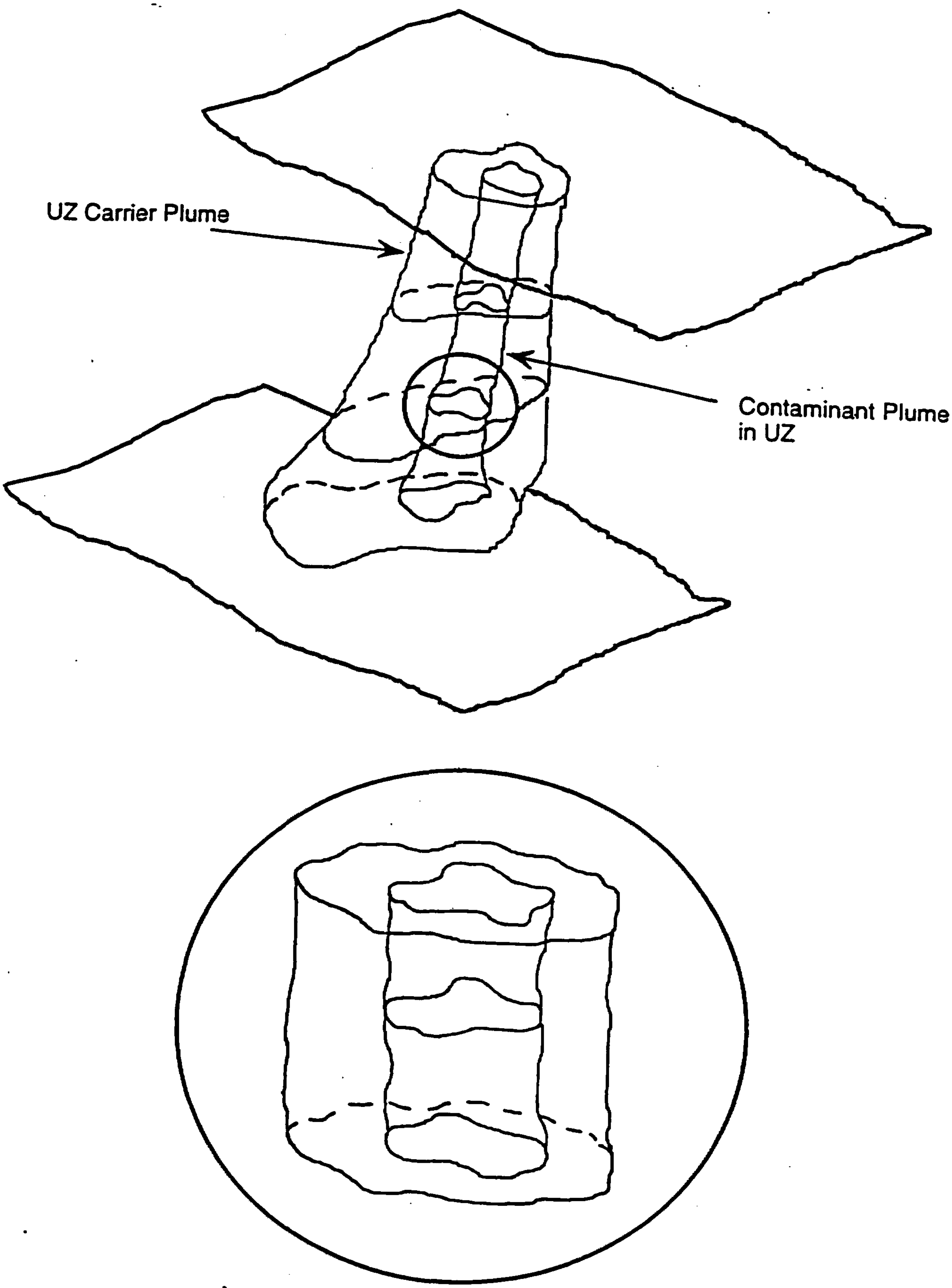
How Mixing Occurs

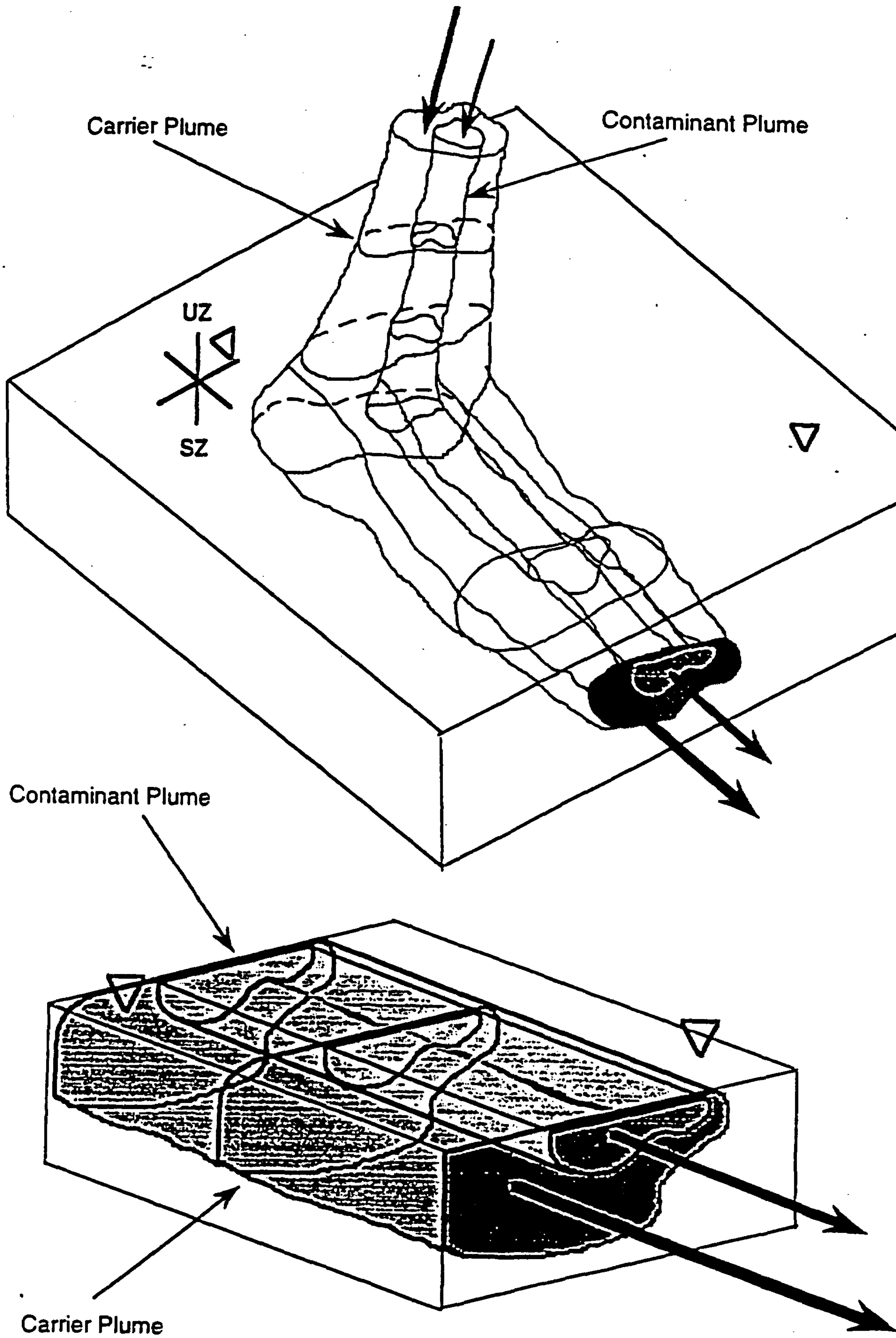


Waste Container
Extent of
Stress-Altered
Region
Weep
Carrier Plume
Filtrated Colloids
Contaminant Plume


Parallel
Fractures
Intersecting
Fractures


z
y
x


UZ Carrier Plume
Contaminant Plume
in UZ

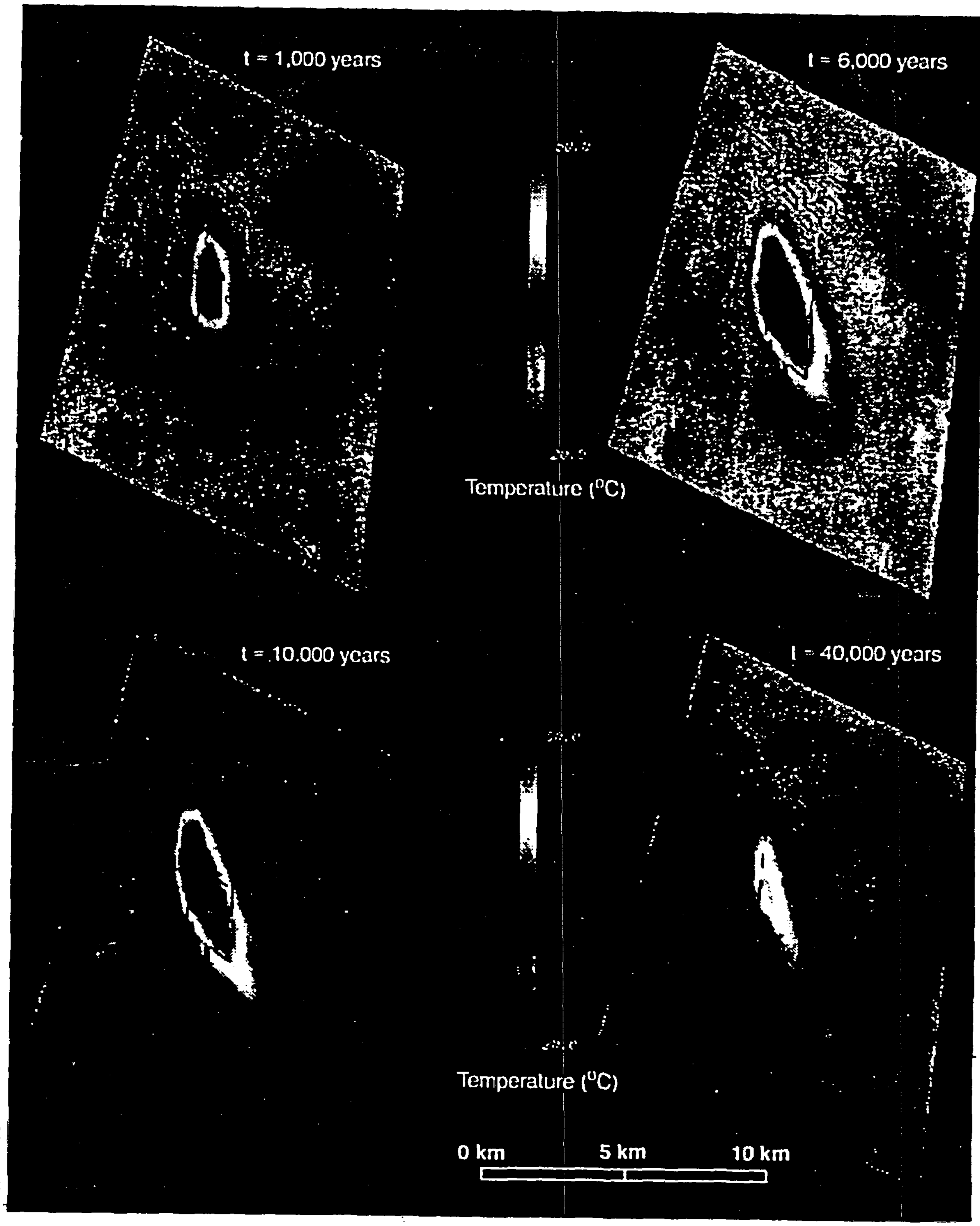

Carrier Plume
Contaminant Plume
UZ
SZ
Contaminant Plume
Carrier Plume

Sandia National Laboratories

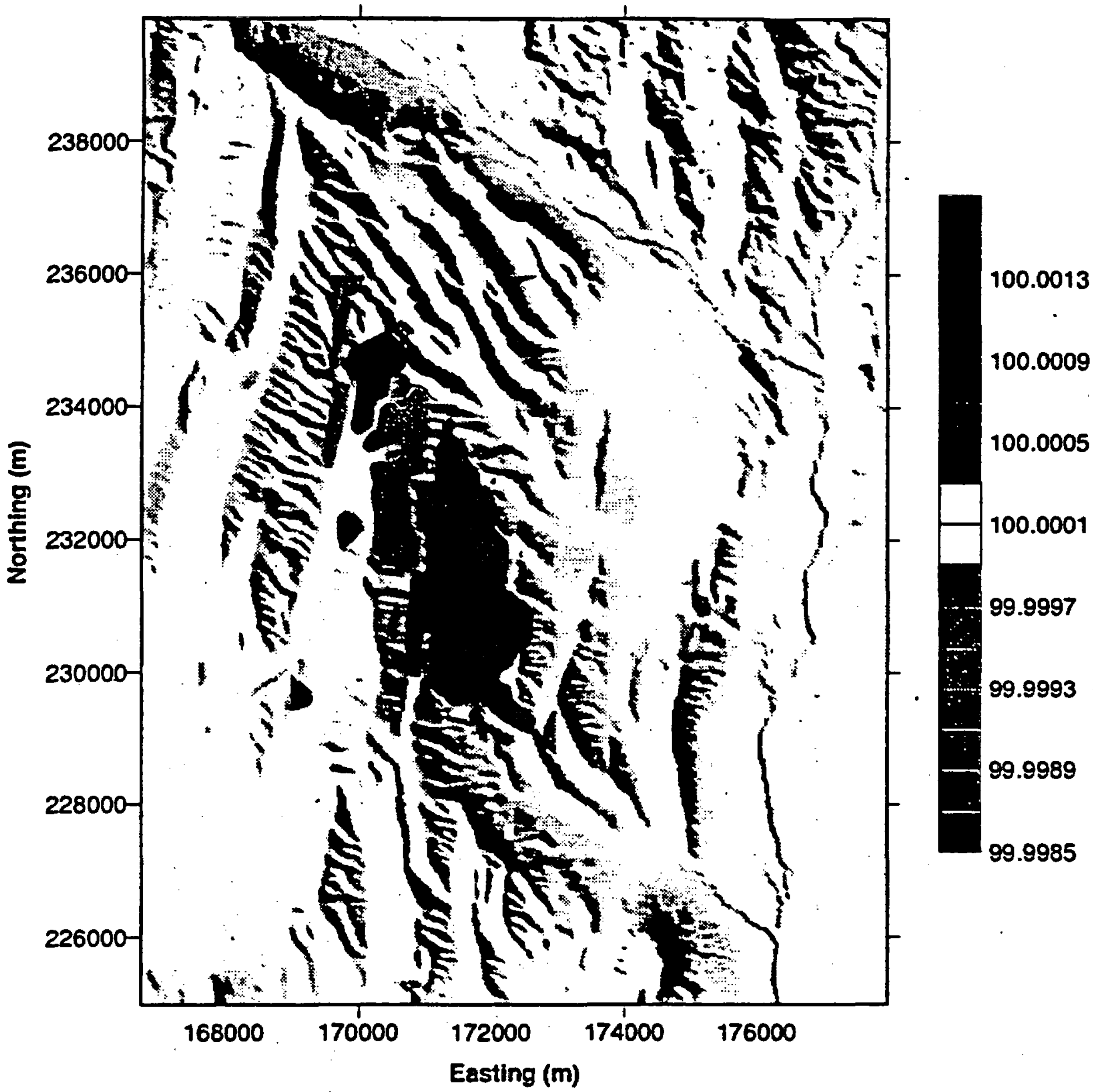
Coupling to Other Components of TSPA (Thermal and Chemical Plume) Issue 4.2

BILL W. ARNOLD
SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NM
April 2, 1997

Simulated Temperature at the Water Table, 3D Thermohydrologic Model



Simulated Cristobalite Dissolution and Precipitation, Time = 20,000 Years After Waste Emplacement, Initial Solid Phase Concentration = 100 moles/m**3



Sandia National Laboratories

- Thermohydrologic modeling of flow and heat transport in the SZ indicates that there may be a significant increase (>30 °C) of temperature at the water table relative to ambient conditions resulting from repository heat (Ho et al., 1996).

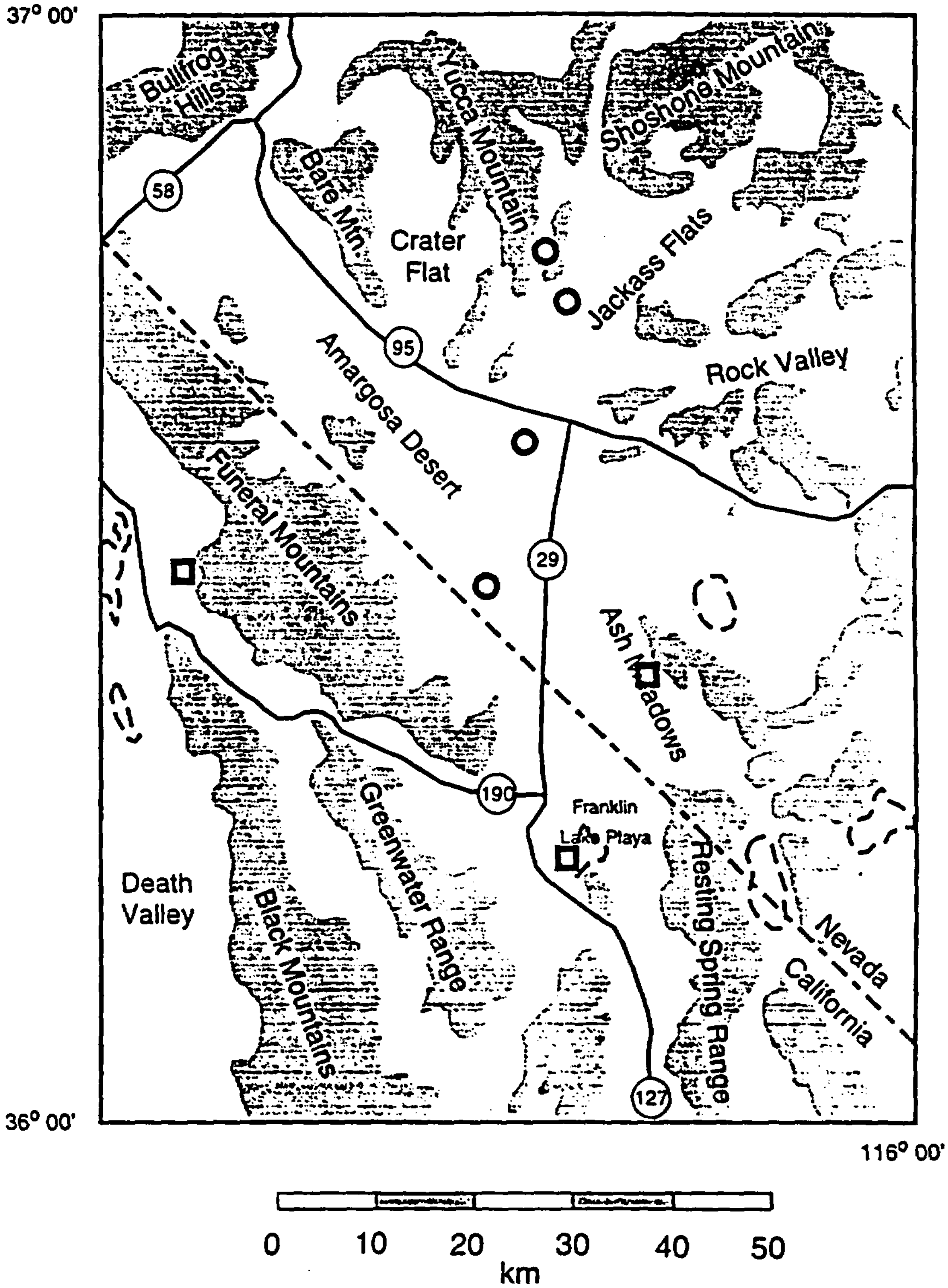
- Preliminary reactive transport modeling of silica dissolution and precipitation in the SZ coupled to thermohydrologic modeling suggests the formation of a zone of relatively concentrated dissolution beneath the repository and a zone of more diffuse precipitation downgradient of the repository.

- The absolute magnitudes of change in cristobalite concentration in the solid phase are relatively small in this preliminary reactive transport model. Simulation of dissolution/precipitation reactions of other mineral phases should also be considered to evaluate possible alterations to hydrologic properties in the SZ related to repository heat.

Sandia National Laboratories

Coupling to Other Components of TSPA (Well Withdrawal Scenarios) Issue 4.3

BILL W. ARNOLD
SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NM
April 2, 1997



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- At a minimum, TSPA-VA calculations should include radionuclide concentrations from wells at approximately 5 km and 30 km from the potential repository.

- Both high-capacity, deeper wells (corresponding to irrigation or municipal wells) and low-capacity, shallow wells (corresponding to domestic or stock wells) should be considered in TSPA-VA simulations.

- Scoping calculations may be warranted to assess the evaporative accumulation of radionuclides at regional SZ discharge areas, such as Franklin Lake Playa.

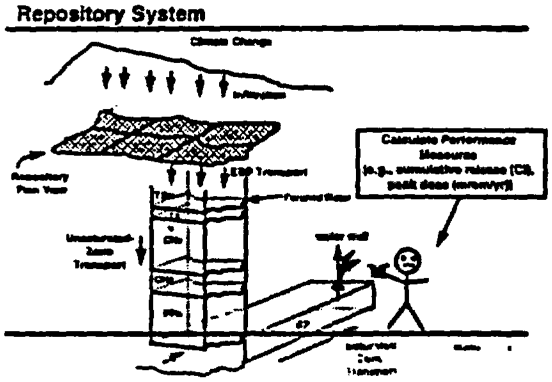
Performance Assessment
and Modeling

Abstraction of Well Withdrawal Scenarios

Category 4. Coupling to Other Components of TSPA
Issue 4.3. Well Withdrawal Scenarios

Jerry McNeish
M&O/Intera (DE&S)
SZ Workshop
April 2, 1997

Schematic of Yucca Mountain Potential Repository System



Proposal for well withdrawal abstraction

- **Problem Statement: NRC rejection of TSPA-95 approach to well withdrawal**
- **Proposed approach to abstraction:**
  - Improved definition of withdrawal zone thickness
  - Detailed local scale modeling
  - Sensitivity analysis of wellbore mixing, length of screened interval, depth of vertical mixing, zone of pumping influence, pumping rates
- **Proposed Abstraction:**
  - Wellbore mixing factor
  - Regional aquifer mixing factor

Bruce A. Robinson
Los Alamos National Laboratory

Title: Coupling to UZ Transport

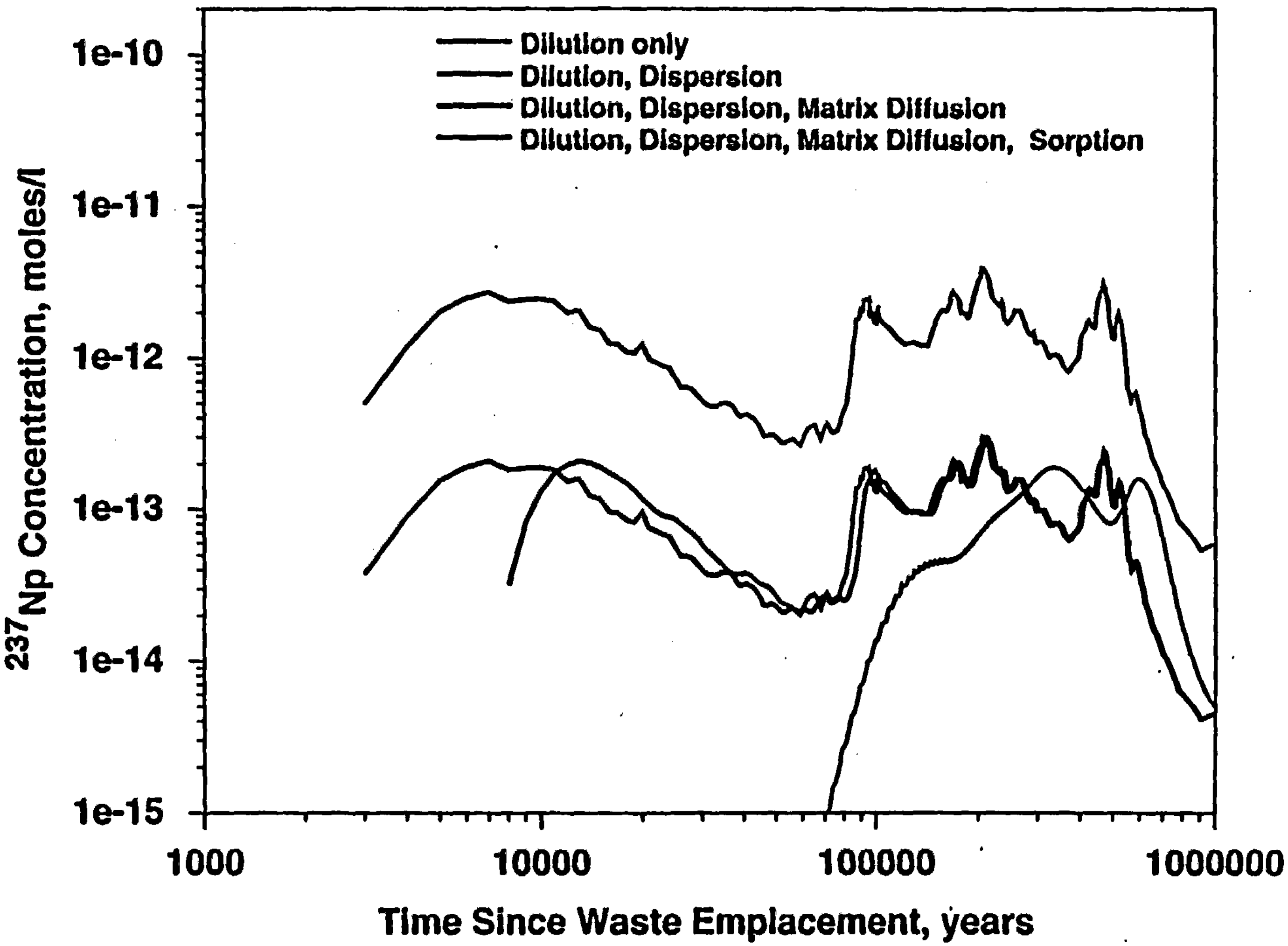
Issue 4, Talk #6

Synopsis

Convolution should be used to couple the UZ and SZ flow and transport models for TSPA. Anything less will fail to take advantage of some of the features of the SZ transport system that enhance predicted performance.

Results of Convolution Procedure

$$C_{SZ}(t) = \int_0^t C_{UZ}(t-t')f_{SZ}(t')dt'$$

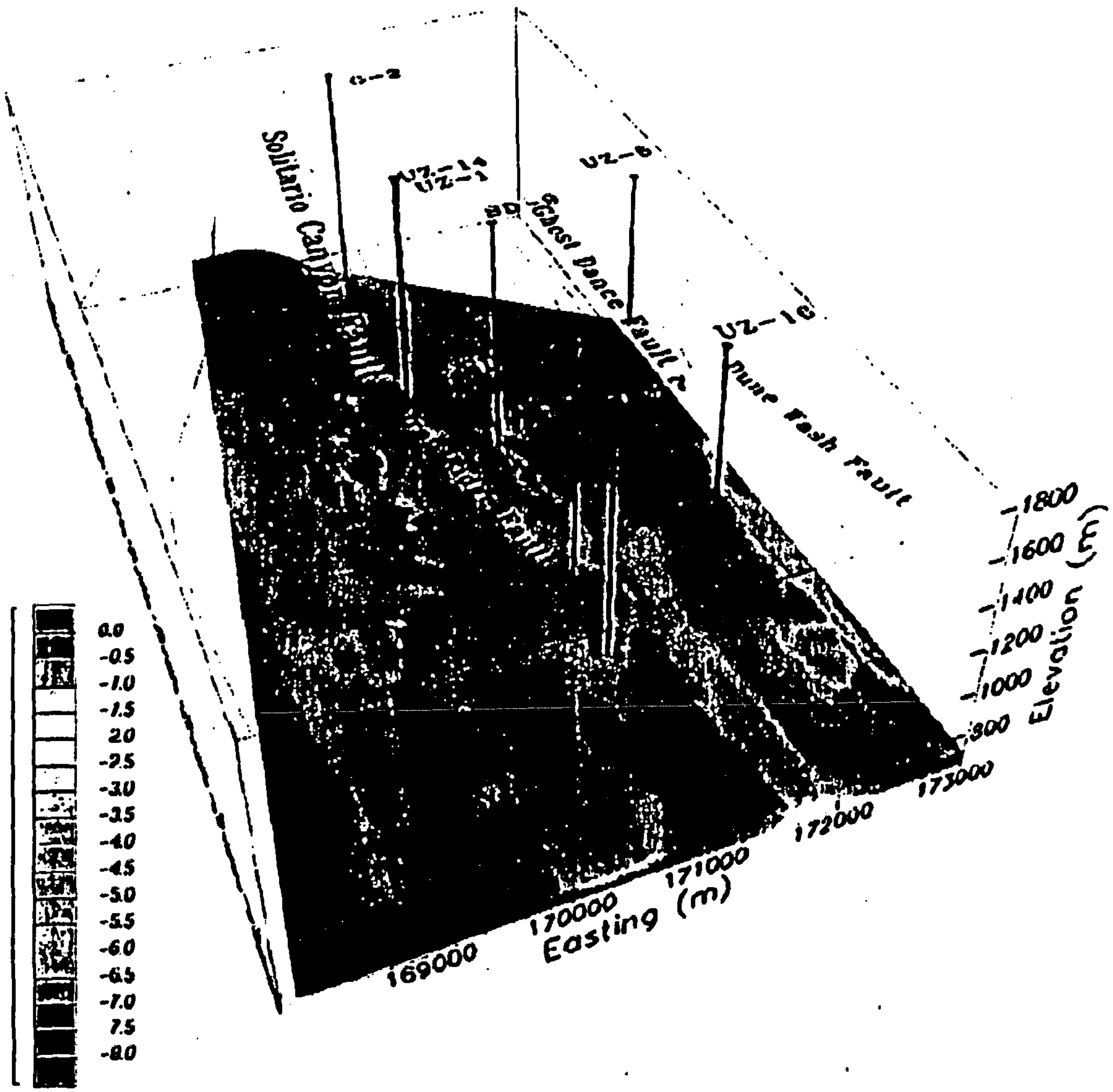


What Can We Learn about the SZ from the UZ flow model?

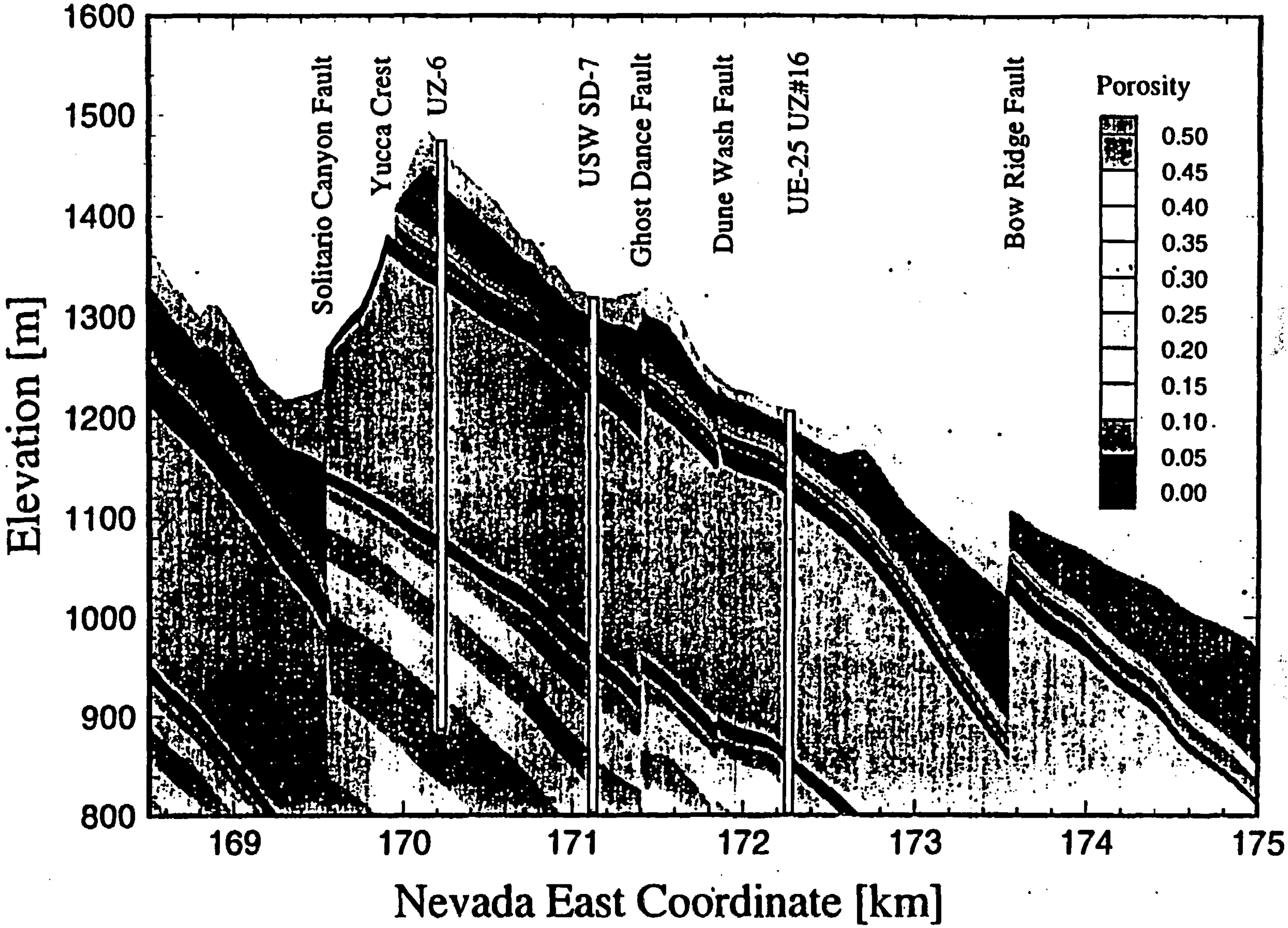
Ardyth Simmons

LBNL

Vertical Matrix Mass Flux at Water Table



Recharge map at the water table, simulated using the dual-permeability model, parameter set #4 and [illegible]ltration map #2



Matrix porosities

Summary of UZ Flow Analysis Plans

Susan J. Altman
Sandia National Laboratory

TSPA-VA Saturated Zone Flow and Transport Abstraction Testing Workshop
April 2, 1997

TSPA-VA Abstraction/Testing Workshop UZ Flow

Issues Focused on in Analyses Plans

- Seepage into the drift
- Infiltration and climate change
- Lateral flow below the repository and perched water
- Model calibration

UZ Flow Abstraction/Testing Workshop
Analyses Plans

- Calibration and Abstraction of the UZ Site-Scale Model
- Flow Seepage into Drifts under Pre-Waste-Emplacement Conditions
- Testing of perched-water concepts and their implications for TSPA-VA calculations
- Sub-Grid Scale Fractures: Lump with Matrix or Fractures?

Analyses Plans
Calibration and Abstraction of the UZ Site-Scale Model

- **Objective:** Determine how to abstract the UZ flow field
  - Produce a simplified model of the unsaturated zone from which numerous simulations can be run for unsaturated zone abstractions for TSPA-VA Determine the ratio of fracture to matrix flux components in all locations in the UZ flow field
  - Conduct sensitivity studies to assist in the prioritization and clarification of certain issues listed as important in workshop
- **Hypothesis:** A simplified model can be created that can capture all of the important processes for TSPA calculations. From this model numerous flow fields (or parameter distributions and domains) can be abstracted for:
  - unsaturated-zone transport calculations from the repository horizon, and
  - a distribution of percolation flux at the repository horizon (drift scale modeling)
- **Inputs to TSPA:** Abstracted UZ flow field
- **Organizations Involved:** LBNL, SNL, Intera

Analyses Plans

Calibration and Abstraction of the UZ Site-Scale Model

Examples of Issues being Addressed by Sensitivity Studies

- Use uncertainty in infiltration rates to bound uncertainty in fracture properties
- Effects of transient vs. steady-state infiltration
- Effects of the use of different formulations of the fracture relative permeability curves
- Effects of different conceptual models of fracture-matrix interactions
  - Function of upstream saturation
  - Function of upstream relative permeability
- Effects of heterogeneities

Analyses Plans

Flow Seepage into Drifts under Pre-Waste-Emplacement Conditions

- **Objective:** To develop a model of seepage into drifts for TSPA. This model would specifically be able to address the spacing of the drips and under what hydrogeological conditions water will drip into the drifts.
- **Hypotheses:**
  - Only fracture/high permeability connected features which intersect the drift can support seeps..
  - Need episodic flux - either ambient transient or thermally driven for drip into drift.
- **Inputs to TSPA:**
  - Estimate the spatial distribution of potential seeps at ambient conditions.
  - Determine of the volume and duration of episodic flux which will give rise to seeps into drift using different conceptual models.
- **Organizations Involved:** LBNL, SNL

Analyses Plans

Flow Seepage into Drifts under Pre-Waste-Emplacement Conditions
Sensitivity Studies

- Alternative conceptual models (SCM vs. DKM).
- Alternative models for fracture properties and characteristic curves will be implemented to account for the effects of fracture coating, aperture closure due to thermal-mechanical-hydrological coupling, flow channeling and fast flow mechanisms such as liquid film flow.
- Alternative conceptualizations for fracture/matrix interactions.
- For each of these sensitivity studies, the effects on the duration and volume of percolation pulse needed for seepage will be examined.

Analyses Plans

Testing of perched-water concepts and their implications for TSPA-VA calculations

- **Objective:** Identify physical controls on perched-water formation, and test hypotheses through numerical simulation using 2D and 3D models.
- **Hypothesis:** The conceptual model of the formation of the perched water plays a key role in understanding the volume and residence times of the perched water bodies.
- **Inputs to TSPA:** Quantitative estimates of spatial extent, volumes, residence times and pathlengths within and around perched water.
- **Organizations Involved:** LBNL, SNL, Intera

Analyses Plans

Sub-Grid Scale Fractures: Lump with Matrix or Fractures?

- **Objective:** Determine the sensitivity of sub-grid scale fractures to transport calculations in order to simplify TSPA calculations
- **Hypothesis:** The details of whether the sub-grid-scale fractures are lumped into the matrix continuum or the fracture continuum when fitting the saturation data are unimportant for transport of radionuclides, as long as these fractures are properly considered in the computation of transport velocities.
- **Inputs to TSPA:** Sensitivity study that could result in supporting the simplification for TSPA calculations as to how they handle sub-grid scale fractures
- **Organizations Involved:** LANL, LBNL, Intera, SNL

Analyses Plans

Sub-Grid Scale Fractures: Lump with Matrix or Fractures?
Model Plan

- Obtain hydrostratigraphic column for SD-7, set up 1D grid based on stratigraphy at this location.
- Perform fit to saturation, water potential data at nominal infiltration rate using DKM using 2 methods:
  - hold fracture continuum properties constant at "typical" values, allow matrix properties to vary;
  - hold matrix properties at values measured in laboratory, allow fracture properties to vary.
- Simulate migration of ^{99}Tc and ^{237}Np to the water table for the two cases, compare breakthrough curves, especially the peak flux of radionuclide at the water table.
- Conduct sensitivity studies based on different fracture-matrix interaction models.

FY97 SZ MODELING MILESTONES

NUMBER	ACCOUNT	LEVEL	DESCRIPTION	DUE DATE	COMPLETED
SPH23AM4	14006	4	Memo to TPO: Climate Scenarios received	1/30/97	1/14/97
SPH23DM4	14006	4	Updated Reg. Framework Model to RPC	3/14/97	~~2/18/97~~ 3/14/97
SPH23BM4	14006	4	Reg. Model Synthesis Report to Review	5/1/97	
SP23OM3	14006	3	Regional Model Synthesis Report to DOE	8/1/97	
SPH23VM4	11004	4	Memo to TPO: Site Synth. Report Annotated Outline	2/28/97	2/11/97
SPH25CM4	11005	4	Memo to TPO: PA Mtg. Summary	2/28/97	2/13/97
SPH24FM4	11003	4	Updated Site Framework Model to Review	4/30/97	
SPH23WM4	11004	4	Site Model Synthesis Report to Review	5/30/97	
SP23CBM3	11003	3	Calibrated Site Flow Model to DOE	6/16/97	
SPH35RM4	11006?	4	Site Framework Model to RPC	7/31/97	
SPH25DM4	11005	4	Memo to TPO: PA Interactions	8/1/97	
SP23NM3	11004	3	Site Model Synthesis Report to DOE	8/29/97	

UZ Transport Abstraction/Testing Plans

- Fracture-Matrix Interaction
- Transient Flow and Transport
- Colloid-Facilitated Radionuclide Transport
- Sorption Models for Radionuclide Transport
- Effects of Dispersion and Fine-Scale Heterogeneity on Radionuclide Transport

Links to SZ Abstraction/Testing Plans

- **Transient Flow and Transport**
  - **Climate changes influence both UZ transport and water table elevation beneath repository - need to link these models**
- **Colloid-Facilitated Radionuclide Transport**
  - **Same transport mechanisms will aply in UZ and SZ**
- **Sorption Models for Radionuclide Transport**
  - **Some of the same sorption models will aply in UZ and SZ**
- **Effects of Dispersion and Fine-Scale Heterogeneity on Radionuclide Transport**
  - **Probably different mechanisms/processes, but should be discussed**

Existing Workscope - LANL

- Sorption and diffusion studies
- C-Wells reactive tracer experiments
- Studies of redox potential of the SZ fluids
- SZ flow and transport model