QA: QA

Model
Administrative Change Notice

Complete only applicable items.

1. Document Number:	MDL-NBS-HS-000011	**2. Revision:**	03	**3. ACN:**	01
4. Title:	Saturated Zone Site-Scale Flow Model				
5. No. of Pages Attached	99				

6. Approvals:

Preparer:	Scott James [signature] Print name and sign	9/27/07 Date
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Responsible Manager:	Stephanie Kuzio for Kenneth Rehfeldt Print name and sign	10/1/07 Date

7. Affected Pages	8. Description of Change:
p. ix	Updated TOC to reflect changes in reference section.
p. xxi	Added ASCII to acronyms list.
p. xxia	Page rollover from change to acronyms list.
p. 1-1	Updated DIRS number and title for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650.
p. 1-2	Updated Figure 1-1.
p. 1-5	Added explanations for CRs 8758 and 10893.
p. 6-1, p. 6-1a	Updated the FEPs reference to MO0706SPAFEPLA.001 [DIRS 181613]).
p. 6-3	Deleted redundant sentence at the beginning of 2nd paragraph, replaced "when" with "whose" in last line of 2nd paragraph, and deleted reference citation to Figure 6-1 in the last paragraph..
p. 6-19	Updated the reference from Table 6-5 to (SNL 2007 [DIRS 174109], Table 6-3)
p. 6-20	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also called out sections specific to the Addendum.
p. 6-21	Corrected typo from "that" to "than"
p. 6-23	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the section specific to the Addendum.
p. 6-26	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the section specific to the Addendum.
p. 6-29	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the section specific to the Addendum.
p. 6-39	Changed "nodes" to "tetrahedral elements" and "as shown" with "which becomes evident"
p. 6-40	Changed m to superscript m^3 in Table 6-5.

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p. 6-42	Elevations added to Figure 6-10 per DOE comment and removed x-axis label.
p. 6-43	Replaced “Top” from Table 6-6, column three title with “Land”.
p. 6-44	Deleted “surface and below.”
p. 6-45	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650.
p. 6-47	Removed phrase, “with geometry described in Table 6-7” in last paragraph.
p. 6-48	Update Figure 6-12 caption to read “Altered Northern Region.”
p. 6-56	Replaced “Watermark Computing” with “STN: 10289-5.5-00.”
p. 6-66	Changed “zone” to “zones.”
p. 6-68	Corrected reference from Table 6-8 to Table 6-10.
p. 6-70	Changed “780-m to 730-m” to “780 to 730-m (~50-m).”
p. 6-75	Changed distance to 4,073,761 and made slight modification as follows “approximately 5 km south of the midpoint of the repository.”
p. 6-75	Deleted the sentence starting with “Mass balance….”
p. 6-77	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 6-83	Changed “will results” to “results.”
p. 6-93	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 6-93	Removed an extraneous semicolon.
p. 6-93	Added STN and PEST reference as follows “STN: 10289-5.5-00; [DIRS 161564], Watermark Numerical Computing 2004 [DIRS 178612]”
p. 6-96	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the Addendum.
p. 6-96	Corrected reference from “Watermark Computing” to “Doherty.”
p. 6-98	Corrected typo from “is” to “in.”
p. 6-99	Inserted “is” before “50-m” in the third paragraph.
p. 6-100	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 6-101	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 6-101	Reorganized sentence to improve readability.
p. 7-7	Corrected typo from “that” to “than.”
p. 7-12	Deleted extraneous “to”
p. 7-14	Changed "... percolation through..." with "... infiltrating into..."
p. 7-14	Changed “average” to “range” and updated numbers
p. 7-14	Replaced obsolete Flint reference with that of SNL 2007 to reflect the latest understanding of infiltration.
p. 7-14	Replaced the second Flint reference with a qualified DTN.
p. 7-16	Deleted extraneous Flint reference.

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p. 7-32	Updated sentence to improve readability as follows: "Specific discharge across the 18-km compliance boundary (see the green line on Figure 6-17) and discussed throughout other documents (SNL 2007 [DIRS 177392]) is…."
p. 7-34	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 7-34	Corrected typo from "theses" to "these."
p. 8-5	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 8-6	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 8-7	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650 and also the portion specific to the addendum.
p. 8-7	Uncapitalized "recharge" and "discharge"
p. 8-11	Updated DIRS number for the Saturated Zone Flow and Transport Model Abstraction from 177390 to 181650. Changed "hydrologic" to "hydrogeologic" in the first sentence of the second paragraph.
pp. 9-1 to 9-36	Rebuilt references section to address the condition identified in CR 10893.
p. A-59	Deleted unnecessary reference to BSC 2004.
p. A-215	Typo in DIRS 170008 changed to 170009.
p. A-218	Corrected "east" to "west" in second paragraph – "Flow Path 8 illustrates leakage to the west across the hydrologic boundary…"
p. A-220	Changes in spacing made (no space between number and %) and non-breaking space added.
p. A-222	Non-breaking space removed.
p. A-224	Typo in DIRS 170008 changed to 170009.
p. B-44	Corrected "eastward" to "westward" in fifth paragraph – "…and an additional arrow indicating westward flow of Flow Path 8 was added."
p. E-1	Minor typos like spacing (or addition of a non-breaking space) corrected.
p. E-2	Minor typos like spacing (or addition of a non-breaking space) corrected.
p. E-3	Minor typos like spacing (or addition of a non-breaking space) corrected.
p. F-1	Added "e" to "Plan."
p. H-1	Corrected date from 2003 to 2002.
p. I-1, I-1a	Added an introductory paragraph.
p. I-3	Corrected date from 2006 to 2005.
p. I-6	Italicized "t."
p. I-6	Added comma after Equation I-15
p. I-6	Added a concluding paragraph.

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ACRONYMS AND ABBREVIATIONS

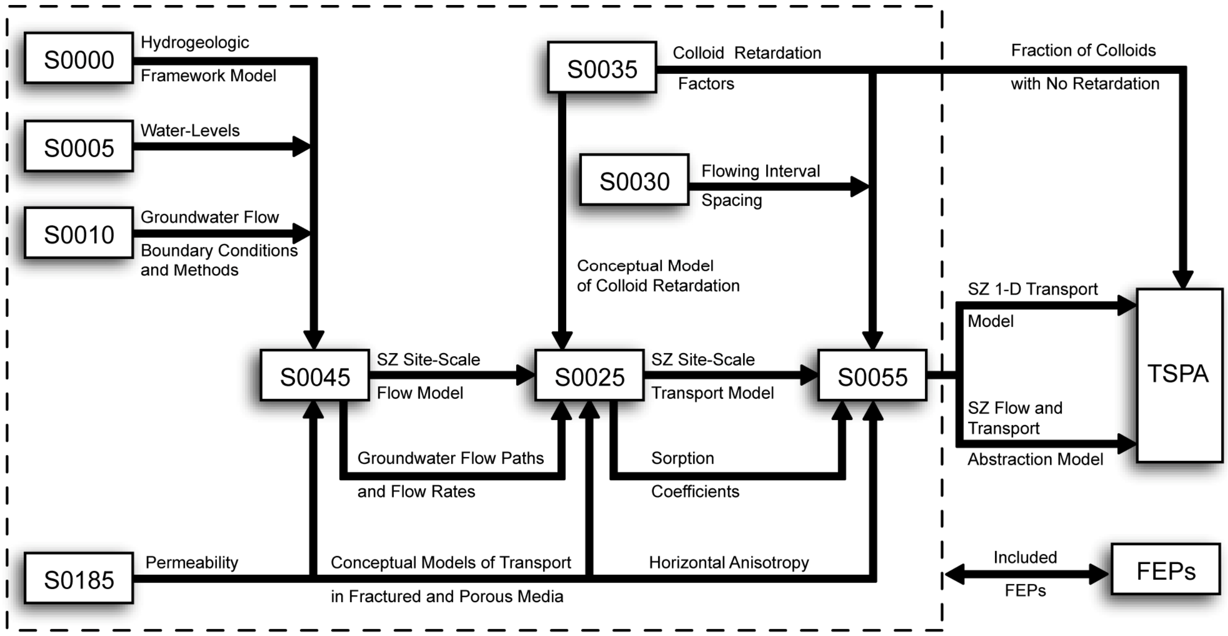
ACC	accession number
ACM	alternative conceptual model
ASCII	American Standard Code for Information Interchange
AR	Amargosa River: group of boreholes located on the west side of Amargosa Desert
AR/FMW	Group of boreholes located near the confluence of the Amargosa River and Fortymile Wash drainages
ASCII	American Standard Code for Information Interchange
ATC	Alluvial Testing Complex
BSC	Bechtel SAIC Company, LLC
CFR	code of federal regulations
CF-SW	Crater Flat Southwest
CMB	chloride mass balance
CR	condition report
CRWW	Coffer Ranch Windmill Well
CVFE	control-volume finite element
DFGP	Desert Farms Garlic Plot
DIC	Dissolved inorganic carbon
DIRS	document reference system
DOC	dissolved organic carbon
DOE	Department of Energy
DOS	disk operating system
DTN	data tracking number
DVRFS	Death Valley Regional (ground water) Flow System
ESF	Exploratory Studies Facility
EWDP	Early Warning Drilling Program
FEHM	finite-element heat and mass transfer numerical analysis computer code
FEPs	features, events, and processes
FMW-E	Fortymile Wash-East: group of boreholes in the Amargosa Desert east of Fortymile Wash
FMW-N	Fortymile Wash-North: group of boreholes east and northeast of Yucca Mountain
FMW-S	Fortymile Wash-South: group of boreholes along or near the main channel of Fortymile Wash in Amargosa Desert
FMW-W	Fortymile Wash-West: group of boreholes in the Amargosa Desert west of Fortymile Wash
GF	Gravity Fault: group of boreholes located on east side of the Amargosa Desert
GSIS	geoscientific information system

HFM	hydrogeologic framework model
HFM2006	revised hydrogeologic framework model

1. PURPOSE

The purpose of this model report is to document revision of *Saturated Zone (SZ) Site-scale Flow Model* (BSC 2004 [DIRS 170037]) for Yucca Mountain, Nevada, in accordance with SCI-PRO-006, *Models*. This report provides validation and confidence in the flow model developed in support of the total system performance assessment (TSPA) for the license application (LA). The output from this report provides the flow model used in *Site-Scale Saturated Zone Transport Model*, (SNL 2007 [DIRS 177392]), which in turn provides output to the *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650]). In particular, the output from the SZ site-scale flow model is used by the SZ site-scale transport model to simulate the groundwater flow pathways and radionuclide transport to the accessible environment for use in *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650]), which feeds the TSPA calculations. Figure 1-1 shows the relationship of this report to other saturated zone reports that also pertain to SZ flow and transport. The figure also depicts the relationship between SZ models and analyses. It should be noted that Figure 1-1 does not contain a complete representation of the data and parameter inputs and outputs of all saturated zone reports, nor does it show inputs external to this suite of saturated zone reports.

Since the development, calibration, and validation of the SZ site-scale flow model (CRWMS M&O 2000 [DIRS 139582]), more data have been gathered and analyses have been completed. The data include new stratigraphic and water–level data from Nye County wells, single- and multiple-well hydraulic testing data (SNL 2007 [DIRS 177394]), and new hydrochemistry data (Appendix B). New analyses include the 2004 transient Death Valley Regional (ground water) Flow System (DVRFS) model (Belcher 2004 [DIRS 173179]), the creation of a new hydrogeologic framework model (HFM), called HFM2006 (SNL 2007 [DIRS 174109], DTN: MO0610MWDHFM06.002 [DIRS 179352]), and the 2003 unsaturated zone (UZ) flow model (BSC 2004 [DIRS 169861]). The new data and analyses were used to construct the SZ site-scale flow model presented in this report to support TSPA-LA. The intended use of this work is to provide a flow model that generates flow fields that are used to simulate radionuclide transport in saturated volcanic rock and alluvium under natural-gradient flow conditions. Simulations of water-table rise were also conducted for use in downstream transport and abstraction modeling. The SZ site-scale flow model simulations were completed using the three-dimensional, finite-element heat and mass transfer computer code, FEHM V2.24, STN: 10086-2.24-02 [DIRS 179539]. Concurrently, the process-level transport model and methodology for calculating radionuclide transport in the SZ at Yucca Mountain using FEHM are described in *Site-Scale Saturated Zone Transport* (SNL 2007 [DIRS 177392]). The velocity fields are calculated by the flow model, described herein, independent of the transport processes, and are then used as inputs to the transport model. Justification for this abstraction is presented in *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650]).



Legend

S0000 -	Hydrogeologic Framework Model	MDL-NBS-HS-000024
S0005 -	Water-Level Data Analysis	ANL-NBS-HS-000034
S0010 -	Recharge and Lateral Groundwater Flow Boundary Conditions	ANL-NBS-MD-000010
S0025 -	Site-Scale Saturated Zone Transport	MDL-NBS-HS-000010
S0030 -	Probability Distribution for Flowing Interval Spacing	ANL-NBS-MD-000003
S0035 -	Saturated Zone Colloid Transport	ANL-NBS-HS-000031
S0045 -	Site-Scale Saturated Zone Flow Model	MDL-NBS-HS-000011
S0055 -	Saturated Zone Flow and Transport Model Abstraction	MDL-NBS-HS-000021
FEPs -	Features, Events, and Processes in SZ Flow and Transport	DTN: MO0706SPAFEPLA.001
S0185 -	Saturated Zone In-Situ Testing	ANL-NBS-HS-000039

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NOTE: This figure is a simplified representation of the flow of information among SZ reports. See the most recent revision of each report for a complete listing of data and parameter inputs. This figure does not show inputs external to this suite of SZ reports.

FEPs = features, events, and processes; SZ = saturated zone; TSPA = total system performance assessment.

Figure 1-1. Generalized Flow of Information among Reports Pertaining to Flow and Transport in the SZ

This model report is governed by *Technical Work Plan: Saturated Zone Flow and Transport Modeling* (BSC 2006 [DIRS 177375]). All activities listed in the technical work plan (TWP) that are appropriate to the SZ site-scale flow model are documented in this report. The TWP (BSC 2006 [DIRS 177375]) cites procedures that were in effect at the time the work described in this report was planned and approved. Following the transition of the science work scope from Bechtel SAIC Company, LLC (BSC) to Sandia National Laboratories (SNL), new procedures have been issued since October 2, 2006.

6. MODEL DISCUSSION

6.1 MODELING OBJECTIVES

The purpose of the SZ site-scale flow model is to describe the steady-state flow of groundwater as it moves from the water table below the repository, through the SZ, and to the accessible environment. The flow model estimates the SZ advective processes that control the movement of groundwater and dissolved radionuclides and colloidal particles that might be present.

The previous versions of the SZ site-scale flow model were developed in support of the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) and the TSPA-LA (BSC 2004 [DIRS 170037]). This model revision includes the following modifications to: (1) reflect the current understanding of SZ flow, (2) enhance model validation and uncertainty analyses, (3) improve locations and definitions of fault zones, (4) enhance grid resolution (500-m grid spacing to 250-m grid spacing), and (5) incorporate new data collected since the TSPA-SR:

- Implementation of the updated hydrogeologic framework model (HFM) that incorporates recent geologic data obtained from the Nye County Early Warning Drilling Program (DTN: MO0610MWDHFM06.002 [DIRS 179352]) and the 2004 DVRFS (Belcher 2004 [DIRS 173179])
- A potentiometric surface updated with water-level data from Phases III and IV of the NC-EWDP (Output DTN: MO0611SCALEFLW.000)
- Additional water-level calibration target data from Phases III and IV of the Nye County Early Warning Drilling Program (Output DTN: SN0702T0510106.007)
- Boundary volumetric/mass flow rates and recharge data from the 2004 DVRFS (Belcher 2004 [DIRS 173179]) and the 2003 UZ flow model (BSC 2004 [DIRS 169861])
- Use of field and laboratory tests (hydraulic and tracer data collected since TSPA-SR) to establish and confirm the conceptual model for flow, constrain model parameter calibration, and provide data for model validation and confidence building (SNL 2007 [DIRS 177394], Section 6).

This modeling analysis is a direct feed to *Site-Scale Saturated Zone Transport* (SNL 2007 [DIRS 177392]) because it provides the SZ flow fields for transport calculations.

6.2 FEATURES, EVENTS, AND PROCESSES CONSIDERED IN THE MODEL

As stipulated in *Technical Work Plan for: Saturated Zone Flow and Transport Modeling* (BSC 2006 [DIRS 177375]), this model report addresses the FEPs pertaining to SZ flow that are included (i.e., Included FEPs) for TSPA-LA listed in Table 6-1. SZ FEPs that were excluded (i.e., Excluded FEPs) for TSPA-LA are described in *Features, Events, and Processes for the Total System Performance Assessment* (SNL 2007 [DIRS 179476]). Table 6-1 provides a list of FEPs that are relevant to this model analysis in accordance with their assignment in the LA FEP list (DTN: MO0706SPAFEPLA.001 [DIRS 181613]). Specific reference to the various sections

6.3 THE CONCEPTUAL MODEL

Yucca Mountain is located in the Great Basin about 150 km northwest of Las Vegas, Nevada. The mountain consists of a series of fault-bounded blocks of ash-flow and ash-fall tuffs and a smaller volume of lava deposited between 14 and 11 Ma (one million years (refers to age)) from a series of calderas located a few to several tens of kilometers to the north (Sawyer et al. 1994 [DIRS 100075]). Yucca Mountain itself extends southward from the Pinnacles Ridge toward the Amargosa Desert, where the tuffs thin and pinch out beneath the alluvium (Figure 6-1). The tuffs dip 5 to 10 degrees to the east over most of Yucca Mountain.

Crater Flat is west of Yucca Mountain and separated from it by Solitario Canyon, which is the surface expression of the Solitario Canyon Fault—a steeply dipping scissors fault with down-to-the-west displacement of as much as 500 m in southern Yucca Mountain (Day et al. 1998 [DIRS 100027], pp. 6 to 7). Underlying Crater Flat are thick sequences of alluvia, lavas, and tuffs that have been locally cut by faults and volcanic dikes. East of Yucca Mountain, and separated from it by Fortymile Wash, is Jackass Flats, which is underlain by a thick sequence of alluvium and volcanic rocks. Timber Mountain, approximately 25 km to the north of the repository area, is a resurgent dome within the larger caldera complex whose eruptions supplied the tuffs at Yucca Mountain.

The SZ site-scale flow model presented in this report describes our current state of knowledge of the saturated flow system. The boundaries of the numerical model for SZ flow and transport are indicated on Figure 6-1 in blue. The domain was selected to be: (1) coincident with grid cells of the DVRFS model (DTN: MO0602SPAMODAR.000 [DIRS 177371]) where site-scale model (FEHM) nodes correspond to regional model (MODFLOW-2000) cell corners in the horizontal plane; (2) sufficiently large to reduce the effects of boundary conditions on estimating permeabilities and calculated flow fields near Yucca Mountain; (3) sufficiently large to assess groundwater flow at distances beyond the 18-km compliance boundary from the repository area; (4) small enough to minimize the model size for computational efficiency and to include structural feature detail affecting flow; (5) thick enough to include part of the regional Paleozoic carbonate aquifer (the bottoms of the site- and regional-scale models are equal at −4,000 m below sea level); and (6) large enough to include borehole data from the Amargosa Desert at the southern end of the modeled area. The hydrogeologic setting of the SZ flow system in the vicinity of Yucca Mountain was summarized by Luckey et al. (1996 [DIRS 100465], p. 13). Yucca Mountain is part of the Alkali Flat-Furnace Creek sub-basin of the Death Valley groundwater basin (Waddell 1982 [DIRS 101062], pp. 15 to 16). Discharge within the sub-basin occurs at Alkali Flat (Franklin Lake Playa) and, possibly, Furnace Creek in Death Valley. Water inputs to the sub-basin include groundwater inflow/outflow along the northern, eastern, and western boundaries of the sub-basin, recharge from precipitation in high-elevation areas of the sub-basin, and recharge from surface runoff in Fortymile Canyon and Fortymile Wash. North and northeast of Yucca Mountain, recharge from precipitation also occurs at Timber Mountain, Pahute Mesa, Rainier Mesa, and Shoshone Mountain (Luckey et al. 1996 [DIRS 100465], p. 13).

porosity, and commonly constitute confining units. Ash fall tuffs have high primary porosity and moderate to low permeability, and they generally act as confining units.

As the tuff deposits cooled, they were subjected to secondary processes, including formation of cooling fractures, recrystallization or devitrification, and alteration of the initial glassy fragments to zeolite minerals and clay minerals, all of which affect the hydrologic properties of the rocks. Beginning with deposition and throughout their subsequent history, the rocks have been subjected to tectonic forces resulting in further fracturing and faulting. They also have been subject to changes in the position of the water table, which greatly affects the degree of alteration of the initially glassy deposits.

The forms of secondary heterogeneity most affecting the SZ are fracturing, faulting, and alteration of glassy materials to zeolites and clay minerals. Fractures, where interconnected, transmit water readily and account for the permeable character of the welded tuffs. Cooling fractures, which are pervasive in welded tuffs, tend to be strata-bound and confined to welded portions of flows, whereas tectonic fractures tend to cut through stratigraphic units, as do faults.

Nonwelded deposits are less subject to fracturing and more subject to alteration of the initial glassy deposits to zeolites and clay minerals, both of which reduce permeability. The presence of perched-water bodies in the UZ is attributed to the ubiquitous presence of a smectite-zeolite interval at the base of the Topopah Spring tuff, which, in the absence of through-going fractures, essentially stops the vertical movement of water (Luckey et al. 1996 [DIRS 100465], p. 46).

The heterogeneity in permeability of different types of deposits led to the subdivision of the Yucca Mountain geologic section into five basic SZ hydrologic units: upper volcanic aquifer, upper volcanic confining unit, lower volcanic aquifer, lower volcanic confining unit, and lower carbonate aquifer. To accommodate the more extensive area of the SZ flow model, HFM2006 (SNL 2007 [DIRS 174109], Table 6-3) includes 22 additional units above and below these basic five units. Near Yucca Mountain, volcanic deposits generally form laterally extensive stratigraphic units; however, due to physical heterogeneity, porosity and permeability are highly variable both laterally and vertically.

In the southern part of the SZ site-scale flow model domain, the volcanic deposits thin and inter-finger with valley fill deposits. The latter are heterogeneous (sand and gravel) because of their mode of deposition (Walker and Eakin 1963 [DIRS 103022], p. 14), but are not subject to the fracturing, faulting, and alteration types of heterogeneity that affect the volcanic rocks.

Within the SZ site-scale model area, little specific information is available on the lower carbonate aquifer. However, information from nearby areas (D'Agnese et al. 1997 [DIRS 100131], p. 90, Figures 46 and 47) suggests that the lower carbonate aquifer is minimally heterogeneous with reasonably high permeability attributed to pervasive solution-enlarged fractures.

Heterogeneity in material properties is a common characteristic of hydrogeologic units at the Yucca Mountain site and it exists at scales ranging from pore scale to regional scale. The larger-scale heterogeneity, at scales of kilometers to tens of kilometers, is effectively addressed via the different units within HFM2006, incorporation of specific hydrogeologic features (e.g., faults and structural zones), and anisotropy. The pore scale heterogeneities are averaged via the concept of macroscopic parameters defined on the basis of a representative elementary volume (Freeze and Cherry 1979 [DIRS 101173], pp. 69 to 70). Groundwater flow equations use parameters defined on the basis of the representative elementary volume. For predominantly porous units such as bedded tuffs and alluvia, the size of the representative elementary volume may be on the order of a few cubic centimeters (de Marsily 1986 [DIRS 100439], p. 15). For fractured rocks (volcanics and carbonates), the size of the representative elementary volume is less well defined, but is typically related to the density of fracturing and is generally much larger than for granular material (Freeze and Cherry 1979 [DIRS 101173], p. 73). The 250-m grid spacing used for the flow model is sufficiently large to allow the use of representative-elementary-volume-defined parameters for groundwater flow. In fact, the grid spacing is large enough that subgrid scale heterogeneity needs to be considered with regard to radionuclide transport. Subgrid heterogeneity leads to enhanced dispersion with increasing scales of transport (de Marsily 1986 [DIRS 100439], pp. 247 to 248). Additionally, the uncertainty in the density of fracturing at the subgrid scale leads to uncertainty in the groundwater velocity and matrix diffusion. Flow modeling accounts for subgrid heterogeneity by defining scaled dispersivities and flowing interval spacing (BSC 2004 [DIRS 170014]) in the transport abstraction modeling (SNL 2007 [DIRS 181650], Section 6.5.2[a]) as random variables characterized by probability density functions.

Heterogeneity at intermediate scales between the grid size of 250 m and the large-scale features of the HFM are addressed using uncertainty in the anisotropy of hydraulic conductivity. A primary concern related to intermediate scale heterogeneity is the possibility of a fast pathway (Freifeld et al. 2006 [DIRS 178611], Table 4) along a relatively continuous path. In the fractured volcanic aquifers beneath Yucca Mountain, the fast path, if it exists, is likely to be related to a fracture or structural feature. The hydraulic testing at the C-wells complex (SNL 2007 [DIRS 177394], Section 6.2) suggest that at a large scale (about 1 km^2), hydraulic conductivity can be characterized as homogeneous, but anisotropic. The direction of anisotropy is primarily related to the dominant direction of fractures and faulting. The impact of possible fast paths at an intermediate scale of heterogeneity is incorporated in the transport simulations through probability distributions of specific discharge, horizontal anisotropy in permeability, and flowing interval spacing (SNL 2007 [DIRS 181650], Section 6.5.2[a]). The aggregate uncertainty in these and other parameters related to radionuclide transport yield simulated SZ transport times for nonsorbing species on the order of 100 years in some Latin Hypercube Sampled realizations of the SZ system (SNL 2007 [DIRS 181650], Figure 6-6[a]).

As noted previously, the properties of each hydrogeologic unit in the model are assumed uniform, but uncertain, with the value assigned during the calibration process. Nevertheless, heterogeneity of material properties at a variety of scales is included in the model via several different mechanisms. First, large-scale heterogeneity is defined by the distribution of units in HFM2006 and the discrete hydrogeologic features incorporated in the SZ site-scale flow model (Table 6-7). Subgrid heterogeneity is included in the transport simulations through the probability distributions for flowing interval spacing and dispersivity. Finally, intermediate scale heterogeneity, which is most likely to be reflected in possible fast paths at scales up to several kilometers, is included as uncertainty in anisotropy. Uncertainty in the HFM is discussed in Section 6.4.3.1.

6.3.1.10 Role of Faults

Faults and fault zones are hydrogeologic features that require special treatment in the SZ site-scale flow and transport models. Faulting and fracturing are pervasive at Yucca Mountain and they affect groundwater flow patterns because they may act as preferred conduits or barriers to groundwater flow. The role that faults play in facilitating or inhibiting groundwater flow depends on the nature of the fault (i.e., whether the faults are in tension, compression, or shear) and other factors such as the juxtaposition of varying geologic units along the fault plane, the rock types involved, fault zone materials, secondary mineralization, and depth below land surface.

Faunt (1997 [DIRS 100146]) investigated the effect of faulting on groundwater movement in the Death Valley region and developed a map of fault traces (Faunt 1997 [DIRS 100146], Figure 10) including diagrams (Faunt 1997 [DIRS 100146], Figure 11) showing the orientation of faults within the principal structural provinces of the region. Faunt (1997 [DIRS 100146], p. 38) grouped the faults into three categories depending on their orientations relative to the present-day stress field (i.e., those in relative tension, compression, or shear).

Faults in relative tension are more likely to be preferential conduits for groundwater, and faults in shear or compression are more likely to impede groundwater movements. Faults modeled to have the most evident effects on groundwater movement, such as effects on potentiometric contours, include the Solitario Canyon, U.S. Highway 95, Crater Flat, and Bare Mountain Faults (see Figure 6-4), all of which appear to act as barriers to groundwater flow. The following features are afforded special consideration in the SZ site-scale flow model: the Crater Flat Fault, the Solitario Canyon (with Windy Wash and Stage Coach splays), the U.S. Highway 95, the Bare Mountain, and Sever Wash Faults. In addition, zones are developed for the Fortymile Wash Structure and Lower Fortymile Wash alluvial regions that appear to act as conduits that focus flow. Other than the Fortymile Wash faults, these features are assigned anisotropic permeabilities that are 10 times more permeable in both directions parallel to the fault (*x*-*z* or *y*-*z* directions).

6.3.1.11 Altered Northern Region

The Claim Canyon caldera is an area of extensive alteration that seems to have resulted in a generalized reduction in permeability in many of the hydrogeologic units in this area (this area is hereinafter referred to as the altered northern region). The concept of the altered northern region allows different permeabilities to be assigned to the same geologic unit depending on whether or not a unit resides within the altered northern region (see Section 6.4.3.7). Deeper units (including the intrusive, crystalline, and lower clastic confining units and the lower carbonate aquifer) are excluded from this alteration because the caldera complex was not present during their genesis. Conceptually, this facilitates modeling of the LHG and it also makes intuitive sense because it is unlikely that permeabilities even within the same geologic unit would have identical values when they are separated by many kilometers (across the model domain from north to south). In the SZ site-scale model formulation, faults that fall within the altered northern region may have diminished impact on the model and could reasonably be removed from consideration here. A notable exception is Sever Wash Fault that retains a distinct permeability

- Horizontal anisotropy in permeability is adequately represented by a permeability tensor that is oriented in the north-south and east-west directions. In support of the TSPA-LA, horizontal anisotropy is considered for radionuclide transport in the SZ (SNL 2007 [DIRS 177394], Section 6.2.6). The numerical grid of the SZ site-scale flow model is aligned north-south and east-west, and values of permeability are specified in directions parallel to the grid. One analysis of the probable direction of horizontal anisotropy shows that the direction of maximum transmissivity is N 33°E (Winterle and La Femina 1999 [DIRS 129796], p. iii), indicating that the anisotropy applied on the SZ site-scale model grid is within approximately 30° of the inferred anisotropy. A detailed description of the horizontal anisotropy calculations is found in *Saturated Zone In-Situ Testing* (BSC 2006 [DIRS 177394], Appendix C6). Sensitivity analyses were performed to assess the impact of uncertainty in the anisotropy and are presented in *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650], Figure 6-1[a]).

- Horizontal anisotropy in permeability may apply to the fractured and faulted volcanic units of the SZ system along the groundwater flowpaths that run from the repository to points south and east of Yucca Mountain. The inferred flowpath from beneath the repository extends to the south and east. This is the area in which potential anisotropy could have an impact on radionuclide transport in the SZ. Given the conceptual basis for the anisotropy model, it is appropriate to apply anisotropy only to those hydrogeologic units that are dominated by groundwater flow in fractures. A more detailed discussion of anisotropy is provided in Section 6.4.3.11.

- Changes in the water-table elevation (due to future climate changes) will have negligible effect on the direction of the groundwater flow near Yucca Mountain although the magnitude of the groundwater flux will change. This supposition has been studied at regional (D'Agnese et al. 1999 [DIRS 120425]; Winterle 2003 [DIRS 178404]; Winterle 2005 [DIRS 178405]) and subregional scales (Czarnecki 1984 [DIRS 101043]). These studies found that the flow direction did not change significantly under increased recharge scenarios. The studies were based on confined aquifer models that did not take into account the free surface boundary at the water table or the saturation of geological units that currently are in the UZ overlying the present-day SZ. These UZ tuffs generally have a lower permeability than those in the SZ, and as such, UZ units that become saturated are not likely to yield faster fluxes in the SZ (BSC 2004 [DIRS 169861], Appendix A).

- Future water supply wells that might be drilled near Yucca Mountain (including outside the regulatory boundary) will have a negligible effect on the hydraulic gradient. Water levels at the southern boundary of the SZ site-scale flow and transport models (in the Amargosa Valley) currently reflect the effect of well pumpage (Luckey et al. 1996 [DIRS 100465], p. 41).

- In the analysis presented in this report, temperature is modeled to be proportional to the depth below the ground surface. Modeling a uniform temperature gradient with depth is equivalent to a model of uniform geothermal heat flux through a medium of homogeneous thermal conductivity. In addition, the temperature at the ground surface is held constant. Data indicate that the temperature gradients generally become more and that permeability values derived from those tests were considered in the validation of the numerical model. It is not expected that the model can reproduce the transient tests, largely due to the 250-m-gridblock sizes. Because transient pumping is not used in any Yucca Mountain radionuclide migration simulations and steady-state gradients are modeled accurately with the model, this does not invalidate the steady-state assumption. Climate change and other transient impacts are incorporated in the SZ flow and transport abstractions (SNL 2007 [DIRS 181650], Tables 6-1[a] and 6-4[a]). Furthermore, the effects of water table rise on flowpaths are investigated here in Section 6.6.4.

The conceptual model of the long-term groundwater flow in this region includes the hypothesis that recharge rates and, consequently, the elevation of the water table and groundwater flow rates, were larger during the last glacial pluvial period. The time required for the flow system to equilibrate to a more arid climate depends primarily on the hydraulic conductivity of the rocks and the amount of water that must be drained from storage to lower the water table.

It is likely that equilibration to the drier climate has occurred given: (1) the long time (thousands of years) since the climate change was completed, (2) the relatively small amount of water stored (small specific yield) in fractured volcanic rocks that make up much of the model domain near the water table, and (3) the relatively large hydraulic conductivity of the fractured volcanic rocks.

The time required for the flow field to arrive at steady-state with respect to pumping from wells is much shorter than the time required for equilibration to climate change. It depends primarily upon the time required for changes in water level to be transmitted through the SZ. Fast transmittal is expected in fractured volcanic rock because of their relatively large hydraulic conductivity and small specific storage. The fact that the modern-day flow system on the scale of this model domain has equilibrated to pumping is supported by the lack of consistent, large-magnitude variations in water levels observed in wells near Yucca Mountain (Luckey et al. 1996 [DIRS 100465], pp. 29 to 32). A transient response to pumping would be expected, instead, to result in a continued decrease in water levels. Overall, pumping rates are typically negligible compared to the total mass of fluid in the system, which is on the order of 10^{16} kg.

6.4.2 Computational Model

The FEHM V2.24 (STN: 10086-2.24-02; [DIRS 179539]) software code is used for SZ site-scale modeling to obtain a numerical solution to the mathematical equation describing groundwater flow, Equation (6-5). FEHM is a nonisothermal, multiphase flow and transport code that simulates the flow of water and air and the transport of heat and solutes in two- and three-dimensional saturated or partially saturated heterogeneous porous media. The code includes comprehensive reactive geochemistry and transport modules and a particle-tracking capability. Fractured media can be simulated using equivalent-continuum, discrete-fracture, dual-porosity, or dual-permeability approaches. A subset of the FEHM code capabilities was used in the SZ site-scale flow model because only a single-phase, isothermal flow model is solved.

Particle tracking is a numerical technique that simulates the transport of fluid “particles.” Particle-tracking techniques have a long history of use in similar applications (e.g., Pollock 1988 units (Table 6-2) provide a geometric representation of hydrogeology and structure and are used as a basis for assigning hydrologic properties within the SZ site-scale flow model domain.

The DVRFS HFM consists of 28 surfaces representing the top elevation of each of the 27 hydrogeologic units plus the base at −4,000-m elevation, and a horizontal grid consisting of a rectangular array of nodes with 125-m spacing (SNL 2007 [DIRS 174109], Section 6). HFM2006 consists of 24 surfaces because unit IDs 10, 13, 22, and 25 are not present in its model area (SNL 2007 [DIRS 174109], Tables 6-2 and 6-3). An important goal of the HFM2006 was to match geologic units with the regional DVRFS HFM. This match allows more direct comparisons with the regional conditions and parameters, without a transition at the site-scale model boundary, and facilitates use of boundary volumetric/mass flow rates extracted from the regional-scale model for use as target boundary conditions during site-scale model calibration. Permeabilities (hydraulic conductivities for the regional model) may not match across model boundaries because these parameters are calibrated independently. The HFM2006 surface grids exactly reproduce the DVRFS Model grid nodes except where more detailed data are available, primarily within the domain of the Geologic Framework Model (GFM) (DTN: MO0012MWDGFM02.002 [DIRS 153777]) and near NC-EWDP boreholes area. These more detailed areas are important considerations in understanding the SZ flow system and they help define the boundaries of the fractured tuff aquifers immediately beneath and down gradient from Yucca Mountain, and the alluvial aquifer from which groundwater discharges in the Amargosa Valley. Data from the NC-EWDP investigations better constrain the location of the tuff-alluvium contact at the water table and better characterize the thickness and lateral extent of the alluvial aquifer north of U.S. Highway 95 (SNL 2007 [DIRS 181650], Section 6.5.2.2[a]).

Recent NC-EWDP drilling revealed a larger formation of alluvial material (Unit 26) in HFM2006 replacing volcanic and sedimentary unit previously thought to be present. It also revealed more of Unit 20 (Timber Mountain Volcanics) to the south of the GFM area than was previously indicated.

This report describes SZ flow modeling using HFM2006, which incorporates the newer DVRFS HFM (Belcher 2004 [DIRS 173179]), GFM2000 (DTN: MO0012MWDGFM02.002 [DIRS 153777]), and all NC-EWDP data through Phase IV.

Table 6-2. Hydrogeologic Units for the Hydrogeologic Framework Model

Hydrogeologic Units in HFM2006				
Unit ID	**Abbreviation**	**Unit Name**	**Description**	**Stacking Order**
28	YAA	Younger alluvial aquifer	Pliocene to Holocene coarse-grained basin-fill deposits	27
27	YACU	Younger alluvial confining unit	Pliocene to Holocene playa and fine-grained basin-fill deposits	26
26	OAA	Older alluvial aquifer	Pliocene to Holocene coarse-grained basin-fill deposits	25
25	OACU	Older alluvial confining unit	Pliocene to Holocene playa and fine-grained basin-fill deposits (not in HFM2006 domain)	24
24	LA	Limestone aquifer	Cenozoic limestone, undivided	23

6.4.3.3 Hydrogeologic Properties

HFM2006 provides the hydrogeologically-defined geometry for SZ flow and transport process models and is used to assign geologic properties to the nodes of the computational grid. The physical hydrogeologic unit present at each node in the computational grid was established during the computational grid construction. The HFM2006 surface files represent the top surface of each hydrogeologic layer in the model framework and were imported into LaGriT to identify the hydrogeologic layer designation for each node and cell of the computational grid. Cells above the ground surface were identified using the HFM2006 surfaces, then they were removed from the grid. Quality checks were performed to ensure that the final grid is correct. These include histograms of element volume and element aspect ratio as described by Bower et al. (2000 [DIRS 149161]). Once the grid geometry was evaluated and the material units conform as needed to the input HFM, FEHM modeling input files are generated. These files include the mesh geometry, lists of nodes on external boundaries, and node lists sorted by material property.

All nodes were automatically and visually checked to ensure that they were assigned the correct material identification corresponding to the input HFM. Lists of the number of nodes associated with each material were compared to the volume of each material in the EARTHVISION framework to confirm that the hydrogeologic units are identified correctly.

When evaluating the computational grid for SZ flow and transport, the hydrogeologic properties of the grid are compared to the hydrogeologic framework used as input. It is expected that the grid units will differ slightly from the HFM due to differences in grid spacing (i.e., 250 versus 125 m). The grid units should still resemble the input HFM and areas of importance should be replicated accurately. The flow pathways are expected to leave the repository and travel in a south-southeasterly direction towards Fortymile Wash and the 18-km compliance boundary. From the 18-km boundary to the end of the model, the flowpaths should trend to the south-southwest and generally follow Fortymile Wash. Outlines of the repository, Fortymile Wash, and U.S. Highway 95 are included on Figure 6-5 as reference to these areas.

6.4.3.4 Evaluation of Hydrogeology represented in the SZ Computational Grid

All nodes were automatically and visually checked to ensure that they were assigned the correct material. The number of tetrahedral elements assigned to each hydrogeologic unit and their associated element volumes are presented in Table 6-5. Lists of the number of nodes associated with each material were compared to the volume of each material in the HFM2006 to confirm that the hydrogeologic units are identified correctly. To check that hydrogeologic properties are being assigned in accord with the HFM2006, relative unit volumes are compared. Differences will occur between the HFM and grid units due to variations in grid element sizes in the computational grid. Volumes represented by the HFM2006 surfaces are included for comparison. Large grid elements less accurately capture thin layers, which becomes evident when comparing unit volumes. Figures showing the grid units are supplied in Appendix G to confirm that differences are reasonable and acceptable.

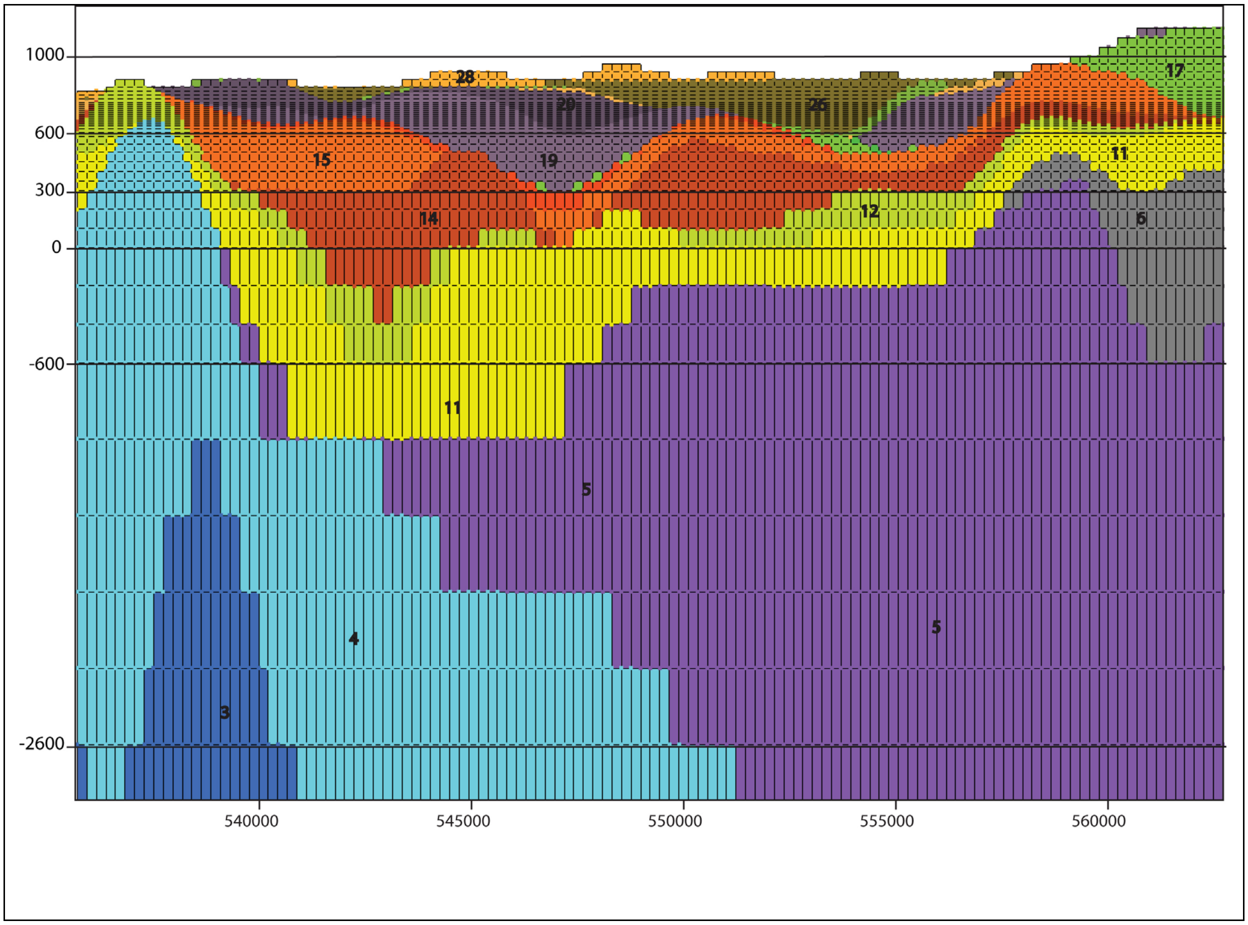
Table 6-5. SZ Computational Grid and HFM2006 Volume Comparisons by Unit

Unit	Names	SZ Computational Grid			HFM2006 Surfaces	
		Tetrahedral Elements Number	Volume of Elements per Unit (m^3)	% Fractional Volume	Volume between Surfaces (m^3)	% Fractional Volume
28	YAA	32,106	4.75×10^9	0.07	1.15×10^{10}	0.17
27	YACU	7,788	8.11×10^8	0.01	9.89×10^8	0.01
26	OAA	137,772	2.09×10^{10}	0.31	2.35×10^{10}	0.34
24	LA	18,834	2.08×10^9	0.03	2.18×10^9	0.03
23	LFU	38,208	8.56×10^9	0.13	1.48×10^{10}	0.22
21	Upper VSU	316,716	5.53×10^{10}	0.81	5.58×10^{10}	0.82
20	TMVA	152,586	3.77×10^{10}	0.56	4.38×10^{10}	0.64
19	PVA	838,668	2.35×10^{11}	3.47	2.45×10^{11}	3.59
18	CHVU	280,368	9.29×10^{10}	1.37	9.45×10^{10}	1.38
17	WVU	122,802	2.52×10^{10}	0.37	2.57×10^{10}	0.38
16	CFPPA	140,064	3.38×10^{10}	0.56	3.78×10^{10}	0.55
15	CFBCU	439,698	1.35×10^{11}	1.98	1.35×10^{11}	1.98
14	CFTA	584,232	2.85×10^{11}	4.20	2.85×10^{11}	4.17
12	OVU	158,982	1.68×10^{11}	2.47	1.69×10^{11}	2.48
11	Lower VSU	461,478	5.97×10^{11}	8.78	5.96×10^{11}	8.72
9	LCA_T1	185,736	3.00×10^{11}	4.42	3.00×10^{11}	4.39
8	LCCU_T1	101,550	2.63×10^{11}	3.87	2.64×10^{11}	3.86
7	UCA	24,900	8.33×10^9	0.12	8.83×10^9	0.12
6	UCCU	238,248	2.18×10^{11}	3.21	2.21×10^{11}	3.24
5	LCA	793,620	2.55×10^{12}	37.59	2.54×10^{12}	37.13
4	LCCU	275,532	1.07×10^{12}	15.77	1.08×10^{12}	15.79
3	XCU	47,490	2.23×10^{11}	3.28	2.26×10^{11}	3.30
2	ICU	106,974	4.50×10^{11}	6.62	4.55×10^{11}	6.67
	Totals	5,504,352	Element Volume 6.79×10^{12}		Sum Volume 6.83×10^{12}	

Source: Output DTN: LA0612TM831231.001.

NOTES: HFM2006 volumes represent the best achievable volumes when matching surface resolutions. The computational grid lengths are 250 m in the horizontal and depths range from 10 to 600 m in the vertical. Units 10, 13, 22, and 25 are not found within the domain of the SZ site-scale flow model.

Figures 6-8 through 6-10 represent sections cut through the computational grid and can be compared to matching sections cut through HFM2006 (SNL 2007 [DIRS 174109], Figures 6-5 and 6-6). The first figure is a north-to-south vertical section cut at an easting of 552,500 m. This section was selected because it is located approximately along the flowpath from Yucca Mountain to the south. The second figure is a west-to-east vertical section cut at a northing of 4,064,000 m and it is located within the area of the newest NC-EWDP well data used in HFM2006. This section cuts across most of the faulting in the area and demonstrates where the faulting is represented in the more widely spaced data of the regional model, which served as the basis for HFM2006. As can be seen in this figure, some of the offsets on the faults are preserved through changes in altitude of a given hydrogeologic unit. Given the depth to which the model extends and the lack of information in most of the modeled volume, this seems to be a rational simplification (SNL 2007 [DIRS 174109], Section 6).



Source: Output DTN: LA0612TM831231.001.

NOTE: Coordinates in UTM, Zone 11, NAD27 meters, 5 × vertical exaggeration. Unit numbers are the hydrogeologic numbers defined by HFM2006 in Table 6-2. This image shows the spacing of the grid in the vertical direction. The grid nodes used in FEHM flow modeling are shown here at the vertices of each grid block. Grid nodes and volumes are colored according to HFM2006 hydrogeology. The colors correspond to those in the legend for Figure 6-7.

UTM = Universal Transverse Mercator.

Figure 6-10. Hydrogeologic Grid Nodes and Spacing at West-East Cross Section in the SZ Computational Grid at UTM Northing = 4,064,000 m

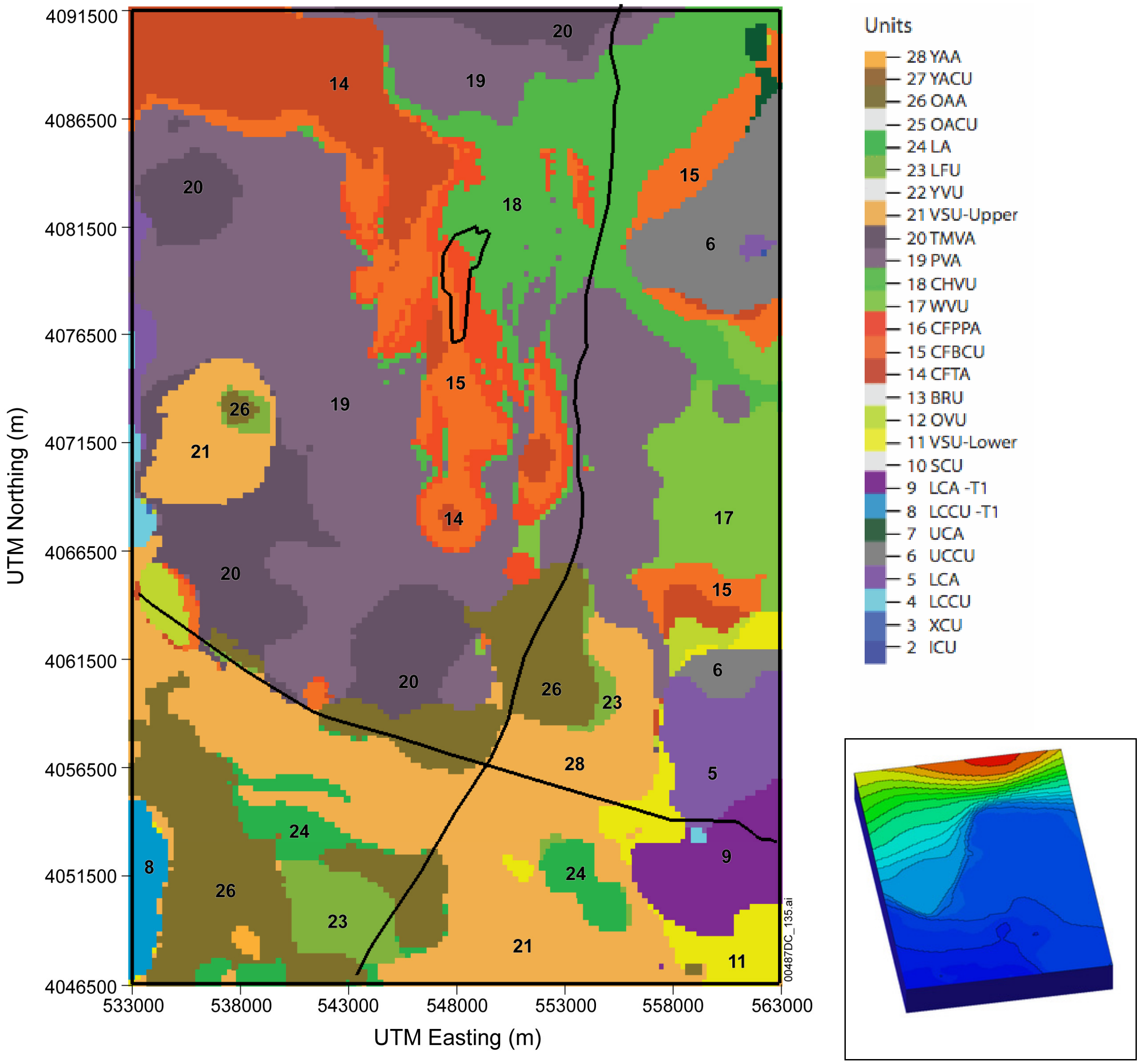
6.4.3.5 Hydrogeology at the Water Table

A new water-table surface is used in conjunction with HFM2006 and is discussed in Appendix E. The water-table surface defines which grid nodes are below and above the water table, those that are above the water table are inactivated in the FEHM flow model. This results in node elevations at the top of the flow model that range from ~1,200 m in the north to ~700 m in the south. The hydrogeologic units at the water table top are shown in Figure 6-11, which compares well with HFM2006 view at the water table (SNL 2007 [DIRS 174109], Figure 6-7c). Table 6-6 lists the numbers of FEHM nodes in the entire model domain (below the land surface) and the number of saturated nodes below the water table.

Table 6-6. SZ Computational Grid Nodes by Unit

Unit	Abbreviation	Nodes per Unit Under Land Surface	Nodes per Unit Under Water Table Surface
28	YAA	9,965	197
27	YACU	1,580	247
26	OAA	24,148	10,637
24	LA	3,289	1,387
23	LFU	8,608	2,751
21	Upper VSU	53,911	42717
20	TMVA	27,940	18,131
19	PVA	143,658	94,149
18	CHVU	47,905	29,189
17	WVU	21,116	14,576
16	CFPPA	23,461	20,242
15	CFBCU	73,939	67,436
14	CFTA	98,162	93,327
12	OVU	27,152	26,691
11	Lower VSU	78,182	76,856
9	LCA_T1	31,608	28,588
8	LCCU_T1	17,848	17,053
7	UCA	4,228	4,201
6	UCCU	40,842	33,533
5	LCA	135,186	131,312
4	LCCU	52,891	52,745
3	XCU	10,018	10,015
2	ICU	20,708	20,708
	Totals	956,345	774,177

Source: Output DTN: LA0612TM831231.001.



Source: Output DTN: LA0612TM831231.001.

NOTE: For illustration purposes only. The figure depicts grid points at the water-table surface. The black lines are used for reference and are the repository outline (SNL 2007 [DIRS 179466]), U.S. Highway 95, and Fortymile Wash. The inset shows the computational grid colored by the water table elevations ranging from 680 m in the south to 1,230 m in the north.

UTM = Universal Transverse Mercator.

Figure 6-11. Hydrogeologic Units Present at the Water-Table Surface in the SZ Computational Grid

The resolution of the computational grid was designed to have the smallest vertical spacing in the vicinity of the water-table below the repository. Therefore, the computational grid honors the hydrogeology of the HFM2006 as can be seen in these figures. Updates to the HFM2006 show differences most evident in the southern part of the model where the volcanic and sedimentary unit replaces the valley-fill aquifer as the most pervasive unit. Updates to the HFM2006 also include increased abundance of the Crater Flat group to the west of Yucca Mountain and the occurrence of Lava Flow unit to the east of Fortymile Wash and to the north of U.S. Highway 95. These changes may have influence on the calibration and specific discharge simulations of the flow model.

Further comparisons can be made across each unit by comparing HFM2006 layer thickness and distribution maps (SNL 2007 [DIRS 174109], Appendix C) to the distribution of grid nodes for each hydrogeologic unit (SNL 2007 [DIRS 174109], Appendix A) and are presented in Appendix G. Figures for each grid unit include the distribution of each unit for the full model domain, and a second figure showing the grid units truncated by the water table surface. The truncated grid units show the active grid nodes for the FEHM modeling domain. Both sets of images are views looking directly down at the top, with south toward the page bottom and showing the horizontal distribution for each unit 1 through 28. The shapes of the HFM2006 maps (SNL 2007 [DIRS 174109], Appendix C) and the grid units (SNL 2007 [DIRS 174109], Appendix A) compare reasonably given that the grid resolution is 250 m and the HFM2006 is 125 m and that vertical grid resolution varies from 10 to 600 m.

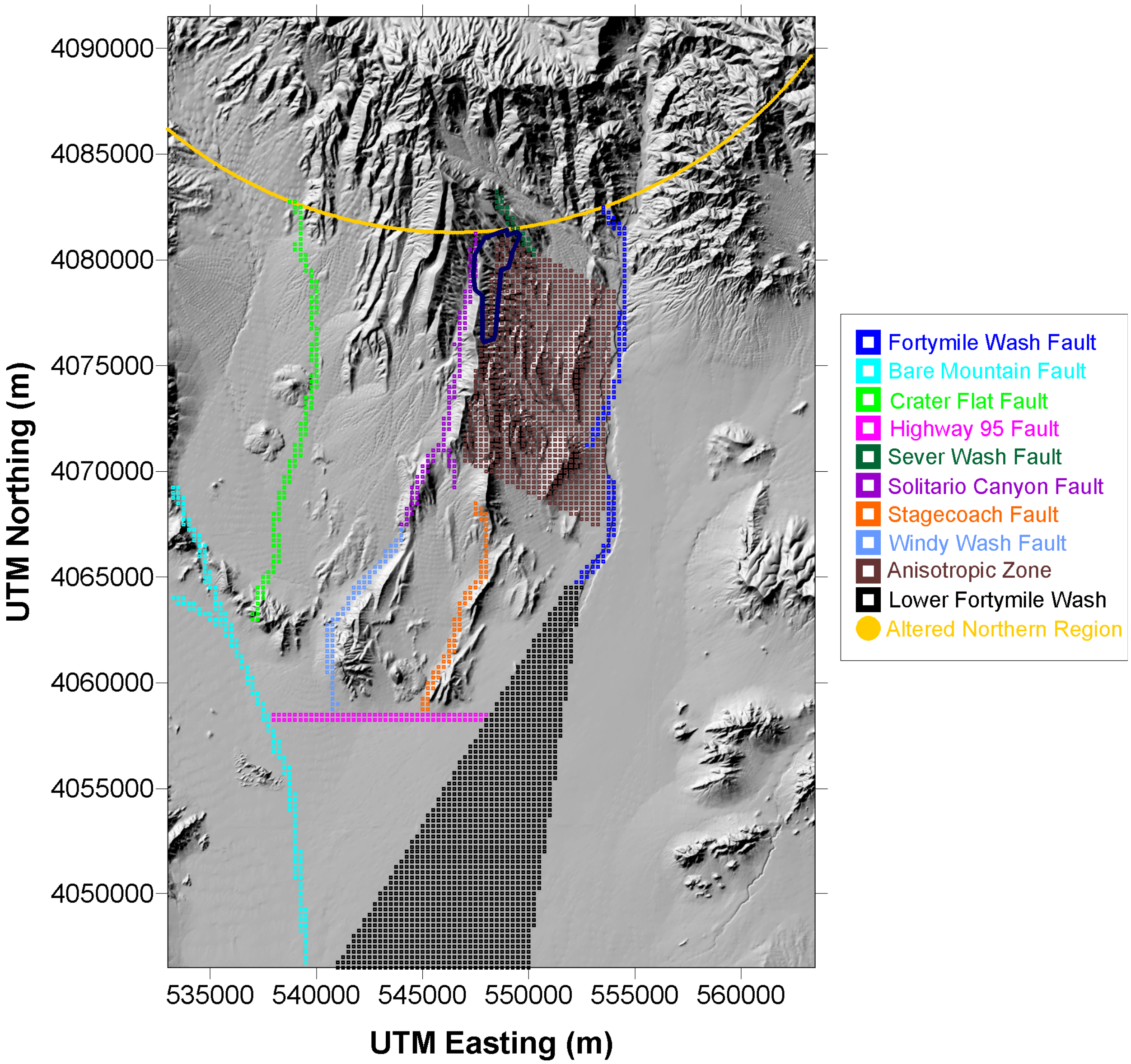
6.4.3.6 Uncertainty

Uncertainty in the SZ computational grid is a function of HFM2006 and the resolution of the grid in relation to the flowpaths. Large grid spacing and associated loss of hydrogeologic unit shape accuracy are chosen to correspond with areas deep in the model and beyond the flowpath regions. Areas of highest resolution were chosen in the shallow units and in the area of the water table below the repository. Uncertainties in the HFM2006 relate most importantly to the quantity and location of available qualified data, and secondly to the interpretation of surfaces and the representation of important faults and structures. Uncertainties due to the definition of the hydrogeologic units are propagated through the flow and transport model abstraction (SNL 2007 [DIRS 181650]).

Model uncertainties in the HFM2006 can be attributed to interpretations and simplifications driven largely by the distribution and availability of data. The data distribution over the SZ area is uneven, much of the volume is unsampled, and many of the inputs are interpretations. As a result, the expected error in the HFM2006 varies significantly over the model area. Some of the surfaces, such as that of the upper volcanic aquifer in the area of the repository, are relatively well defined by more than one data set (derived from the surface hydrogeologic unit map and borehole lithologic logs). Others, especially the units that crop out less commonly, are less well defined and are extrapolated from sparse data. In the area of the repository, the unit locations are relatively well known. Even in this area, however, only one borehole penetrates the Paleozoic rocks. Data uncertainty increases with depth and distance from the repository as data become sparse and the effects of faults deeper in the system become unknown. As a result, the model contains an inherent level of uncertainty that is a function of data distribution and geologic complexity. Additional limitations include data-poor regions in the deeper Paleozoic carbonate region (SNL 2007 [DIRS 174109], Section 6.4.3).

HFM2006 is constructed with a horizontal grid spacing of 125 m, but most of the model domain does not contain sufficient geologic detail to support this resolution. This results in smoothly interpreted or interpolated surfaces at a resolution finer than justified by the geologic data. This finer resolution does not add any additional error. Specific borehole data and other measured volcanic units (Units 12, 14, 15, 16, 17, 18, 19, 20, and 25), and to provide boundaries for a zone of enhanced permeabilitiy in the Crater Flat tuffs to better approximate the small haydraulic gradient in the region. The zone was defined based on responses of USW H-4, UE-25 C#1, UE-25 WT#14, and UE-25 WT#3 to pumping at the C-holes from May 1996 to November 1997. Furthermore, this zone did not include wells USW H-5, G-1, and UZ-14 because, although these wells are located east of the Solitario Canyon Fault, they showed anomlaous heads closer to those observed in wells located west of Solitario Canyon Fault (USW H-6, WT-7, and WT-14). This indicates that some non-characterized feature or process is impacting the water levels just to the east of Solitario Canyon Fault and the newly defined zone allows the model to better represent these data The quadrilateral is defined to encompass the small-gradient area southeast of the repository between Solitario Canyon and Fortymile Wash Faults without including wells USW H-5, G-1, and UZ-14, but including wells USW H-4, UE-25 C#1, UE-25 WT#14, and UE-25 WT#3.

Most hydrogeologic units (the 19 units with areal extents that reach into the north of the model including all units except the lower clastic confining unit thrust, lower carbonate aquifer thrust, Wahmonie volcanic unit, limestone aquifer, and the young alluvial confining unit) have been divided into northern and southern zones near the Claim Canyon caldera boundary to represent the altered northern zone (see Section 6.3.1.11). This zone of decreased permeability facilitates model representation of the LHG north of Yucca Mountain. Except for Sever Wash Fault, fault nodes do not reside in this region. The altered northern region is defined with an arc that intersects the model domain and it is defined by a circle with center 546,500; 4,102,400 (UTM easting and northing) and radius 21,100 m. This designation was selected such that the defining circle roughly corresponds to the center of the caldera complex and the radial extent includes wells: GEXA Well #4, UE-29 a#2, UE-29 UNZ#91, UE-25 WT#6, USW G-2, and USW WT-24. Breaking the hydrogeologic units into independent northern and southern zones yields 19 additional calibration parameters. Figure 6-13 illustrates the radial extent of the altered northern region.



Source: Output DTN: SN0612T0510106.004, *feature_set.zonn* and *aniso.zonn*).

NOTE: Source for repository outline: SNL 2007 [DIRS 179 466]. Fault traces are labeled in the legend. FEHM zone number correspond to the following regions: 39 – Anisotropic zone; 40 – Fortymile Wash Fault; 41 – Bare Mountain Fault; 42 – Crater Flat Fault; 43 – U.S. Highway 95 Fault; 44 – the Solitario Canyon Fault; 45 – Sever Wash Fault; 46 – Stagecoach Fault; 47 – Windy Wash Fault; 50 – Lower Fortymile Wash.

UTM = Universal Transverse Mercator.

Figure 6-12. Geologic Features Included in the SZ Site-Scale Flow Model and vertical) multiplied by 10 (e.g., Solitario Canyon fault permeabilities in the *y*- and *z*-directions are 10 times that in the cross-fault direction). The permeabilities of major faults are used as calibration parameters; however, the anisotropy ratios were constant during the calibration process. A 10:1 horizontal to vertical anisotropy was also assigned in the Lower Fortymile Wash Alluvial Zone.

6.5 SZ SITE-SCALE FLOW MODEL RESULTS

6.5.1 Model Calibration

Calibration is the process by which values of important model parameters are estimated and optimized to produce the best fit between model output and observed data. Calibration is generally accomplished by adjusting model input parameters (e.g., permeabilities) to minimize the difference between observed and simulated conditions (in this case, comparing simulated and observed head values and lateral boundary volumetric/mass flow rates). Model calibration may be performed manually or through automated optimization procedures. Automated optimization procedures generally employ a carefully prescribed mathematical process that selects the optimal set of parameters based on minimizing an objective function describing the difference between observed and simulated conditions. These procedures typically provide the most structured and thorough means of calibrating a model, and, frequently, they provide useful additional information regarding model sensitivity to parameters and other useful statistical measures. Consequently, an automated optimization procedure is used to calibrate the SZ site-scale flow model. However, manual adjustments to the calibration are also performed to ensure accurate representation of the small hydraulic gradient region southeast of the repository by ensuring that simulated particle pathlines do not contradict flow directions inferred from the potentiometric map.

A description of the calibration technique includes discussions of: optimization procedures; model outputs, whose differences between observed values (calibration targets) were minimized; and parameters that were varied during calibration.

6.5.1.1 Calibration Criteria

Proper calibration of the SZ site-scale flow model requires consideration of the full range of available data, which include field data for water levels and hydraulic heads, permeability data from field and laboratory tests, locations of known faults and other geologic data, and hydrochemical data. Opinions expressed by the Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353]) must also be considered. The goal during development of the SZ site-scale flow model was to deliver to performance assessment a model that, given data sparseness, is as realistic as possible.

6.5.1.2 Parameter Optimization Procedure

The SZ site-scale flow model was calibrated with the commercial parameter estimation code, PEST (STN: 10289-5.5-00; [DIRS 161564]). PEST is a Levenberg-Marquardt (LM)-based optimization algorithm. The LM package is a well-established algorithm (Press et al. 1992 [DIRS 103316], pp. 678 to 683), it is robust, and widely applicable. It will search for the minima of a multidimensional function. In this case, the features or faults. The zone sizes were fixed based on data from HFM2006. Uncertainty associated with geologic contacts is discussed in Section 6.7.3.

Recall that vertical anisotropy is assigned a value of 10:1 (horizontal to vertical) in the volcanic and valley-fill units (above Unit 9). Lower permeability in the vertical direction than in the horizontal direction typically occurs in stratified media, and the ratio of 10:1 is in the generally accepted range (CRWMS M&O 1998 [DIRS 100353], Table 3-2). For a site-specific example, the relatively high vertical gradient observed in well UE-25 p#1 suggests that vertical permeability is lower than horizontal permeability (minimal hydraulic connectivity). Nine wells (see Section 6.3.1.5) exhibited vertical gradients (BSC 2004 [DIRS 170009], Table 6-4). The uncertainty associated with the vertical anisotropy is discussed in Section 6.7.2.

Specific hydrogeologic features thought to potentially impact groundwater flow are classified as distinct permeability zones. The permeability variable or permeability multiplication factor used for a specific feature was assigned to all of the nodes within that feature. The hydrogeologic features for which special permeability zones were established are primarily faults, fault zones, and areas of hydrogeologic alteration (Section 6.5.2). As previously discussed, these features are distinct from the subhorizontal hydrogeologic units identified in HFM2006. Each of the identified hydrogeologic features includes multiple geologic formations and represents a zone of altered permeability within individual formations.

Twenty-three permeability zones were established based on the geologic units within the SZ site-scale model domain from HFM2006 for model calibration. Additional (usually low) permeability zones reflecting altered northern region were added to the model to help establish known system characteristics (like the LHG). These were established by dividing existing (base) geologic units into altered northern regions with permeabilities defined by multipliers. These permeability multipliers are calibration parameters that modify the permeability values assigned to geologic units in the altered northern regions. Eight additional zones representing faults and the Lower Fortymile Wash alluvium were established because they were identified as important structural features (e.g., the Solitario Canyon Fault) or were necessary for some conceptual feature, such as the LHG north of Yucca Mountain (which is partially established in the model domain with help from the altered northern region).

As required by PEST, upper and lower bounds were placed on each permeability variable during parameter optimization with limits chosen to reflect maximum and minimum field values (permeability) or a realistic range of values (permeability multipliers). A list identifying permeability zones, its calibrated permeability parameter, and the upper and lower bounds specified for the parameter is provided in Table 6-9.

Table 6-9. Calibration Parameters Used in the SZ Site-Scale Flow Model

Parameter Name (zone number)	Geologic Unit or Feature	Calibrated Value (m^2)	Minimum Value (m^2)	Maximum Value (m^2)
ICU (2)	Intrusive Confining Unit (granite)	9.9×10^{-17}	1.0×10^{-19}	1.0×10^{-10}
XCU (3)	Crystalline Confining Unit (granite)	1.0×10^{-16}	1.0×10^{-19}	1.0×10^{-10}
LCCU (4)	Lower Clastic Confining Unit	9.7×10^{-17}	1.0×10^{-19}	1.0×10^{-10}
LCA (5)	Lower Carbonate Aquifer	9.7×10^{-15}	2.0×10^{-15}	1.0×10^{-10}

Table 6-9. Calibration Parameters Used in the SZ Site-Scale Flow Model (Continued)

Parameter Name (zone number)	Geologic Unit or Feature	Calibrated Value (m^2)	Minimum Value (m^2)	Maximum Value (m^2)
wwfz (47)	Windy Wash Fault Zone	4.8×10^{-16}	1.0×10^{-19}	1.0×10^{-10}
wash (50)	Lower Fortymile Wash	2.0×10^{-11}	1.0×10^{-19}	1.0×10^{-10}

Output DTN: SN0612T0510106.004, *sz_site_2006.pst*.

In addition to the PEST optimization described above, several manual adjustments were made to improve the model in ways that were not possible during the PEST run. Specifically, during calibration, only water levels (and lateral volumetric/mass flows) were considered in the objective function and hence head gradients or important head differences between wells were not explicitly considered. Manual adjustments were made to ensure that the flow direction southeast of the repository (in the small-gradient, anisotropic region) matched the direction inferred from the range and distribution of head values in this area. These adjustments modified the direction of particle paths emanating from the repository (to match the direction inferred from differences in the measured water levels) while maintaining good calibration (low objective function and low weighted RMSE for heads). The specific discharge was adjusted by changing the permeability of several units as listed in Table 6-10. Specific discharges were manipulated without adversely affecting the heads or gradient in the small hydraulic gradient area near Yucca Mountain. Table 6-10 shows the units that were adjusted during hand calibration, their PEST-optimized permeability values, and their hand calibrated values. It should be noted that an additional zone corresponding to the Bullfrog Tuff within the quadrilateral defined by the Yucca Mountain zone was added during hand calibration with a permeability of 5×10^{-13} m^2 to ensure that the small hydraulic gradient region observed southeast of the repository is honored by the model and the flow paths from below the repository did not terminate along the eastern model boundary.

Table 6-10. Hand Calibration Results used in the SZ Site-Scale Flow Model

Parameter Name (unit/zone number)	Geologic Unit or Feature	Hand-Calibrated Value (m^2)	PEST-Calibrated Value (m^2)
LCAT1 (9)	Lower Carbonate Aquifer	5.6×10^{-12}	5.6×10^{-14}
CFBCU (15)	Bullfrog Tuff	$5.2. \times 10^{-14}$	5.2×10^{-14}
CFPPA (16)	Prow Pass Tuff	3.1×10^{-12}	1.1×10^{-13}
PVA (19)	Paintbrush Volcanic Aquifer	6.5×10^{-14}	2.5×10^{-13}
VSU (21)	Volcanic and Sedimentary Unit	8.7×10^{-13}	8.7×10^{-16}
OAA (26)	Older Alluvial Aquifer	1.5×10^{-13}	8.8×10^{-13}
CFPPAm (116)	Prow Pass Tuff Multiplier	1.4×10^{-3}	9.4×10^{-3}
CHVUm (117)	Crater Hills Volcanic Unit Multiplier	2.3×10^{-3}	2.3×10^{-3}
4wfz (40)	Fortymile Wash Fault Zone	1.4×10^{-10}	6.4×10^{-11}
wash (50)	Lower Fortymile Wash Alluvial Zone	2.0×10^{-11}	5.2×10^{-13}

Output DTN: SN0612T0510106.004, *sz_site_2006_calibrated.pst*.

RMSE for calibrated model is only 18% worse than the best-fit potentiometric surface (24.39 m compared to 20.70 m). Moreover, the weighted RMSE of the calibrated model is an order of magnitude better than the best-fit potentiometric surface and this indicates excellent model agreement in high weight areas of the model domain—areas felt to be the most important to get accurate model simulations (i.e., downgradient from the repository). Because of the 10-m minimum layer thickness, head differences of less than this magnitude are within the uncertainty range of the model.

As can be seen in Figure 6-15, the largest head residuals (~100 m) are in the northern part of the model in the altered northern region and in the vicinity of the moderate hydraulic gradient. These residuals are largely the result of the low weighting factor of (0.1) and the possibility that they reflect perched conditions (see Section 6.5.2.1 for a description and Section 6.7.7 for a discussion of perched water effects). In the figure, a negative residual means that the calibrated value was lower than the target data (note that the PEST record file shows opposite signs; a negative residual means that the calibrated value was higher than observed). The next highest head residuals border the Crater Flat and Solitario Canyon Faults. These residuals (~25 m) are most likely the result of 250-m grid blocks not being able to resolve the 780 to 730-m (~50-m) drop in head in the short distance just east of the above-mentioned features. There may be additional complicating factors such as varied hydrologic characteristics in the Solitario Canyon Fault along its north-south transect. In the model, the fault acts as a barrier, but is defined with only one calibration parameter. This may not be adequate to represent the local behavior of such a long feature. For example, well USW G-1, about 1,000 m from the Solitario Canyon fault, shows an 8-m difference between measured and simulated heads. The measured head for this well (754 m), located on the east side of the fault, is closer to measured head values on the west side of the fault. Because the majority of wells on the east side have heads of approximately 745 m, the simulated head for USW G-1 has a calibrated result close to that value. Overall results indicate that the model adequately represents the water table near Yucca Mountain. In the vicinity of the 18-km compliance boundary and south, the modeled potentiometric surface is typically on the order of 5 m higher than the observed water levels although the estimated gradients match well (see Section 7.2.1).

6.5.2.4 Specific Discharge

Using the calibrated SZ site-scale flow model, specific discharge was estimated as the average over 100 particles. These particles were randomly distributed below the repository and tracked until they traveled across UTM Northing 4,073,761 m (approximately 5 km south of the midpoint of the repository). Pathlength divided by travel time yields the specific discharge for a particle and the average across 100 particles was 0.36 m/yr (1.08 ft/yr) for the calibrated model. End members of the 100-particle plume had specific discharges of 0.11 and 0.66 m/yr. The Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353], Figure 3-2e) estimated a median specific discharge of 0.6 m/yr (2.0 ft/yr) for the 5-km (3-mile) distance. Thus, reasonable agreement is found between the specific discharge simulated by the calibrated SZ site-scale flow model and that estimated by the Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353]).

6.6 CONSIDERATION OF ALTERNATIVE CONCEPTUAL MODELS

The SZ site-scale flow model propagates information through the SZ flow and transport model abstraction (SNL 2007 [DIRS 181650]) to the performance assessment calculations, which are used to evaluate potential risks to groundwater users downgradient from the repository area. The results of these performance assessment calculations depend upon the specific discharge of groundwater leaving the repository area as well as on the flow paths and the distribution of flow among the various hydrostratigraphic units that carry, deflect, or otherwise affect the flow. For this report only, the specific discharge was evaluated with SPDIS.EXE (STN: 611598-00-00 [DIRS 180546]), which calculates the average travel distance divided by corresponding travel time to reach a specified northing location (e.g., 5 km downgradient) across 100 particles. It is important to note that SPDIS.EXE yields a convenient metric to compare specific discharges, which represents surrogates for flow fields generated from the model. The alternative conceptual models (ACMs) presented here were investigated because they represented a hydrologic concern such as water table rise due to climate change or were related to a model feature (anisotropy) that had a possibility of affecting the specific discharge calculations. This section presents analyses of the ACMs, their representation in the numerical model, and a discussion about possible impacts on the model outputs. ACMs affecting model outputs are discussed here, although this uncertainty is not directly propagated to the radionuclide breakthrough curves in the TSPA calculations. Specifically, it should be noted that the SZ flow and transport abstraction model does not use the SZ site-scale flow model as a source of direct input to the assessment of uncertainty in groundwater specific discharge. The two direct inputs used to establish the groundwater specific discharge multiplier are DTNs: MO0003SZFWTEEP.000 [DIRS 148744] and LA0303PR831231.002 [DIRS 163561] (SNL 2007 [DIRS 181650], Figure 6-2[a]).

The calibrated SZ site-scale flow model described in detail in Section 6.5 also provides the basis for the ACMs discussed here. That is, the same numerical grid and HFM were used throughout this section. Various parameterization schemes were used to define the ACMs (e.g., change in potentiometric surface). The following ACMs were evaluated:

- Removal of vertical anisotropy: This ACM relates to removal of vertical anisotropy in permeability

- Removal of horizontal anisotropy: This ACM relates to removal of horizontal anisotropy in the volcanic units downgradient from Yucca Mountain

- Removal of the altered northern region: This ACM relates to removal of the permeability multipliers that reduce the permeability in the northern region, which help the model honor the observed high head

- Increase in permeability in the *z*-direction for the Solitario Canyon Fault

- Water table rise: This ACM relates to future water table rise.

unsaturated and saturated zones at Yucca Mountain indicated previous water-table elevations of 85 m (279 ft) higher than present (Marshall et al. 1993 [DIRS 101142], p. 1,948). Recently completed wells at paleospring discharge locations near the southern end of Crater Flat, which are inactive sites of Pleistocene spring discharge, revealed shallower-than-expected groundwater with depths of only 17 to 30 m (56 to 100 ft) to the water table (Paces and Whelan 2001 [DIRS 154724]; BSC 2004 [DIRS 168473], Table I-1). These findings indicate that the water-table rise during the Pleistocene at these paleospring locations could not have been more than about 30 m (100 feet) due to formation of discharge locations. The results of the mineralogical and geochemical studies showing a maximum water-table rise of up to 85 m reflect evolution of past climates for the last 1 million years, which included the effects of glacial climates. The maximum water-table rise under monsoon and glacial-transition climates is, therefore, expected to be less than 85 m because the monsoon and glacial-transition climates are warmer and dryer than the glacial climate (Sharpe 2003 [DIRS 161591]).

Interpretation of the water levels in wells at the southern end of Crater Flat, in relation to water-table rise, is complicated by several factors. The paleospring discharge locations at the southern end of Crater Flat are not along the flow path from Yucca Mountain. Also, a higher groundwater flow rate (increased hydraulic gradient) is expected under future wetter climatic conditions. However, the principles of hydrogeology specify that a uniform rise in the water table could only occur if the increased saturated thickness (and its effect on transmissivity) accommodates the additional groundwater flow through the aquifer. For the geology within the model domain, an increase in gradient to accommodate the increase in flow results in a nonuniform water-table rise with higher increases upgradient of flow. A higher groundwater flow rate implies a higher hydraulic gradient, a larger transmissivity, or both along any given flow line. Thus, the water table at upgradient locations would be expected to rise more than the water table at downgradient locations, resulting in a nonuniform rise in the water table across the flow system.

Two-dimensional groundwater flow modeling of the response to doubling mean annual precipitation indicated a maximum water table rise of 130 m (430 ft) in the vicinity of Yucca Mountain (Czarnecki 1985 [DIRS 160149]). This result is potentially overestimated because the analysis by Czarnecki (1985 [DIRS 160149]) was limited to two dimensions. In addition, average precipitation under monsoon and glacial-transition climates is less than twice the present-day value in the Yucca Mountain area, and the percolation flux resulting from the precipitation increase was also conservatively modeled (Czarnecki 1985 [DIRS 160149]). More recent groundwater flow modeling of the regional flow system under paleoclimate conditions (the DVRFS) simulated water levels of 60 to 150 m (200 to 490 ft) higher than present below Yucca Mountain (D'Agnese et al. 1999 [DIRS 120425], p. 2). Coarse resolution of the numerical grid in this model is believed to have resulted in potential overestimation of water table rise (150 m).

The uncertainty in water-table rise has been evaluated by considering these multiple lines of evidence and new geochemical data using a multidisciplinary workshop approach, as documented by *Total System Performance Assessment Model/Analysis for the License Application* (SNL 2007 [DIRS 178871]). Given that these various sources of information on water-table rise result in significant variations in the estimate and that none of the sources is clearly definitive, a subjective approach to quantifying uncertainty was used and a consensus

6.7 UNCERTAINTY

Characterizing and understanding the flow through the saturated zone is important for assessing the overall containment strategy for safely sequestering radioactive materials at the Yucca Mountain repository. Uncertainty in flow modeling arises from a number of sources including, but not limited to, the conceptual model of the processes affecting groundwater flow, water–level measurements and simplifications of the model geometry, boundary conditions, hydrogeologic unit extent and depth, and the values of permeability assigned to hydrogeologic units. This section discusses and attempts to quantify uncertainties in the SZ site-scale flow model because all uncertainty contributes to inaccuracy in system representation and response (uncertainty in model predictions). Such uncertainty is an inescapable aspect of geologic modeling. In addition to the discussion in this section, parameter uncertainty is addressed in the model abstraction document (SNL 2007 [DIRS 181650], Table 6-7[a]) and a thorough discussion of uncertainty analysis is given in Appendices H and I. *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650], Sections 6.5.2.1 and Figure 6-2[a]) includes additional quantitative analysis on horizontal anisotropy in permeability and groundwater specific discharge. *Saturated Zone In-Situ Testing* (SNL 2007 [DIRS 177394]) addresses the uncertainty related to the spatial distribution of the observation wells. Overall, it is understood that model predictions are always uncertain, thus it is important to minimize and quantify this uncertainty. It should be noted that the uses of PEST V11.1 (STN: 611582-11.1-00; [DIRS 179480]) and SPDIS (STN: 611598-00-00; [DIRS 180546]) are non-quality affecting analyses of the qualified results produced by PEST V5.5 (STN: 10289-5.5-00 [DIRS 161564]) and that they in no way change the conclusions of this report. Instead, this analysis sheds light on some of the details going on behind the scenes during the calibration process (e.g., differentiating null from solution space errors and evaluating data worth and parameter importance).

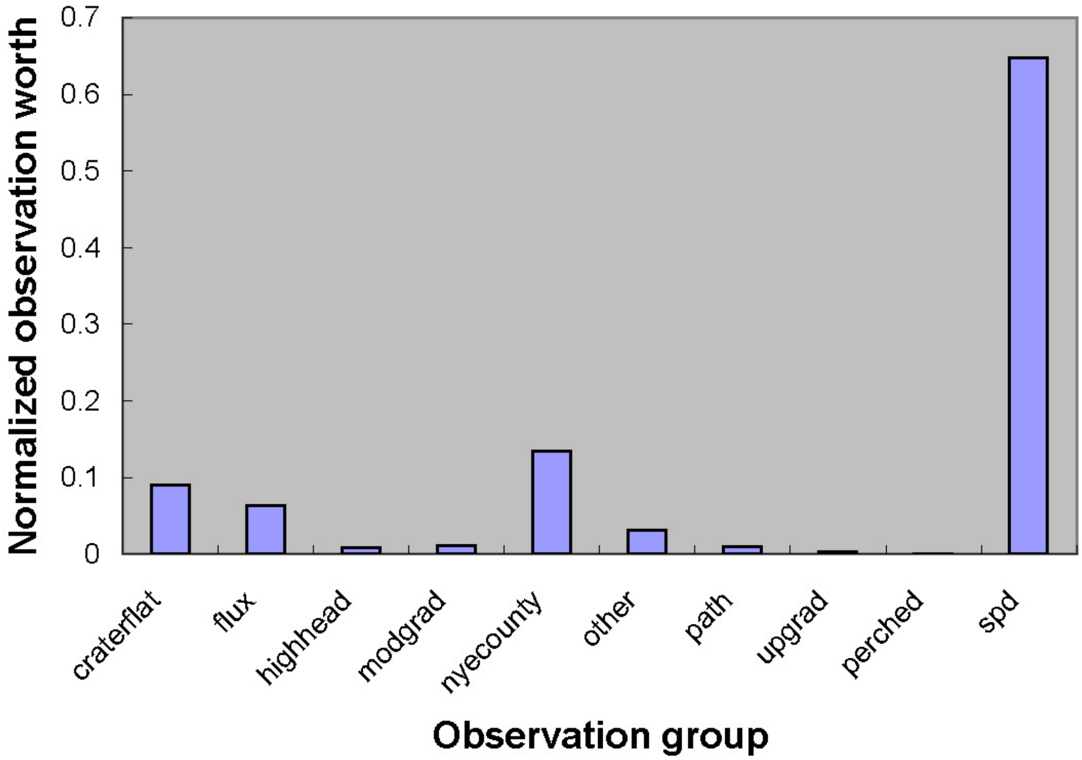
Estimating uncertainty in a modeled process is a wide ranging field of active research spanning many disciplines including hydrologic modeling, surface water flow and transport, medical imaging, geophysics, etc. A fundamental aspect of geologic modeling is the calibration phase where model parameters (in this case permeabilities) are adjusted until the model's replication of historical field measurements is judged to be "reasonably good." It is then assumed that this constitutes sufficient justification to use the model to make predictions to be used in site management. For the SZ site-scale flow model developed here, PEST (STN: 10289-5.5-00; [DIRS 161564], Watermark Numerical Computing 2004 [DIRS 178612]) was used to minimize the objective function comprising a weighted sum of squares of water-level measurements and fluxes across the lateral model boundaries (minimize the differences between measured and modeled data). Additional information was also used to hand calibrate the model, namely gradients that indicate that flowpaths emanating from below the repository should travel in a southeasterly direction. Future efforts could explicitly include soft data (e.g., local specific discharge estimates from well tests or elicitation) in the PEST calibration process.

When performing an uncertainty assessment on model results, which are solely dependent upon the parameter values supplied to the model, it is important to recognize two fundamental types of uncertainty in a model: null space and solution space uncertainties (see Appendix H). Null space uncertainty is that which arises in a calibrated model prediction due to the necessary simplifications made during model development (e.g., using a predefined HFM, applying constant BCs, representing heterogeneity with a homogenized geologic unit, single porosity significantly different predicted model metrics, like specific discharge). Thus, null space uncertainty is the uncertainty in the prediction from a calibrated model due to the inability of the calibrating data set to inform those parameters that contribute to the model output metric (in this case, prediction of specific discharge). Recent advances in uncertainty assessment facilitate quantification of the null space error despite the inability to reduce it (given a specified, calibrated model and data set).

6.7.1 Uncertainty in Specific Discharge

In previous flow and transport and abstraction models of the SZ, the specific discharge was varied from one-tenth of its nominal value to ten times its nominal value in performance assessment calculations (BSC 2001 [DIRS 157132], Section 6.2.5). Based on recent calibration experience and the evaluation of permeability data from Yucca Mountain and other sites, the range was reduced to 1/8.93 times its nominal value to 8.93 times the nominal value (SNL 2007 [DIRS 181650], Figure 6-2[a]). The nominal value is obtained from a predictive run of the calibrated SZ site-scale flow model (Section 6.5). It should be noted that because the numerical model is linear, the calibration of the model can be preserved by scaling the fluxes, recharge, and permeabilities by exactly the same ratio. A new uncertainty analysis procedure is available in recent releases of the PEST software. Although PEST V11.1 is not qualified, it is still extremely useful in analyzing and describing the results from qualified codes. A general introduction and discussion of the latest techniques in uncertainty and sensitivity analyses is presented in Appendices H and I.

The PEST V11.1 (STN: 611582-11.1-00; [DIRS 179480]) PREDVAR suite of codes (Doherty 2006 [DIRS 178613]) was used to analyze FEHM's predictive uncertainty for specific discharge. First, null space and solution space uncertainties are quantified. This analysis, if done a priori, can help to determine if calibrating the conceptual model to the existing dataset will significantly reduce uncertainty in the selected predictive model metric. The effect of calibrating each model parameter (or each set of parameters when considering the permeability multipliers for the altered northern region, which were lumped) in reducing uncertainty in specific discharge 5 km from the repository is presented in Figure 6-26. Red bars are normalized contributions to uncertainty (they have unit sum) in specific discharge from uncalibrated parameters and blue bars are the same contribution from calibrated parameters. This figure can be interpreted as the answer to the following question: Assuming perfect knowledge of a parameter, how do the rest contribute to reduction in uncertainty of a prediction? Specifically, the contribution of calibrating each parameter with respect to reducing uncertainty in specific discharge is illustrated. There is seemingly little value gained in reducing uncertainty in specific discharge across the 5-km boundary through the calibration process. The uncertainty for specific discharge decreased 56% after calibration. It is not surprising to see such a small reduction in predictive uncertainty for specific discharge because calibration data did not include an estimate for specific discharge. If a specific discharge measurement was explicitly included in the automatic calibration process, a greater reduction in uncertainty would be expected. In these figures, a parameter's "contribution" to uncertainty is assessed through repeating the predictive uncertainty analysis under an assumption of perfect knowledge of that parameter type and measuring the decrease in predictive error thereby incurred. That is, each parameter is sequentially assigned it calibrated value with zero error bars and the resulting impact on decreased uncertainty in a prediction is assessed. In some circumstances, post-calibration analysis of its potential worth to the calibration process. Figure 6-27 shows the relative worth of groups of observations for reducing specific discharge uncertainty. Not surprisingly, observation groups NYE COUNTY, CRATER FLAT, and FLUX are important observations for reducing predictive uncertainty in specific discharge. FLUX is important because it directly impacts overall flows through the model and should therefore be important to specific discharges throughout the model domain. Head observations in the altered northern region (HIGH HEAD), along the inferred flow path (PATH), and those considered perched (PERCHED) are of lesser importance in reducing uncertainty in specific discharge.



Source: Output DTN: SN0705T0510106.009.

NOTE: Observation groups are listed and defined in Table 6-9, "flux" are the boundary flux target observations and "spd" Is a hypothetical specific discharge observation that could be used in calibration.

Figure 6-27. Value of Observation Group to Reducing Uncertainty in Specific Discharge

6.7.2 Nonlinear Analysis

A methodology for nonlinear analysis of predictive error was applied to the Yucca Mountain model. Its theoretical basis is described in Appendix I. Applying the nonlinear analysis to the specific discharge prediction made by the SZ flow model yielded a maximum of 1.60 m/yr across the 5-km boundary (less than a factor of three times the maximum value of 0.66 m/yr). The nonlinear analysis is undertaken such that model calibration is maintained and only the null space is modified. By changing combinations of parameters that make no impact on the calibration objective function (weighted RMSE between modeled and measured head data and boundary fluxes), the specific discharge was maximized to a value of 1.60 m/yr (Output DTN: SN0705T0510106.009). This indicates that even a model maintaining calibration can have significant "wiggle room" in its predictions. Note also that this maximization process was undertaken with the specific intent of seeing just how high the specific discharge could go for a nominally calibrated model. The chances for the exact combination of (null space) parameters required to make this happen in real life is low and this maximized specific discharge therefore represents a reasonable upper bound for this calibrated model. Furthermore, visualization of the flow field arising from this combination of permeabilities yielded an unrealistic scenario where flow exited the eastern boundary of the model.

6.7.3 Discussion of the Effect of Hydrogeologic Contact Uncertainty on Specific Discharge

The HFM conceptual model for the SZ site-scale flow model was created from a variety of field data and exists in electronic form as Earthvision surfaces (SNL 2007 [DIRS 174109]). There is uncertainty in the spatial positions of these surfaces primarily due to lack of data. These surfaces were used to generate the finite-element mesh such that each element is assigned those hydrogeologic properties found at the center of the element as discussed in Section 6.4.3.1. There is interest in how uncertainties in the representation of hydrogeologic-unit horizontal locations affect flux or specific discharge calculations. Due to the coarseness of the finite-element mesh, some horizontal uncertainty in the HFM can be entertained. As long as the horizontal spatial ambiguity in the location of hydrogeologic contacts is less than 125 m (one-half the grid block dimension), there is essentially zero impact on model specific discharge or flux calculations.

Because flow leaving the repository area is confined to a few of the most permeable units, the vertical dimension deserves special consideration. From the SZ site-scale flow model, it is known that the fluid leaves the repository area through the Crater Flat Tuffs and migrates to alluvial units. The flow paths in areal and vertical views are reproduced in Figure 6-17. Note that the vertical thickness of the flowing zone varies between 25 and 400 m, and the elevation changes from 400 to 700 m above sea level. From Table 6-4, the spacing in this part of the finite element mesh varies from 10 to 50 m. Consider, for example, that the uncertainty in the vertical location of a geologic contact is 50 m in the portion of the model where the flow path is 400 m thick. Changing a single element's hydrogeologic designation, either to or from one unit to another could not result in a change to the average local specific discharge by more than a factor of 50/400 (13%). This is well within the overall specific discharge uncertainty range (Section 6.7.1). The vertically thin flow path south of UTM Northing coordinates 4,065,000 m (Figure 6-17) results in a greater impact from geologic uncertainty. Here the fluid flow is vertically constrained to about 25 m. If the bottom contact of the local hydrogeologic unit were to change by 10 m (the thickness of a single layer), this could result in a change to the average specific discharge in that area of up to 40%. Integrated specific discharge calculations will be affected to a lesser degree. A study of the impacts of hydrogeologic contact location uncertainty reveals:

- Sensitivity to uncertainty in the hydrogeologic contact surfaces in the horizontal directions is much less than in the vertical direction due to the averaging effect of 250-m grid block spacing

- The change in specific discharge due to the 50-m uncertainty in the vertical hydrogeologic surface can produce up to a 13% change in the local specific discharge near the repository and in the alluvial flow regions
- 10-m uncertainty in the vertical hydrogeologic surface can produce up to a 40% change in the local specific discharge in the transitional zone (south of UTM Northing 4,065,000 m).

Because of the averaging effect across elements in the integrated specific-discharge calculations (0 to 18 km), a 50% regional change in a relatively small portion of the 0- to 18-km compliance boundary affects model results only moderately. The range of uncertainty considered for specific discharge in the SZ flow and transport abstractions model is significantly greater than the uncertainty in the HFM (SNL 2007 [DIRS 174109], Section 6.4.3).

6.7.4 Site Data

In the 18-km compliance region (green line on Figure 6-17), performance assessment calculations are also strongly influenced by travel of fluid in the alluvial aquifer. Estimates of groundwater specific discharge in the SZ have been obtained from field-testing at the ATC (SNL 2007 [DIRS 177394], Section 6.4.5). The ATC is approximately located at the boundary of the accessible environment, as specified in regulations for the Yucca Mountain Project, 10 CFR 63.302 [DIRS 176544]. The location of the ATC is approximately 18 km from Yucca Mountain, and testing was performed in the alluvium aquifer. Estimates of groundwater specific discharge at the ATC range from 0.47 to 5.4 m/yr (DTN: LA0303PR831231.002 [DIRS 163561]; SNL 2007 [DIRS 177394], Table 6.5-6). From the calibrated SZ site-scale flow model, the specific discharge to the 18-km compliance boundary is 0.55 m/yr. This calculation integrates transport through all volcanic and alluvial units from introduction below the repository to the 18-km compliance boundary and its relatively low value can partially be attributed to slow flows through the volcanic units.

In addition to the information from the Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353]) (related to specific discharge in the volcanics), other data are available for specific discharge in the alluvium (SNL 2007 [DIRS 177394], Tables 6.5-5 and 6.5-6). The measured specific discharge at the ATC spans a factor of 7.8 (i.e., 1.2 to 9.4 m/yr) while at NC-EWDP-22S the range was 11.5 (0.47 to 5.4 m/yr). There are no site data available for specific discharge in volcanic units, but the Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353], p. 3-43) typically suggested larger ranges (approximately two orders of magnitude or more). A factor of 1/8.93 to 8.93 times the nominal value that combines volcanic and alluvial uncertainties with Bayesian updating is used as a multiplier for the specific discharge throughout the model domain in the latest performance assessment calculations (SNL 2007 [DIRS 181650], Figure 6-2[a]). It is worth noting that the specific discharge is variable along any given flowpath and that it can either increase or decrease locally due to flow focusing, hence significant variability and uncertainty is expected locally, but these fluctuations are smoothed when averaged over kilometer-scale portions of the model domain. For example, across the 100 flow paths in the calibrated model, the range of specific discharges spans approximately an order of magnitude across both the 5- and 18-km boundaries. Nevertheless, the overarching criterion that the range in uncertainty of specific discharge encapsulate uncertainty within the domain (with minimal overestimation) is met by TSPA. Historical details of the specific discharge multiplier distribution and associated sampling techniques, including figures, are contained in *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650], Figure 6-2[a]) and no differentiation is made between specific discharge in the volcanics or alluvium.

6.7.5 Remaining Uncertainties in Specific Discharge Estimates

The analyses and corresponding assignment of an uncertainty range for the groundwater specific discharge assume that the porous continuum approach is appropriate for the fractured volcanic tuffs. A remaining uncertainty is whether or not the continuum approach can be employed at the scale of the model. An alternative conceptual model not yet explicitly examined is one in which most of the flow from Yucca Mountain moves through faults rather than through the unfaulted rock. To test this alternative model, the known faults need to be included explicitly in the numerical grid of the SZ site-scale flow and transport models. Although the grid-generation and flow-calculation capabilities exist to do this, the need to calibrate the model efficiently and perform particle-tracking transport simulations has taken priority and led to the adoption of structured grids that make explicit inclusion of faults difficult. Important faults are included in the model to capture their impact on flow and transport. Furthermore, the adoption of a range that includes larger specific discharge values and smaller effective porosities introduces realizations that replicate the behavior of a fault-dominated flow and transport system. Therefore, the suite of performance assessment transport simulations currently used likely encompasses the range of behavior that would be obtained with a fault-based flow and transport model.

Finally, it is noted that model linearity assures that a global, constant-multiplier increase in permeability and corresponding increase in infiltration will yield an equal increase in specific discharge throughout the model domain without impacting the head RMSE. Although the net infiltration was defined by specified data sets (Belcher 2004 [DIRS 173179]; BSC 2004 [DIRS 169861]; Savard 1998 [DIRS 102213]), model permeabilities could be globally adjusted such that flux through the southern boundary increased to match that of the regional model (discussed in Section 6.5.2.2). The resulting 23% increase in specific discharge throughout the model domain is still within the uncertainty range of the entire SZ site-scale flow model and well within the specific discharge multiplier used in TSPA (SNL 2007 [DIRS 181650]); also see Sections 6.7.1, 6.7.4, 7.2.3, and 8.3.1 of this document).

6.7.6 Effect of Perched Water on Flow Paths and Specific Discharge

Perched water was not explicitly modeled in the SZ site-scale flow model because the weights applied to these observations were insignificant (0.1). It is noted that the conceptualization of the LHG through introduction of the altered northern region yielded water levels in wells UE-25 WT#6 and USW G-2 (suspected to be perched) that were much lower than the reported water levels. From Table 6-8, it can be seen that some modeled water levels are about 150 m lower than the data in this area to the north of Yucca Mountain; but this is consistent with the perched water-level interpretation in that area (BSC 2004 [DIRS 170009], Section 5). The area of suspected perched water is near the steepest hydraulic gradient in the model and these hydraulic gradients occur over only a few model elements. Thus, if there is some specific reason

7.1.3 Confidence Building After Model Development to Support the Scientific Basis of the Model

Model validation requires that mathematical models be validated by one or more of several methods given in Section 6.3.2 (1st and 9th bullets) of SCI-PRO-006. Validation of the SZ site-scale flow model as related to the procedural requirements mandates the following:

1. SCI-PRO-006, Section 6.3.2 (1st bullet): Corroboration of model results with the laboratory, field experiments, analog studies, or other relevant observations, not previously used to develop or calibrate the model.

   The SZ site-scale flow model was validated by comparing results from this model with the laboratory and field experiment and other observations. The validation criteria, testing, and results are described in detail in Section 7.2 of this report. Based on material presented in these sections, this criterion is considered satisfied.

2. SCI-PRO-006, Section 6.3.2 (9th bullet): Technical review through publication in a refereed professional journal. Although this is not required by the TWP, this post-development model validation activity adds to the confidence in the SZ site-scale flow model.

   A previous version of the SZ site-scale flow model and its results are described in the referenced professional publications by Eddebbarh et al. (2003 [DIRS 163577]) and Zyvoloski et al. (2003 [DIRS 163341]). These publications demonstrate additional confidence in the model, when taken in conjunction with the model validation activity described in Item 1 above because the same modeling techniques were used in this report. Moreover, this revision is based on an improved and updated HFM with more accurate fault locations, more than four times as many grid nodes, and a calibration that yielded a lower residual (weighted RMSE).

7.2 VALIDATION RESULTS

The validation activities for the SZ site-scale flow model are carried out according to *Technical Work Plan for Saturated Zone Flow and Transport Modeling* (SNL 2007 [DIRS 177375], Section 2.2), which requires Level II model validation of the SZ site-scale flow model based on its relative importance to the performance assessment for the repository. The TWP states that the validation will include confidence building activities implemented during model development. In addition, it states that post-development model validation will consist of a comparison of simulated flowpaths to those derived from hydrochemistry and isotope analyses, plus two or more other comparisons as indicated in the technical work plan.

Water levels and gradients. For purposes of postdevelopment model validation, a comparison of simulated and observed water levels for all new water-level data is presented in Section 7.2.1. This comparison focuses on the NC-EWDP Phase V water-level data (DTN: MO0612NYE07122.370 [DIRS 179337]). A comparison of simulated and observed gradients along the flowpath from the repository is also presented to evaluate the impact of the difference between observed and simulated water levels on the estimates of specific discharge. Specific discharge is directly proportional to the hydraulic gradient. As previously established in

To further validate the SZ site-scale flow model, a comparison was made of the hydraulic gradients along the flowpath using water-level data from two wells that were not used during calibration (NC-EWDP-22PC and -32P). Table 7-3 presents gradients calculated for postdevelopment model validation. Predicted gradients are about a factor of two lower than observed because the model does not capture the rapid water level change near U.S. Highway 95 fault. However, this region is south of the region of primary interest and, as discussed in Section 7.1.3, the model reproduces observed gradients over the relevant portion of the flowpath from the repository through Fortymile Wash to U.S. Highway 95 quite well. The validation is considered successful because the simulated hydraulic gradient agrees to within 50% with gradient calculations from data.

Table 7-3. Predicted and Observed Hydraulic Gradients for Post-Development Validation

Flow Segment	$\Delta H/\Delta L$ (Measured)	$\Delta H/\Delta L$ (Simulated)	Relative Error
NC-EWDP-24PB to NC-EWDP-32P	3.22×10^{-3}	1.81×10^{-3}	−0.44
NC-EWDP-22PC to NC-EWDP-32P	2.49×10^{-3}	1.39×10^{-3}	−0.44

Sources: DTNs: GS010908312332.002 [DIRS 163555] (non-NC-EWDP wells); SN0612T0510106.004 (modeled heads).

Output DTN: SN0702T0510106.007 (NC-EWDP aggregated Phase III, IV, and V well data).

NOTE: Calculations are from data in Table 7-2.

7.2.2 Comparison of Calibrated Effective Permeabilities to Field Test Results

The numerical model was calibrated by adjusting permeability values for individual hydrogeologic units in the model until the sum of the weighted residuals squared (the objective function) was minimized. The residuals include the differences between the measured and simulated hydraulic heads and the differences between the groundwater fluxes simulated with the SZ regional- and the site-scale models. Permeabilities estimated from hydraulic tests were neither formally included in the calibration nor considered in the calculation of the objective function. The field-derived permeabilities were instead used to check on the reasonableness of the final permeability estimates produced by the calibration.

Discussions of the permeability data from the Yucca Mountain area and nearby NTS as well as the Apache Leap site in Arizona are presented in the following subsections. A discussion of the general inferences about permeability that can be drawn from regional observations is also presented. Following these discussions, a comparison of calibrated effective permeabilities with the 95% confidence interval on the mean of measured permeability values is presented, including the analysis of the potential impact of calibrated permeability values on groundwater specific discharge.

7.2.2.1 General Permeability Data

Many factors affect the permeability of volcanic rocks at Yucca Mountain including: (1) the tendency of the rock either to fracture or to deform plastically in response to stress; (2) the ability of the rock to maintain open fractures, which is a function of the strength of the rock and overburden stress; (3) proximity to major zones of deformation, such as fault zones; and, (4) the degree of mineralization or alteration that would tend to seal fractures and faults. Other factors

(Patterson 1999 [DIRS 158824]) indicates that the formation generally has low permeability compared to the rate of water infiltrating into the unsaturated zone, which has been estimated to range between 1.5 and 48.2 mm/yr in the vicinity of the repository under the present climate (SNL 2007 [DIRS 174294], Table 6.5.7.1-2). Water flowing under a unit gradient at a rate of 10 mm/yr (3.17×10^{-10} m/s) would seep through a rock having a permeability of $0.0000323 \times 10^{-12}$ m^2 (assuming a viscosity of 0.001 N-s/m^2 and a water density of 1,000 kg/m^3); so the field-scale vertical permeability of the Calico Hills Formation, which includes the effects of fracturing, presumably has permeabilities less than this value. Based on core measurements, the geometric-mean hydraulic conductivity for the zeolitic Calico Hills Formation is 2.2×10^{-11} m/s (DTN: MO0605SPAFABRP.004 [DIRS 180539], file: *Analysis of source data.zip*), which is significantly higher than the low permeability ($0.0000323 \times 10^{-12}$ m^2) thought necessary for perched water. The calibrated effective permeability for the Calico Hills Volcanic unit was 0.46×10^{-12} m^2, which is on par with results from cross-hole testing.

7.2.2.1.2 Alluvial Testing Complex

From July through November 2000, pumping tests were conducted in well NC-EWDP-19D. The first test involved production from the entire saturated thickness of 136 m. The results indicated a transmissivity of about 21 m^2/day and an average hydraulic conductivity of 0.15 m/day, approximately equivalent to a permeability of 0.2×10^{-12} m^2 (SNL 2007 [DIRS 177394], Section 6.4.5 and Appendix F7). Subsequently, four screened intervals having a combined thickness of 84 m were tested individually. The combined transmissivities of these intervals totaled about 145 m^2/day, greatly exceeding the transmissivity determined for the initial open-hole test. There are at least two likely causes for the discrepancy. First, pumping apparently resulted in further well development, as fine materials were drawn into the well and discharged with the water. Second, the screened intervals are probably interconnected hydraulically, consistent with the complexity of fluvial-alluvial depositional environments, so that actual thicknesses of the producing zones were significantly greater than the screened intervals. The average permeability of the section is probably greater than the initial permeability determined from the open-hole test (0.2×10^{-12} m^2) but less than those calculated for the two deeper screened intervals, 1.5×10^{-12} and 3.3×10^{-12} m^2. Although thin, discontinuous zones may locally have higher permeabilities, these results indicate that significantly thick (greater than 10 m) and areally extensive zones at NC-EWDP-19D probably have average permeabilities between 0.1×10^{-12} and 1×10^{-12} m^2 (SNL 2007 [DIRS 177394], Sections 6.4.5 and Appendix F7).

7.2.2.1.3 Apache Leap

Fractured welded tuffs and relatively unfractured nonwelded tuffs occur both above and below the water table. Permeabilities measured in the unsaturated zone at Yucca Mountain using air may, therefore, have some relevance to the permeability values of similar rocks located below the water table. In the unsaturated zone, air-injection tests have been conducted from surface-based boreholes in both welded and nonwelded tuffs (LeCain 1997 [DIRS 100153]) and from test alcoves in and adjacent to the Ghost Dance Fault zone in the densely welded Topopah Spring tuff (LeCain et al. 2000 [DIRS 144612]). At Yucca Mountain, no water-injection tests were done in these same intervals to directly compare to the results of the air-injection tests. However, some understanding of the probable relation between permeabilities estimated from account for heterogeneity and departures of the actual flow field from the assumed flow geometry.

7.2.2.1.4 Tuffaceous Formations

The Prow Pass, Bullfrog, and Tram tuffs of the Crater Flat group contain both nonwelded to partially welded margins and partially to densely welded interiors (Bish and Chipera 1989 [DIRS 101195]; Loeven 1993 [DIRS 101258]). The initially vitric nonwelded to partially welded margins of these units have been largely altered to zeolites during hydrothermal events as a result of their thermodynamically unstable glass composition and their initially high permeabilities (Broxton et al. 1987 [DIRS 102004]). The partially to densely welded parts of these units have devitrified to mostly quartz and feldspar and have higher matrix permeabilities than the nonwelded to partially welded zeolitized margins (Loeven 1993 [DIRS 101258]). Additionally, because the welded parts of the tuffs have a greater tendency to fracture, the densely welded parts of these units generally have higher secondary permeability. Thus, unless faults are locally present, the densely welded parts of the Prow Pass, Bullfrog, and Tram tuffs are expected to have substantially higher permeability than the nonwelded margins.

The densely welded parts of the Prow Pass, Bullfrog, and Tram tuffs are likely to have mean permeabilities that are less than the mean air permeabilities of the Tiva Canyon ($k = 4.7 \times 10^{-12}$ m^2) or Topopah Spring ($k = 0.75 \times 10^{-12}$ m^2) tuffs estimated from air-permeability tests (see Section 7.2.2.1.3). This likelihood is because greater lithostatic stresses at depth tend to close fractures and successive hydrothermal events have caused increasing degrees of alteration with depth (Broxton et al. 1987 [DIRS 102004]). Figure 7-3 shows the geometric-mean permeabilities from the single-hole air-permeability tests for the Tiva Canyon and Topopah Spring tuffs and the geometric-mean single-hole water permeabilities calculated for the Calico Hills Formation and the Prow Pass, Bullfrog, Tram, and Lithic Ridge tuffs. The single-hole permeabilities show the expected trends of decreasing permeability with depth. Conversely, the trends in the cross-hole permeability data from the C-wells (see Section 7.2.2.3.2 and Section 7.2.2.6, Figure 7-4) are exactly opposite those expected based on geologic reasoning; these trends could, however, reflect the proximity of each hydrogeologic unit to the Midway Valley fault, which intersects the C-wells in the upper part of the Tram tuff (Geldon et al. 1998 [DIRS 129721], Figure 3). Thus, it appears that permeability trends with depth at the C-wells are controlled by local conditions and do not reflect general trends in permeability established by the single-hole tests and expected from geologic reasoning.

permeability, the Lower Carbonate Aquifer remained the primary water bearing unit in the model.

Overall, the calibrated effective permeabilities show trends consistent with permeability data from Yucca Mountain and elsewhere at the NTS. The calibrated effective permeability of the three Crater Flat tuffs and Calico Hills formation are all within the values measured in the field. The relatively high permeability estimated for the Tram tuff from the cross-hole tests may be at least partially attributable to local conditions at the site of these tests. A breccia zone is present in the Tram tuff at boreholes UE-25 c#2 and UE-25 c#3 (Geldon et al. 1997 [DIRS 100397], Figure 3) that may have contributed to a local enhancement in the permeability of the Tram tuff.

Calibrated effective permeabilities for units corresponding to the Lava Flow Aquifer and the valley fill aquifer are within the range of measured permeabilities. The calibrated effective permeabilities of units corresponding to the Welded Tuff Aquifer are more than an order of magnitude lower than field estimates, but no confidence intervals are available and calibrated values would probably fall within these limits if they were available.

7.2.3 Specific Discharge

Although the calibrated permeabilities of any geologic unit or feature in the SZ site-scale flow model indirectly influence the simulated specific discharge, those geologic units along the flowpath from the repository to the compliance boundary directly determine the simulated specific discharge. Particle tracking using the SZ site-scale model (see Section 6.5.2.4) indicates that fluid particles migrating from the repository generally enter the SZ in the Crater Flat units (see Figure 6-22). Because of the high permeabilities of these units and the small hydraulic gradient, the particles remain in those units until reaching their southern ends. At this point, flow generally enters the alluvial portion of the flow system after briefly transitioning through the Paintbrush Volcanic Aquifer. The flowpath through the alluvial deposits is represented in the SZ site-scale model by the Lower Fortymile Wash alluvium. Thus, those calibrated permeabilities that most directly control the simulation of specific discharge by the SZ site-scale model are those for the Crater Flat units and the Lower Fortymile Wash alluvia.

Specific discharge across the 18-km compliance boundary (see the green line on Figure 6-17) and discussed throughout other documents (SNL 2007 [DIRS 177392]) is strongly influenced by groundwater flow in alluvium. Estimates of specific discharge in the SZ were recently obtained from field-testing at the ATC (SNL 2007 [DIRS 177394], Section 6.5.5). The ATC is located approximately 18 km from Yucca Mountain at the boundary of the accessible environment as specified at 10 CFR 63.302 [DIRS 176544]. The specific discharge from the repository to the 18-km compliance boundary was 0.55 m/yr (average across all flowpath lengths divided by travel times), although much of the time along this flowpath is spent in the slower flowing volcanic units indicating that the specific discharge in the alluvial material is higher than in the volcanics. The technique used to estimate specific discharge at locations within the SZ site-scale flow model corresponding to the locations where measurements are available (UE-25 c#3, NC-EWDP-22S, and NC-EWDP-19P) was to isolate a cubic volume within 1,000 m of the well location extended to 10 m above and below the entire open interval and to calculate the average specific discharge across all flowing nodes. The ATC testing was performed in the alluvium aquifer and estimates of groundwater specific discharge at the ATC range from 0.5 to 12 m/yr.

The simulated average specific discharge across the 5-km boundary ranges from 0.35 to 0.38 m/yr for differing values of horizontal anisotropy in permeability ranging from 20 to 0.05 (0.36 m/yr for the expected horizontal anisotropy values of 5:1 N-S to E-W with end members of the 100-particle distribution of 0.11 to 0.66 m/yr). This compares to the 0.6 m/yr derived by the Expert Elicitation Panel (CRWMS M&O 1998 [DIRS 100353], Section 3.2) and is also within their range, which actually spans nearly five orders of magnitude. The data from ATC field testing yielded specific discharge estimates ranging from 1.2 to 9.4 m/yr while testing at NC-EWDP-22S ranged from 0.47 to 5.4 m/yr. A distribution of specific discharge multipliers was developed (SNL 2007 [DIRS 181650], Figure 6-7) that ranged from 1/30th to 10 times the nominal value. Recently, that range was reduced to 1/8.93 and 8.93 times nominal specific discharge (SNL 2007 [DIRS 181650], Figure 6-2[a]). In addition to a distribution in specific discharge, uncertainty in effective porosity (variable effective porosity in conjunction with specific discharge can result in highly variable flow velocities through the SZ) is implemented through the use of a truncated normal distribution in the SZ transport abstraction model (SNL 2007 [DIRS 181650], Section 6.5.2.3). The details of the uncertainty distributions of specific discharge multiplier and effective porosity in the alluvium and their associated sampling techniques are contained in the SZ flow and transport abstraction model (SNL 2007 [DIRS 181650], Table 6-7[a]).

7.2.4 Comparison of Hydrochemical Data Trends with Calculated Particle Pathways

Groundwater flowpaths and mixing zones were identified in Appendices A and B in the analyses of the areal distributions of measured and calculated geochemical and isotopic parameters, scatter plots, and inverse mixing and reaction models Flowpaths of tracer particles were calculated with the SZ site-scale flow model. The particles were started below the repository footprint and allowed to transport downstream to the model boundary. These flow pathways are compared to flowpaths deduced from hydrochemical data shown in Figure 7-5. These flowpaths must be evaluated in the context of the hydraulic gradient while considering the possibility that flowpaths can be oblique to the potentiometric gradient because of anisotropy in permeability. These flowpaths were drawn by first using chemical and isotopic constituents generally considered to behave conservatively in groundwater such as chloride (Cl^-) and sulfate (SO_4^{2-}) ions. However, because no single chemical or isotopic species varies sufficiently to determine flowpaths everywhere in the study area, multiple lines of evidence were used to construct the flowpaths. This evidence includes the areal distribution of chemical and isotopic species, sources of recharge, groundwater ages and evaluation of mixing/groundwater evolution through scatter plots, and inverse mixing and reaction models as presented in Appendices A and B. The derivation of flow pathways from hydrochemical data is developed in detail in Appendices A and B and summarized in Sections B6.6 and B7.

Of particular interest are the Flow Paths 2 and 7 from this analysis. As shown in Figure 7-5, Flow Path 7 originates in the vicinity of the repository footprint and overlaps the model-calculated flowpaths. Flow Path 2 is also of interest, although it originates northeast of the repository, because it closely bounds Flow Path 7 to the east. Although flow pathways derived from hydrochemical data do not originate in the same location as particle tracks derived from the site-scale model, the paths converge east and south of the repository.

Table 8-1. Output Data

DTN	Intermediary?	Description
LA0612RR150304.001	Yes	NC-EWDP UTM coordinates
LA0612RR150304.002	Yes	Underground Testing Area geochemical data
LA0612RR150304.003	Yes	NC-EWDP geochemical data
LA0612RR150304.004	Yes	Hydrochemical flowpaths
LA0612RR150304.005	Yes	Uranium activity ratios for groundwaters
LA0612TM831231.001	No	LaGriT HFM2006 surfaces
MO0611SCALEFLW.000	No	Potentiometric surface
SN0610T0510106.001	Yes	NC-EWDP well location and water-level data
SN0612T0510106.003	Yes	Infiltration data
SN0612T0510106.004	No	SZ site-scale flow model output
SN0702T0510106.006	No	FEHM model of water table rise
SN0702T0510106.007	Yes	NC-EWDP well data used for SZ flow model potentiometric surface, calibration and validation
SN0704T0510106.008	No	Water-level and particle-track output from the calibrated model
SN0705T0510106.009	Yes	PEST v11.1 analyses

8.3 OUTPUT UNCERTAINTY

This section describes remaining uncertainties associated with the nominal flow field. Specifically, the section recommends how the uncertainty in metrics associated with model outputs (specific discharge and flowpaths) should be considered.

8.3.1 Specific Discharge Uncertainty Range

Because uncertainty in permeability translates into uncertainty in specific discharge (given a constant head gradient), insight gained when investigating permeability values during calibration has relevance to specific discharge estimates. Also, recall that for linear models such as this, calibration to hydraulic heads is preserved when scaling the fluxes, recharge, and permeabilities proportionally. The 95% confidence interval for calibrated permeabilities (Output DTN: SN0612T0510106.004, *sz_site_2006.rec*) typically spans 3 or more orders of magnitude. While this range could yield major changes in specific discharge in a homogeneous system, no single change in permeability by up to an order of magnitude yielded even a factor of 2 change in specific discharge because surrounding permeability values strongly impact the flow into/out of the altered unit. It can be concluded that even if calibrated permeabilities are in error by more than an order of magnitude for any given unit, the specific discharge output from the model will remain within the uncertainty limits developed elsewhere for use in TSPA (e.g., 1/8.93 to 8.93 times nominal value (SNL 2007 [DIRS 181650], Figure 6-2[a])). Experience with the calibrated SZ site-scale flow model indicates that the range of specific discharges used for TSPA is large enough to encapsulate all the uncertainties assumed during the development and calibration of this model.

The specific discharge from the repository to the 18-km compliance boundary is 0.55 m/yr, although much of the distance along this flowpath is in the slower flowing volcanic units indicating that the specific discharge in the alluvial material is higher than in the volcanics. The technique used to estimate specific discharge at locations within the SZ site-scale flow model alluvial material corresponding to the locations where measurements are available (NC-EWDP-22S, and NC-EWDP-19P) was to isolate a cubic volume within 1,000 m of the well location extending 10 m above and below the entire open interval and to calculate the average specific discharge across all flowing nodes. Measured groundwater specific discharges from alluvial pump tests range from 0.47 to 9.4 m/yr (SNL 2007 [DIRS 177394], Tables 6.5-5 and 6.5-6). For the expected flow porosity in the alluvium of 0.18 (SNL 2007 [DIRS 177394], Section 6.4), the field-test-derived specific discharges ranged from 0.89 m/yr at NC-EWDP-22S to 7.3 m/yr at NC-EWDP-19P. Model-simulated specific discharges at NC-EWDP-22S and -19P are 20.97 and 11.75 m/yr, respectively. These relatively high modeled values correspond to the high effective permeability assigned to the model unit for the Lower Fortymile Wash alluvium, but they are still within the factor of 3 of the upper end of test-derived expected value (7.3 m/yr) and therefore meet the validation criterion established by the TWP (BSC 2006 [DIRS 177375, Section 2.2.2.1). Comparatively little sensitivity was seen to horizontal anisotropy in the volcanics; the modeled average specific discharge across the 5-km boundary ranges from 0.35 to 0.38 m/yr for values of N-S to E-W horizontal anisotropy in permeability of 0.05 to 20, respectively (SNL 2007 [DIRS 177394], Section 6.2.6). Although there were no specific discharge measurements from the C-wells tests, the modeled value was estimated at 1.75 m/yr within 1,000 m of the C-wells. Finally, the nonlinear maximum calibrated specific discharge estimated across the 5-km boundary downgradient from the repository is 1.60 m/yr (Section 6.7.2 and Appendix I), which is just less than 3 times the maximum value of 0.66 m/yr. This combination of permeabilities was specifically selected to maximize specific discharge, which is still well within the range established by the specific discharge multiplier used in SZ abstraction models. That is, an uncertainty distribution in specific discharge is constructed where the nominal specific discharge is multiplied by 1/8.93 and 8.93 (SNL 2007 [DIRS 181650], Figure 6-2[a]). The details of the uncertainty distributions of specific discharge and effective porosity in the alluvium and their associated sampling techniques are outlined in the SZ abstraction model (SNL 2007 [DIRS 181650], Table 6-7[a]).

8.3.2 Flowpaths Uncertainty

The flowpaths from the water table beneath the repository to the accessible environment directly affect breakthrough curves and associated radionuclide transport times (recall that flowpath length is used to calculate specific discharge). Because the flowpaths are close to the water table and transition from the volcanic tuffs to the alluvium, flowpath uncertainty directly affects the length of flow in the volcanic tuffs and in the alluvium.

Uncertainty in flowpaths is affected by anisotropy in hydraulic properties of the volcanic tuffs. Large-scale anisotropy and heterogeneity were implemented in the SZ site-scale flow model through direct incorporation of known hydraulic features, faults, and fractures (see Section 6.7.10). Horizontal anisotropy in the volcanic units was derived from analysis of hydraulic testing at the C-wells (SNL 2007 [DIRS 177394], Section 6.2.6 and Appendix C6). This scientific analysis report also recommends an uncertainty range in anisotropy that should be used in the SZ site-scale flow model to account for uncertainty in the flowpaths and this parameter was carried forward through to SZ abstraction modeling (SNL 2007 [DIRS 181650], Figure 6-2[a]). For isotropic permeability, average flowpath length to the 18-km compliance boundary is approximately 22.9 km. For anisotropy ratios of 20:1 and 0.05:1 (N-S:E-W), average flowpath lengths are 29.7 and 22.8 km, respectively. This is an acceptable range of variability in model results in light of the bounds established by geochemical analyses (Figure 7-5). Also, recall that 5 km of this difference can be attributed solely to the random initial distribution of particles below the repository.

The model is adequate for its intended use of providing flow-field simulations as input to the SZ site-scale transport model necessary to generate radionuclide breakthrough curves.

8.4 HOW THE APPLICABLE ACCEPTANCE CRITERIA ARE ADDRESSED

This section describes how the acceptance criteria in the YMRP (NRC 2003 [DIRS 163274], Section 2.2.1.3.8.3), *Flowpaths in the Saturated Zone*, are addressed by this report.

Acceptance Criteria from Section 2.2.1.3.8.3, *Flowpaths in the Saturated Zone*

Acceptance Criterion 1: *System Description and Model Integration Are Adequate.*

Subcriterion (1): Section 1 explains that this model generates SZ velocity fields which are used as inputs for the model of transport in the SZ and are abstracted in the TSPA. The important physical phenomena are adequately incorporated in the SZ abstraction process as described in the following subsections: hydraulic gradients (Section 6.3.1.4); vertical gradients (Section 6.3.1.5); lateral boundary conditions (Section 6.3.1.6); recharge (Section 6.3.1.7); discharge (Section 6.3.1.8); heterogeneity (Section 6.3.1.9); faults (Section 6.3.1.10); and groundwater flow processes (Section 6.3.2.). The discussion of groundwater table rise in Section 6.6.4 uses consistent and appropriate assumptions about climate change.

Subcriterion (2): Aspects of hydrology, geology and geochemistry that may affect flowpaths in the SZ are described adequately in Section 6.3 and Appendices A and B.

Subcriterion (4): Section 6.3.1.7 states that the recharge to the flow model was derived from three sources: regional-scale SZ model (Belcher 2004 [DIRS 173179]), 2003 UZ flow model (BSC 2004 [DIRS 169861]), and Fortymile Wash data (Savard 1998 [DIRS 102213]). Recharge from the UZ site-scale model (percolation flux) was taken as the flow through the base of that model, the domain of which includes approximately 40 km^2 (19.3 mi^2) that encompasses an area only slightly larger than the footprint of Yucca Mountain, a small fraction of the SZ model domain. The SZ site-scale flow model uses appropriate recharge values from flow in the unsaturated zone.

Subcriterion (5): Section 6.2 provides a road map to sections and FEPs document where sufficient data and technical bases to assess the degree to which FEPs have been included in the flowpaths.

Uncertainty in the quantification of specific discharge is discussed in Sections 6.7 and Appendix H. A nonlinear analysis is presented in Section 6.7.2 and Appendix I. There is general consistency between the specific discharge simulated by the model and the median of values of uncertainty ranges estimated by the SZ expert panel from testing data. Uncertainty in specific discharge is propagated forward to the TSPA.

Uncertainty in the hydrogeologic contacts is discussed in Section 6.7.3 and shown to have moderate effects in some cases. Accordingly, this uncertainty was determined not to warrant propagation to the TSPA. Additional uncertainties due to limitation in site data, conceptualization of the LHG, and representation of potentially perched water-level measurements, and fault conceptualizations are discussed in Sections 6.7.4 through 6.7.8. None of these uncertainties warrants propagation to TSPA.

Uncertainty due to scaling is discussed in Section 6.7.9 where it is concluded that such uncertainty does not significantly affect flow modeling.

Subcriterion (3): The conceptual model uncertainty considered in this report is consistent with available site characterization data and field measurements. The genesis of the conceptual model is discussed in Section 6.3. Alternative conceptual models are considered in Section 6.6. A thorough description of uncertainty, especially uncertainty associated with specific discharge estimates, is given in Section 6.7. Furthermore, an introduction on predictive variance uncertainty minimization and quantification is given in Appendix H. An extension of this theory to nonlinear predictive variance is outlined in Appendix I.

Subcriterion (4): Alternative modeling approaches are appropriate and consistent with available data and current scientific knowledge, and appropriately consider their results and limitations, using analyses that are sensitive to the processes modeled, as discussed above.

Acceptance Criteria from Section 2.2.1.1.3, *System Description and Demonstration of Multiple Barriers*

Acceptance Criterion 3: *Technical Basis for Barrier Capability is Adequately Presented.*

When considered together, reports associated with the saturated zone including this report, *Site-Scale Saturated Zone Transport* (SNL 2007 [DIRS 177392]), and *Saturated Zone Flow and Transport Model Abstraction* (SNL 2007 [DIRS 181650]) constitute an adequate description (including thorough discussions of uncertainty) of the saturated zone as a natural barrier to radionuclide release.

9. INPUTS AND REFERENCES

The following is a list of the references cited in this document. Column 1 contains the unique six-digit numerical identifiers (the Document Input Reference System numbers), which are placed in the text following the reference callout (e.g., Ahlers et al. 1999 [DIRS 109715]). The purpose of these numbers is to assist in locating a specific reference. Multiple sources by the same author (e.g., SNL 2007) are sorted alphabetically by title.

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172396 GS040208312322.003. Uranium Concentrations and 234U/238U Ratios from Spring, Well, Runoff, and Rain Waters Collected from the Nevada Test Site and Death Valley Vicinities and Analyzed between 01/15/98 and 08/15/98. Submittal date: 04/01/2004.

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180317 LA0202EK831231.004. Calculation of the Maximum Possible Percentage of 1000 Year-Old Water Present in Selected Yucca Mountain Area Groundwater Samples. Submittal date: 02/25/2002.

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163788 LA0304TM831231.002. SZ Site-Scale Flow Model, FEHM Files for Base Case. Submittal date: 04/14/2003.

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151492 MO0007GNDWTRIS.002. Isotopic Content of Groundwater from Yucca Mountain Project Borehole, USW G-2, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151493 MO0007GNDWTRIS.003. Isotopic Content of Groundwater from Yucca Mountain Project Boreholes UZ-14, WT-17, and WT #3, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151494 MO0007GNDWTRIS.004. Isotopic Content of Groundwater from Borehole TW-5 Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151495 MO0007GNDWTRIS.005. Isotopic Content of Groundwater from Yucca Mountain Project Borehole JF #3, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151496 MO0007GNDWTRIS.006. Isotopic Content of Groundwater from Selected Yucca Mountain Project WT Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151497 MO0007GNDWTRIS.007. Isotopic Content of Groundwater from Yucca Mountain Project Boreholes WT #14, WT #15, and WT #12, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151508 MO0007GNDWTRIS.008. Isotopic Content of Groundwater from Yucca Mountain Project Borehole UE-25 P #1 Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151509 MO0007GNDWTRIS.009. Isotopic Content of Groundwater from Selected Yucca Mountain Project Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151500 MO0007GNDWTRIS.010. Isotopic Content of Groundwater from Selected Yucca Mountain Project Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151501 MO0007GNDWTRIS.011. Isotopic Content of Groundwater from Selected Boreholes Not Drilled for the Yucca Mountain Project Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151504 MO0007GNDWTRIS.013. Isotopic Content of Perched Groundwater from Yucca Mountain Project Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151507 MO0007MAJIONPH.002. Major Ion Content of Groundwater from Borehole TW-5 Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151513 MO0007MAJIONPH.003. Major Ion Content of Groundwater from Yucca Mountain Project Borehole USW G-2, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151516 MO0007MAJIONPH.004. Major Ion Content of Groundwater from Borehole ONC #1, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151517 MO0007MAJIONPH.005. Major Ion Content of Groundwater from Boreholes UZ-14, WT-17 and WT #3, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151518 MO0007MAJIONPH.006. Major Ion Content of Groundwater from Selected Boreholes Not Drilled on the Yucca Mountain Project, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/25/2000.

151519 MO0007MAJIONPH.007. Major Ion Content of Groundwater from Yucca Mountain Project Borehole UE-25 UZ #16, Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151521 MO0007MAJIONPH.008. Major Ion Content of Groundwater from Selected YMP and Other Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151522 MO0007MAJIONPH.009. Major Ion Content of Groundwater from Borehole NDOT Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151523 MO0007MAJIONPH.010. Major Ion Content of Groundwater from Borehole UE-25 P #1 Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151524 MO0007MAJIONPH.011. Major Ion Content of Groundwater from Selected Yucca Mountain Project Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151529 MO0007MAJIONPH.012. Major Ion Content of Groundwater from Selected YMP and Other Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151530 MO0007MAJIONPH.013. Major Ion Content of Groundwater from Selected YMP and Other Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151531 MO0007MAJIONPH.014. Major Ion Content of Groundwater from Selected Boreholes Not Drilled on the Yucca Mountain Project Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151532 MO0007MAJIONPH.015. Major Ion Content of Groundwater from NC-EWDP Boreholes Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/27/2000.

151533 MO0007MAJIONPH.016. Major Ion Content of Perched Groundwater from Selected YMP Boreholes with Perched Water Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 07/28/2000.

151534 MO0008MAJIONPH.017. Major Ion Content of Groundwater from Selected WT Boreholes Drilled for the Yucca Mountain Project Extracted from ANL-NBS-HS-000021, Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing and Recharge at Yucca Mountain, Nevada. Submittal date: 08/02/2000.

153777 MO0012MWDGFM02.002. Geologic Framework Model (GFM2000). Submittal date: 12/18/2000.

153384 MO0012URANISOT.000. Water - Selected Uranium Abundance and Isotope Ratios. Submittal date: 12/06/2000.

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155523 MO0102DQRGWREC.001. Groundwater Recharge Rate Data for the Four Reaches of Fortymile Wash Near Yucca Mountain, Nevada. Submittal date: 02/26/2001.

179436 MO0110NYE03848.087. NC-EWDP-WASHBURN 1X Well Completion Diagram. Submittal date: 10/17/2001.

157184 MO0112DQRWLNYE.014. Well Completion Diagram for Borehole NC-EWDP-19P. Submittal date: 12/04/2001.

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165876 MO0306NYE05259.165. Revised NC-EWDP-19IM1 Well Completion Diagram. Submittal date: 07/02/2003.

165877 MO0306NYE05260.166. Revised NC-EWDP-19IM2 Well Completion Diagram. Submittal date: 07/02/2003.

179373 MO0306NYE05261.167. Revised NC-EWDP-10S Well Completion Diagram. Submittal date: 07/03/2003.

179374 MO0306NYE05262.168. Revised NC-EWDP-10P Well Completion Diagram. Submittal date: 07/03/2003.

179375 MO0306NYE05263.169. Revised NC-EWDP-18P Well Completion Diagram. Submittal date: 07/03/2003.

179376 MO0306NYE05264.170. Revised NC-EWDP-22S Well Completion Diagram. Submittal date: 07/03/2003.

179377 MO0306NYE05265.171. Revised NC-EWDP-22PA Well Completion Diagram. Submittal date: 07/03/2003.

179378 MO0306NYE05266.172. Revised NC-EWDP-22PB Well Completion Diagram. Submittal date: 07/03/2003.

179379 MO0306NYE05267.173. Revised NC-EWDP-23P Well Completion Diagram. Submittal date: 07/03/2003.

170556 MO0307GSC03094.000. As-Built Survey of Nye County Early Warning Drilling Program Phase IV Boreholes EWDP-16P, EWDP-27P & EWDP-28P. Submittal date: 07/14/2003.

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179381 MO0312NYE05718.202. NC-EWDP-28P Well Completion Diagram. Submittal date: 12/09/2003.

174102 MO0408GSC04123.000. Nye County Early Warning Drilling Program, Phase IV, As-Built Location of NC-EWDP-19PB Borehole. Submittal date: 08/12/2004.

179382 MO0409NYE06093.241. NC-EWDP-29P Well Completion Diagram. Submittal date: 09/08/2004.

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180021 MO0608ABEWDPPV.000. As-Built Location of Nye County Early Warning Drilling Program (EWDP) Phase V, Boreholes #NC-EWDP-24PA, NC-EWDP-24PB, NC-EWDP-32P, and NC-EWDP-33P. Submittal date: 08/08/2006.

179352 MO0610MWDHFM06.002. Hydrogeologic Framework Model (HFM2006) Stratigraphic Horizon Grids. Submittal date: 11/01/2006.

180022 MO0611NYE06947.344. NC-EWDP-13P Well Completion Diagram. Submittal date: 11/17/2006.

179486 MO0612NYE07008.366. NC-EWDP-32P Well Completion Diagram. Submittal date: 12/04/2006.

179487 MO0612NYE07011.368. NC-EWDP-33P Well Completion Diagram. Submittal date: 12/04/2006.

179337 MO0612NYE07122.370. EWDP Manual Water Level Measurements through November 2006. Submittal date: 12/15/2006.

179443 MO0702NYE05714.375. NC-EWDP-16P Well Completion Diagram. Submittal date: 02/27/2007.

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LA0612RR150304.002. Hydrochemical Data Obtained from the Underground Test Area (UGTA) Program's Geochem05 Database. Submittal date: 12/18/2006.

LA0612RR150304.003. Geochemical and Isotopic Data for Selected NC-EWDP Wells, Phases II, III, and IV. Submittal date: 01/02/2007.

LA0612RR150304.004. Regional Groundwater Flow Pathways In The Yucca Mountain Area Inferred From Hydrochemical And Isotopic Data. Submittal date: 01/02/2007.

LA0612RR150304.005. Uranium Activity Ratios Calculated from Isotopic Ratios Reported for Nye County EWDP Boreholes and McCracken Well by Geochron Laboratories, for Samples Collected between November 1999 and June 2000. Submittal date: 12/21/2006.

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MO0611SCALEFLW.000. Water Table for the Saturated Zone Site Scale Flow Model. Submittal date: 11/15/2006.

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SN0612T0510106.003. Recharge and Lateral Groundwater Flow Boundary Conditions for the Saturated Zone (SZ) Site-Scale Flow Model. Submittal date: 12/04/2006.

SN0612T0510106.004. Saturated Zone (SZ) Site-Scale Flow Model PEST and FEHM Files Using HFM2006. Submittal date: 01/17/2007.

SN0702T0510106.006. Saturated Zone (SZ) Site-Scale Flow Model with "Water Table Rise" Alternate Conceptual Model - FEHM Files Using HFM2006. Submittal date: 02/19/2007.

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167994 EARTHVISION V. 5.1. 2000. IRIX 6.5. STN: 10174-5.1-00.

163072 EXT_RECH V. 1.0. 2002. Sun O.S. 5.7. STN: 10958-1.0-00.

161725 FEHM V. 2.20. 2003. SUN 9.S. 5.7 & 5.8, Windows 2000, RedHat Linux 7.1. STN: 10086-2.20-00.

179539 FEHM V. 2.24-02. 2006. WINDOWS XP. STN: 10086-2.24-02-00.

173140 LaGriT V. 1.1. 2004. Sun OS 5.7, 5.8, 5.9, IRIX64 OS 6.5. STN: 10212-1.1-00.

179480 PEST V. 11.1. 2007. Windows. STN: 611582-11.1-00.

161564 PEST V. 5.5. 2002. SUN O.S. 5.7 & 5.8, WINDOWS 2000, RedHat 7.3. STN: 10289-5.5-00.

155323 PHREEQC V. 2.3. 2001. WINDOWS 95/98/NT, Redhat 6.2. STN: 10068-2.3-00.

163070 Software Code: Extract V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10955-1.0-00.

163071 Software Code: Extract V. 1.1. 2002. Sun UltraSPARC - SunOS 5.7. 10955-1.1-00.

164654 Software Code: fehm2tec V. 1.0. 2003. Sun, Solaris 2.7 and 2.8. 11092-1.0-00.

164653 Software Code: maketrac V. 1.1. 2003. Sun, SunOS 5.7 and 5.8. 11078-1.1-00.

163073 Software Code: Mult_Rech V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10959-1.0-00.

164652 Software Code: reformat_sz V. 1.0. 2003. Sun, Solaris 2.7 and 2.8. 11079-1.0-00.

163074 Software Code: Xread_Distr_Rech V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10960-1.0-00.

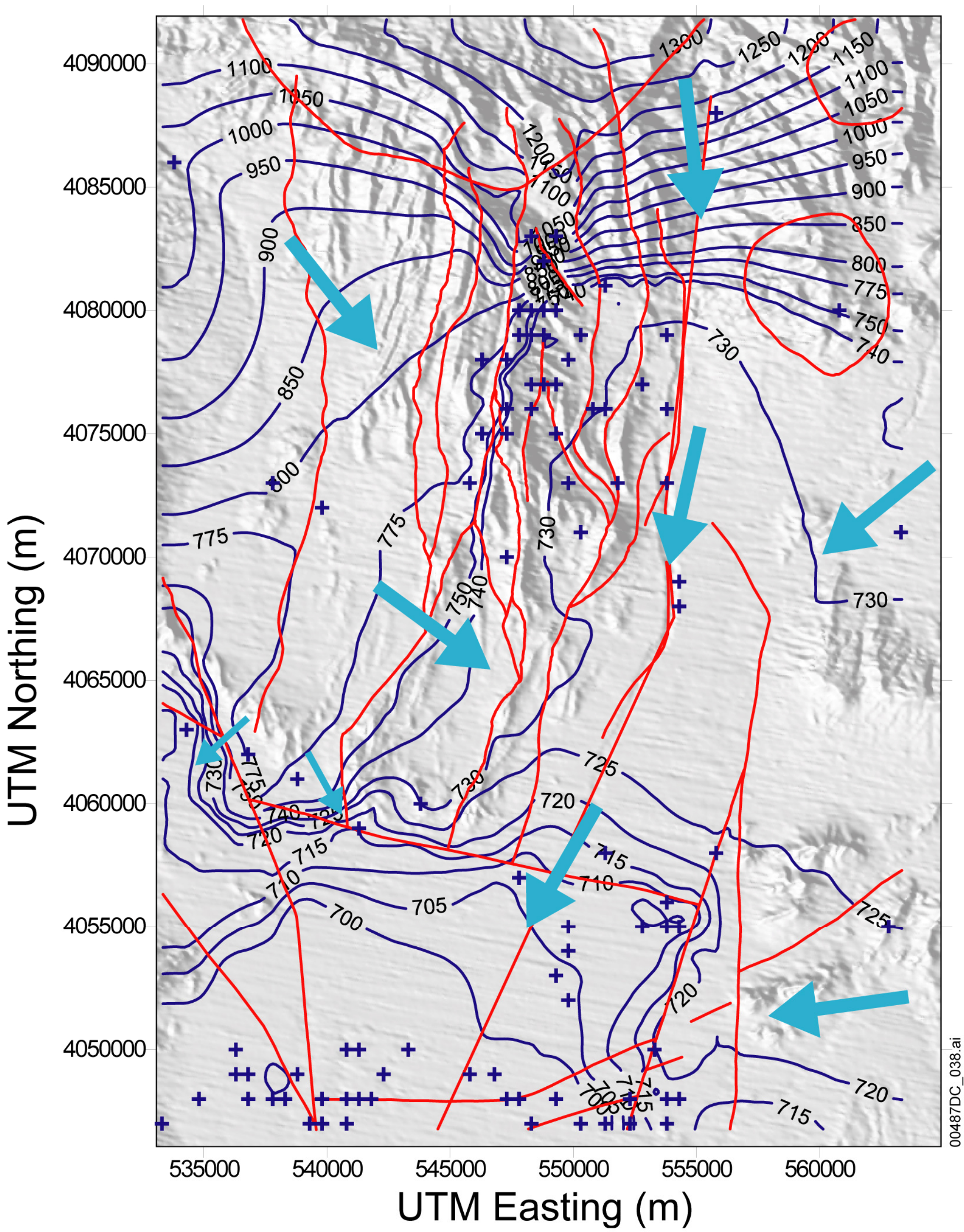
163075 Software Code: Xread_Distr_Rech_-UZ V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10961-1.0-00.

163076 Software Code: Xread_Reaches V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10962-1.0-00.

163077 Software Code: Xwrite_Flow_New V. 1.0-125. 2002. Sun UltraSPARC - SunOS 5.7. 10963-1.0-125-00.

163078 Software Code: Zone V. 1.0. 2002. Sun UltraSPARC - SunOS 5.7. 10957-1.0-00.

180546 SPDIS.EXE V0.0. 2007. Windows XP. 611598-00-00.



Source: USGS (2001 [DIRS 154625], Figure 1-2); DTNs: GS010908314221.001 [DIRS 145263] (Tertiary faults); GS000508312332.001 [DIRS 149947] (Water-level contours).

NOTE: The inferred groundwater flow directions are based on Assumption 1 in Table A5-1. The circular areas outlined in red near the Calico Hills in the northeast corner of the map are zones of hydrothermal alteration associated with granitic intrusions, and the semicircular area along the central northern portion of the map is the southern boundary of the Claim Canyon caldera (BSC 2004 ([DIRS 170037], Table 6-17; Zyvoloski et al. 2003 [DIRS 163341], Figure 2b). The other red lines are selected faults; blue crosses indicated the location of hydraulic head measurements. Blue lines are contours showing elevation (in meters above sea level) of the potentiometric surface; contour intervals vary. UTM=Universal Transverse Mercator. For illustrative/historical perspective purposes only.

Figure A6-3. Potentiometric Surface and Inferred Flow Directions (light blue arrows) for Yucca Mountain and Vicinity

An important conclusion derived from identification of these mixing zones is that they qualitatively illustrate the extent of transverse dispersivity along certain flow pathways. The mixing zones also illustrate that, although some flow pathways may remain intact for great distances (e.g., paths 1 and 2), even these most-persistent flow paths eventually loose their distinct character, largely through mixing. This effect is best illustrated in southern Amargosa desert where flow paths 1, 2, and 3, with contributions from 8, converge and mix. The distinct end member groundwater of the AR and FMW-S groups, representing flow paths 1 and 2, appears to be absent at the southern boundary of the study area. Whereas it is possible that these end member groundwaters have not yet been sampled, the proximity of mixed groundwater samples in the southern part of the study area (samples 141, 174, 175, 183, 184, and 185) leaves little room for unmixed (end member) groundwater to move through the area. The hydrochemical data are interpreted to indicate that groundwaters from distinct sources that merge in the Amargosa Desert eventually lose their hydrochemically distinct character and flow southward as partially mixed groundwater.

A7. SUMMARY, DATA TRACKING NUMBERS, AND UNCERTAINTIES

A7.1 SUMMARY

Hydrochemical data from the saturated zone in the Yucca Mountain region were compiled, documented, and analyzed in this appendix. The hydrochemical data are used together with physical hydraulic data to evaluate the local and regional flow system at Yucca Mountain. This report provides an independent assessment of the flow patterns (Section A6.3.11) and recharge rates (Section A6.3.6) near Yucca Mountain that can be compared with flow paths and recharge rates associated with the SZ site-scale flow model documented in *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]), and for which the model input/output files are in DTN: LA0304TM831231.002 [DIRS 163788]. This report also provides an independent basis for calculating groundwater residence times (Section A6.3.9) that can be compared with particle breakthrough curves calculated using the site-scale SZ transport model. Additionally, this appendix contributes to the resolution of technical issues associated with groundwater residence times and flow path lengths in alluvium and tuff, as discussed below. The methods used in this appendix are widely accepted, the data are sufficient and the analysis appropriate for the intended use if this document.

A7.1.1 Summary of Overview Sections (Sections A6.3.1 to A6.3.5)

Areal distributions of chemical and isotopic data as well as calculated parameters show many consistent patterns throughout the study area. Groundwater that has low concentration of most solutes characterizes groundwater beneath Yucca Mountain and in Fortymile Wash. Dilute groundwaters characterize the northern part of Fortymile Wash as well as the southern part in the Amargosa Desert. Increases in most solute concentrations occur to the west of Yucca Mountain and along the southern margin of Yucca Mountain near U.S. Highway 95. Dilute groundwaters are flanked by less dilute groundwaters to the east and west in the Amargosa Desert. Hydrochemical data presented in these sections provide first-order constraints on flow pathways. Groundwater beneath Yucca Mountain and in Fortymile Wash is characterized by low concentrations of most solutes.

A7.1.4 Summary of Flow Pathways (Section A6.3.11)

Flow paths can be traced using areal plots and scatterplots of geochemical and isotopic data, inverse mixing and water/rock interaction analyses involving PHREEQC, and simulations done with the SZ flow model. Because no single chemical or isotopic species varies sufficiently to determine flow paths everywhere in the study area, multiple chemical and isotopic species were considered.

Flow Path 1 (Figure A6-62) shows groundwater moving roughly parallel to the Amargosa River from an area west of Bare Mountain toward the southwest corner of the site model area. Flow Path 2 indicates that groundwater flows parallel to Fortymile Wash to connect upgradient areas in Fortymile Canyon with downgradient areas in the Amargosa Desert. Groundwater following Flow Path 3 flows from central Jackass Flats near well J-11 through the eastern part of the Amargosa Desert. Flow Paths 4 and 5 shows groundwater moving predominantly south-southeast through Crater Flat. Mixing relations and modeling suggest that these groundwaters leak across a region with a steep hydraulic gradient to mix with more dilute groundwaters to the southeast. Flow Paths 6 and 7 show groundwater flow from the Solitario Canyon area to the south. Again, leakage to the southeast across a steep hydraulic gradient coincident with the Solitario Canyon fault is suggested by hydrochemical trends. Groundwater from northern Yucca Mountain is interpreted to flow southeast toward lower Dune Wash and then southwestward toward wells located west of Fortymile Wash near U.S. Highway 95 (Flow Path 7). The location of Flow Path 7 implies that groundwater from the repository area will flow further to the west of this path. Flow Path 8 illustrates leakage to the west across the hydrologic boundary between the carbonate aquifer to the east and the alluvial aquifer in Amargosa Desert. Flow Path 9 schematically illustrates deep underflow of groundwater from the carbonate aquifer, east of and including the GF and AF groups, beneath the Amargosa Desert and Funeral Mountains to the discharge points in Death Valley.

Regions where mixing relations are strongly suggested by hydrochemical data are also shown in Figure A6-62. An important conclusion derived from drawing these mixing zones is that they document and qualitatively illustrate the extent of transverse dispersivity along certain flow pathways. The mixing zones also illustrate that although some flow pathways may remain intact for great distances (e.g., Paths 1 and 2), even these most persistent flow paths eventually lose their distinct character largely through mixing as is demonstrated in southern Amargosa Desert along the southern border of the map area.

A7.2 DATA TRACKING NUMBERS

Several data tracking numbers (DTNs), generated in this appendix are cited elsewhere in this report where they are used as indirect input. These intermediary output DTNs are listed below in an order that coincides with the structure of the appendix. These results are not qualified and cannot be used as direct input without qualification:

- Regional groundwater hydrochemical data: DTNs: LA0309RR831233.001 [DIRS 166546] and LA0309RR831233.002 [DIRS 166548]
- Calculated hydrochemical parameters: DTN: LA0310EK831232.001 [DIRS 165995]

affect groundwater chemistry. Most sample data presented herein were collected by the United States Geological Survey (or by their contractors), who have a long and proven record of groundwater sampling using proven techniques. Furthermore, Yucca Mountain Project Quality Assurance Programs also govern many of these sampling procedures. This program is designed to assure that methods utilized are appropriate for the desired purpose. Thus, the data are accepted to be representative of in situ conditions. All analytical data presented herein have uncertainty associated with the individual values. These uncertainties reflect limits of precision of the analytical technique combined with accuracy of the measurement, which is typically determined by replicate analysis of samples (standards) with known values. The data presented herein were determined using a variety of analytical techniques by a number of laboratories, collected over a span of more than 20 years, during which time analytical techniques and associated uncertainties have changed. In some cases, uncertainties for individual analytes or groups of analytes are presented in the original data sources, however, in other data sets analytical uncertainties are neither given nor discussed. Some examples of stated uncertainties are presented below.

The National Water Quality Laboratory produced many of the data presented herein for the Yucca Mountain Program at the United States Geological Survey and uncertainties are stated in some of the DTNs. For example, accuracy for major anions, cations and strontium concentration is estimated to be better than 10% except for fluoride, which is estimated at 15% (DTN: GS000308312322.003 [DIRS 149155]). Uncertainty in concentration of major anions and cations as well as strontium concentration is quoted at less than 10% in DTN: GS011108312322.006 [DIRS 162911]. This DTN also presents uncertainties for isotopic measurements as follows (all given in per mil): deuterium 3.0, ^{18}O 0.2, ^{13}C 0.2, and ^{34}S 0.2. In some cases, strontium was determined by isotope dilution, mass spectrometry methods, for which data are more precise (e.g. 0.5%, DTN: GS970708315215.008 [DIRS 164674]). Uncertainties for ^{14}C are 0.1 pmc for data presented in DTN: GS011108312322.006 [DIRS 162911]. Uncertainties for uranium concentration are given as better than 1% (Paces et al. 2002 [DIRS 158817]). Uncertainties in uranium isotope ratios (^{234}U/^{238}U) are typically given with each individual analysis in the original data source. For example, uncertainties presented in Paces et al. (2002 [DIRS 158817], Table 2) range from 0.09% to 4.5% with a mean of 0.73% (with the exception of a single analysis of a rainfall sample with small U concentration for which uncertainty in the ^{234}U/^{238}U ratio is 9.8%). Uncertainties for strontium isotope ratios (^{87}Sr/^{86}Sr) are typically quoted at 0.00001 for absolute values (e.g., DTN: GS011108312322.006 [DIRS 162911] and for Nye County wells), which translates to an uncertainty of approximately 0.01 in δ^{87}Sr units.

For the purpose of this report, uncertainties assigned to analytical data are based on one or more of the following: (1) stated uncertainties in the original data set; (2) consideration that data produced by the same facility, for which no uncertainties are stated, are likely to have similar uncertainties to data with stated uncertainties; (3) typical uncertainties given in the literature; or (4) the authors' personal experience with typical uncertainties associated for various analytical techniques and analytes. Where uncertainties are not stated, the following uncertainties are assigned to the analytical data: Major anions and anions and strontium concentration: 10%; fluoride concentration: 15%; stable isotopes of hydrogen, oxygen, sulfur, and carbon (expressed as δH, δO, δS, and δC in per mil): 0.2; and ^{14}C: 0.2 pmc. Uncertainties in uranium concentration and uranium and strontium isotope ratios are given in the original data sets.

Another source of uncertainty in the calculated saturation indices of alumino-silicate minerals concerns the assumption that total dissolved Al^{3+} concentrations are in equilibrium with kaolinite. This assumption was based on an empirical fit to dissolved Al^{3+} concentrations from a subset of the Yucca Mountain area wells for which dissolved Al^{3+} data exist (see Section A6.3.5). Estimates of Al^{3+} concentrations that rely on assumed equilibrium with kaolinite underestimate measured Al^{3+} concentrations by –3.0 ±2.9 ppb. If the actual Al^{3+} concentrations were approximately 3 ppb higher than was estimated for the Yucca Mountain area, the saturation indices of all Al-bearing minerals would increase. Assuming Al^{3+} equilibrium with kaolinite, most groundwaters in the Yucca Mountain area are estimated to be saturated with smectite and Ca-clinoptilolite (Figures A6-38 and A6-39). With higher Al^{3+} concentrations, these groundwaters would be even more supersaturated with these minerals. Groundwaters in the Yucca Mountain area are presently estimated to be both undersaturated and supersaturated with K-feldspar (Figure A6-37). With higher Al^{3+} concentrations, some groundwaters that are estimated to be undersaturated with K-feldspar might be calculated to be saturated or supersaturated with K-feldspar.

A7.3.3 Calculated ^{14}C Ages

The calculations of ^{14}C ages used the downgradient increase in the DIC concentrations of selected Yucca Mountain area groundwaters, relative to the DIC concentrations of Yucca Mountain perched waters to estimate the extent of ^{14}C dilution by calcite dissolution in the saturated zone (Section A6.3.6.6.2). The selected groundwater samples were chosen because they, like the perched water samples, had high $^{234}U/^{238}U$ activity ratios relative to many Yucca Mountain area groundwaters, thus indicating the likelihood of a common origin. The estimated increases in the DIC concentrations of the groundwaters were then used to reduce the initial ^{14}C activities to below their original atmospheric values to calculate a "corrected" ^{14}C age for the groundwater. The critical assumptions in this analysis are that (1) the perched water itself required no age corrections and (2) that the measured increases in groundwater DIC relative to perched water limit the amount of ^{14}C dilution by calcite. Assumption (1) appears to be valid based on the historic variations of $^{36}Cl/Cl$ and ^{14}C activities measured on organic carbon in pack-rat middens and similar relations between $^{36}Cl/Cl$ and ^{14}C activities measured for inorganic carbon in perched water. Assumption (2) requires that no reductions in groundwater DIC concentrations take place through exsolution of CO_2 during groundwater flow or during sampling. Although CO_2 losses from groundwater to the unsaturated zone are estimated to be small because of the low diffusion of CO_2 in groundwater, exsolution of CO_2 during groundwater sampling may be a more significant effect. However, groundwater at the wells where ^{14}C age corrections were made typically had relatively low (< 7.8) pH values, indicating that the effects of degassing on DIC concentrations during sample collection were minimal.

A7.3.4 Calculations of the Fractions of "Young" Water in Yucca Mountain Groundwaters

These calculations interpret the measured ^{14}C activities of groundwater beneath Yucca Mountain to result from the mixing of groundwater that has been recharged at different times from the unsaturated zone at Yucca Mountain. Although recharge may have been added continuously over time at varying rates to Yucca Mountain groundwater, the calculations simplify the actual distribution by assuming that the measured ^{14}C activities result from the mixing of an "old"

Conceptual-model uncertainty includes the choice of mineral phases to be considered in a particular model, any constraints on the precipitation/dissolution or exchange reactions imposed on these phases, and the choice of groundwaters considered in these models as potential mixing components. The rationale behind selection of these various parameters is discussed in Section A6.3.8. It is acknowledged; however, that all possible combinations of these parameters were not exhaustively evaluated. Other combinations of end-member mixing components and reaction history could possibly be modeled to yield a particular downgradient water chemistry. Given all the potential combinations of mixing end members and reaction models, it is impossible to quantify uncertainty related to uncertainties in the conceptual model.

A7.3.6 Groundwater Velocities

The groundwater velocities calculated in Section A6.3.9 were based on the measured groundwater ^{14}C activities at wells defining a flow path segment, the linear distance between the wells, and the water-rock interactions identified by the PHREEQC models for that flow-path segment. The calculated velocities are, therefore, affected by the accuracy and representativeness of the groundwater ^{14}C measurements (see Section A7.3.1), the assumption that groundwater flows along a straight path between the wells defining the flow-path segment, and the uncertainties associated with the PHREEQC models, as described in Section A7.3.5. An indication of the quantitative uncertainty associated with transit times is provided by the standard deviations associated with transport times based on the PHREEQC models and differences between the means of these estimates and estimates made based on downgradient increases in DIC concentrations (Table A6-11). An additional uncertainty that may impact these calculations concerns the implicit assumption that no additional ^{14}C is added to the groundwater from downgradient recharge as the groundwater moves from the upgradient to downgradient wells defining a flow-path segment. Recharge at Yucca Mountain may not vary enough spatially to guarantee that upgradient and downgradient recharge could be recognized in a mixture.

A7.3.7 FEHM Groundwater Models of Nonreactive Tracer Transport in the Yucca Mountain Area

The FEHM simulations of nonreactive tracer transport described in Section A6.3.10 used the Yucca Mountain site-scale saturated zone flow model documented in *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]), using the model input/output files in DTN: LA0304TM831231.002 [DIRS 163788]. Uncertainty in flow modeling arises from a number of sources including, but not limited to, the conceptual model of the processes affecting groundwater flow, water–level measurements and simplifications of the model geometry, boundary conditions, hydrogeologic unit extent and depth, and the values of permeability assigned to hydrogeologic units. Such uncertainties associated with this flow model are identified and quantified in *Saturated Zone Site-Scale Flow Model* (BSC 2004 [DIRS 170037], Section 6.8). An additional uncertainty that pertains to the tracer simulations but not the flow model itself concerns numerical dispersion associated with the advection/dispersion equation. Numerical dispersion would tend to cause greater apparent mixing and dilution than would be present solely because of hydraulic conductivity variations in the model. These effects are likely to have influenced the tracer concentration distributions shown in Section A6.3.10 and, in particular, the relatively dilute concentrations near the edges of these tracer plumes may be an artifact of this numerical dispersion.

Areal distributions of bicarbonate (as a surrogate for DIC), $\delta^{13}C$, and ^{14}C (measured on the DIC fraction) are shown in Figures B6-6, B6-9, and B6-10, respectively. These new inorganic-carbon data are generally consistent with data presented in Appendix A. Although these new data do not show consistent north to south trends, there is a general west to east increase in ^{14}C activity among the new Nye County boreholes (Figure B6-10). This shift corresponds to a decrease in bicarbonate concentration and decrease in $\delta^{13}C$ values. These data are consistent with a greater component of carbonate-derived groundwater in the west compared to the east and a greater component of more recently recharged water along Fortymile Wash.

Preliminary results of uncorrected radiocarbon ages based on ^{14}C activities measured for the total DOC fraction of several groundwaters are reported in DTN: GS031208312322.004 [DIRS 179431]. Figure B6-14 compares these uncorrected ^{14}C-TDOC ages, along with uncorrected radiocarbon ages calculated from separate analyses of the light and heavy molecular-weight DOC fractions, to uncorrected ^{14}C-DIC ages.

^{14}C ages determined from ^{14}C activities in DIC and TDOC fractions are in reasonable agreement for samples UE-29a#1, UE-29a#2, -22PA-1 (although the DOC fraction used for the -22PA-1 age estimate was not specified), -19P, and WT-3, all of which are located near Fortymile Wash. However, ^{14}C ages for these same samples determined from the low or high molecular weight fractions are in poor agreement with ages determined using ^{14}C-DIC. These data plot in fields that indicate a smaller percentage of ^{14}C activity (relative to that in modern carbon) in the DOC fraction relative to that in the DIC fraction and correspondingly older ^{14}C ages. The reason for this shift is unknown at this time. Several other samples plot in fields indicating smaller DIC percentages compared to those of TDOC, which yield older uncorrected ^{14}C ages based on DIC. Many of these samples (-1DX, -12PA, -12PC, and -9SX) are located in the CF-SW region, which hosts groundwater with a distinct carbonate signature. The age relationship noted is consistent with addition of dead carbon as inorganic carbon.

B6.6 REGIONAL FLOWPATHS INFERRED FROM HYDROCHEMICAL DATA

Hydrochemical data from the new boreholes presented above validate many of the flow pathways presented previously (Figure A6-62) and also allow minor refinements of that figure. The new boreholes are located in the region bounded between Flow Path 4 and Flow Path 3. A slightly modified version of the regional flowpath figure (Figure A6-62) is presented in Figure B6-15. The rationale underlying each modification is described below.

New hydrochemical data from -23P further validate Flow Path 3. In particular, sulfate/chloride ratios and high sulfate concentrations in -23P are similar to those from borehole J-11 (Jackass Flat grouping), strengthening the argument that water from Jackass Flat flows southwesterly to this region. Boreholes -23P and Washburn-1X constrain the position of Flow Path 3. Only minor adjustments were made to this flowpath. Based on interpretation of new data from -23P, mixing zone C was extended slightly to the north, and an additional arrow indicating westward flow of Flow Path 8 was added.

New hydrochemical data from boreholes -27P, -16P, and -28P confirm a southerly flow from the Solitario Canyon Wash (Grouping SCW) area along Flow Path 6. Slightly elevated sulfate and chloride values in two samples suggest that groundwater from regions to the northwest and/or

E1. PURPOSE

The purpose of this appendix is to describe the potentiometric surface developed for use with the SZ site-scale flow model described within this report. Also included is the process used to develop or construct the potentiometric surface. The description includes background, software used, inputs, analysis with uncertainty and limitations, and conclusions.

Previous potentiometric surfaces and analyses have been presented by *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (USGS 2001 [DIRS 154625], 2004 [DIRS 168473]; BSC 2004 [DIRS 170009]). The initial version of the potentiometric surface (USGS 2001 [DIRS 154625]) was used for the calibration of the SZ site-scale flow model (BSC 2004 [DIRS 170037]).

The USGS (2004 [DIRS 168473]) used updated water-level data for selected wells through the year 2000 as the basis for estimating water-level altitudes and the potentiometric surface in the SZ site-scale flow and transport model domain based on an alternative interpretation of perched water conditions. The updated water-level data presented by the USGS (2004 [DIRS 168473]) include data obtained from NC-EWDP Phases I and II and data from USW WT-24. That revision developed computer files containing:

- Water-level data within the model area (DTN: GS010908312332.002 [DIRS 163555])
- A table of known vertical head differences (DTN: GS010908312332.003 [DIRS 168699])
- A potentiometric-surface map (DTN: GS010608312332.001 [DIRS 155307]) using an alternative concept from that presented by the USGS (2001 [DIRS 154625]) for the area north of Yucca Mountain.

The water-level data analysis (BSC 2004 [DIRS 170009]) was based on work by the USGS (2004 [DIRS 168473]) and includes an analysis of the impact of more recent water-level data and the impact of adding data from the NC-EWDP Phases III and IV wells. It also expands the discussion of uncertainty in the potentiometric-surface map.

The current potentiometric surface presented in this appendix builds on the potentiometric surface as represented by contour lines presented by the USGS (2004 [DIRS 168473], Figure 6-1) as modified by *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009], Figure 6-2), which includes data from two additional recently completed wells, NC-EWDP-24P and NC-EWDP-29P as found in DTN: MO0409SEPPSMPC.000 [DIRS 179336] and illustrated in Figure 6-16.

Output DTN: MO0611SCALEFLW.000 represents the current potentiometric surface and includes representations of the surface in addition to the contours as shown in Figure 6-4.

E2. USE OF SOFTWARE

The potentiometric surface was constructed primarily using EarthVision 5.1 (STN: 10174-5.1-000, [DIRS 167994],) on a Silicon Graphics Octane workstation running IRIX 6.5. EarthVision is a product of Dynamic Graphics, Inc. and is designed for the preparation of three-dimensional geologic surfaces and models. The use of EarthVision to prepare this surface is consistent with the intended use of the software. There are no limitations on the use of this potentiometric surface due to the use of EarthVision.

EarthVision 5.1 can create regularly spaced grids from irregularly spaced data points to create surfaces that represent the top of specific hydrogeological units or the saturated zone. Up to 10,000,000 data points can be used to produce a grid with dimensions up to 1,201 × 1,201 (*GS_EV_5_0.pdf*, pp. 22 and 24). The surface constructed was within the range of these limits.

Several commercially available software packages (exempt per IM-PRO-003) were also used for data handling, formatting, and data visualization in the preparation of the potentiometric surface. These software packages were Microsoft Access (97 and 2000), Microsoft Excel (97 and 2003), AutoCad (2002), EarthVision (7.5.2), and UltraEdit (11.10) by IDM Computer Solutions, Inc. Each of these software packages were used on the Windows 2000 platform. No calculations were performed by these commercial software packages and the only output was in the form of visualizations. AutoCad and EarthVision 7.5.2 were used for data visualization and are therefore exempt per IM-PRO-003. Access, Excel, and UltraEdit were used for formatting data and were also exempt per IM-PRO-003. Each of these exempt software packages is controlled by YMP Software Configuration Management.

E3. INPUTS

The inputs for the construction of the potentiometric surface consist of water level measurements and the contour lines from previous potentiometric surfaces as shown in DTN: MO0409SEPPSMPC.000 [DIRS 179336].

Water level measurements used for the construction of the latest potentiometric surface were obtained from Output DTN: SN0610T0510106.001. In some cases, more than one water-level value is given for a single well and some wells and intervals are not considered appropriate for use in construction of a potentiometric surface. Table A-2 of *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]) was used to determine which wells and intervals were appropriate for use in the construction of the potentiometric surface. For wells or intervals not included in Appendix A of *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]), the value for the uppermost interval found in Output DTN: SN0610T0510106.001 was used.

Contour lines from Figure 6-2 of *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]) and found in DTN: MO0409SEPPSMPC.000 [DIRS 179336] were digitized and included as input data except in the immediate vicinity of the two recently completed wells, NC-EWDP-24P and NC-EWDP-29P.

E4. ANALYSIS

The potentiometric surface discussed herein is intended to be suitable for the needs of the saturated zone site-scale flow model described in this report. The area for which this potentiometric surface was constructed is identical to the area of the Hydrogeologic Framework Model HFM2006 (SNL 2007 [DIRS 174109]) and the SZ site-scale flow model of this report. The area covers about 1,350 km^2 and extends from 533,000 to 563,000 m (west to east) and 4,046,500 to 4,091,500 m (south to north), UTM (Zone 11, North American Datum 1927). The resolution, horizontal spacing, of the potentiometric surface was also established to match the Hydrogeologic Framework Model HFM2006 (SNL 2007 [DIRS 174109]) at 125 m.

The minimum tension method, generally recognized as providing geologically reasonable surfaces except where very steep surfaces are encountered (vertical distances many times greater than the horizontal data spacing), was used to construct the potentiometric surface. Control points were used to limit the tendency to overshoot in areas of very steep gradients. Some smoothing was also applied to minimize the effects of uneven data distribution.

The resulting potentiometric surface was checked at the water level measurement locations by determining the absolute value of the difference between the input value and the value indicated by the new potentiometric surface. The median difference was 0.2 m with a standard deviation of 1.9 m. This difference was determined to be suitable for use with the flow model described in this report. The potentiometric surface is intended for use with the SZ site-scale flow model and may not be suitable for other purposes. This surface does not replicate the input data exactly.

The uncertainty in the previously developed potentiometric surface map discussed in Section 6.5 of *Water-Level Data Analysis for the Saturated Zone Site-Scale Flow and Transport Model* (BSC 2004 [DIRS 170009]) is applicable to the current potentiometric surface. Uncertainty within the potentiometric surface is mostly related to the accuracy of the water-level measurements, distribution of data and relative variations of the surface. In areas of limited data and steep gradients, such as in the northwest portion of the model, uncertainty is greater than in the immediate vicinity of the repository. In general, the relatively flat portion of the potentiometric surface located just south of the repository is relatively less uncertain due to more wells located in the area. This area, from the repository extending to the south, is the most likely general direction of groundwater flow and is of more interest than the northwest portion of the model area.

The potentiometric surface intended for use with the SZ site-scale flow model is contained in Output DTN: MO0611SCALEFLW.000.

E5 CONCLUSIONS

The potentiometric surface found in Output DTN: MO0611SCALEFLW.000 has been prepared using the previous potentiometric surface (BSC 2004 [DIRS 170009]) and the most recently available water level information to create a surface suitable for use in the SZ site-scale flow model.

F1. PURPOSE

The purpose of these calculations is to convert qualified survey coordinates from Nevada State Plane (NSP) to UTM coordinates for selected NC-EWDP boreholes. Qualified borehole coordinates are required to support development of the new site-scale saturated-zone flow model.

The scope of these calculations covers NC-EWDP boreholes, through Phase IV, for which qualified UTM coordinates do not already exist in the Technical Data Management System (TDMS).

This activity is conducted under *Technical Work Plan for Saturated Zone Flow and Transport Modeling* (BSC 2006 [DIRS 177375]). It is a deviation from this TWP insofar as the conversion software used to conduct the activity is not identified in Section 9 of the TWP as software to be used for performing calculations, modeling or analyses for the work covered by the TWP. However, the software used for this activity is qualified, and the software package used to conduct the work was obtained from Software Configuration Management.

F2. QUALITY ASSURANCE

All activities in the governing TWP (BSC 2006 [DIRS 177375]) have been determined to be subject to *Quality Assurance Requirements and Description* (QARD) (DOE 2006 [DIRS 177092]), except for administrative activities. The calculations presented in this report are considered to be an analysis of data to support performance assessment and is therefore subject to the QARD (DOE 2006 [DIRS 177092]). No new data have been collected as part of this work scope. A prerequisite for this task is that all necessary qualified data are obtained from the TDMS.

In addition to the QARD (DOE 2006 [DIRS 177092]), the following procedures are used to perform this task:

- DM-PRO-001, *Document Control*
- DM-PRO-002, *Records Management*
- IM-PRO-002, *Control of the Electronic Management of Information*
- IM-PRO-003, *Software Management*
- RM-PRO-2001, *Document Control*
- SCI-PRO-004, *Managing Technical Product Inputs*
- SCI-PRO-006, *Models*
- TST-PRO-001, *Submittal and Incorporation of Data to the Technical Data Management System*.

H1. INTRODUCTION

Models are calibrated so that they make better predictions than if they were not calibrated. Unfortunately, calibrated model predictions can still be wrong. Furthermore, it is now being fully understood that a calibrated model can make even worse predictions than it did before calibration. With traditional approaches to model calibration, there is no way to find out: (1) whether a calibrated model's predictions are better than those before calibration, (2) if the predictions are better how much better they are, and (3) if their predictions are wrong how wrong they are. Traditional approaches to calibration are not able to ensure that calibrated models minimize "potential predictive wrongness" while quantifying the remaining uncertainty in the potential predictive wrongness.

The traditional approach to model calibration follows the tenet of the "principal of parsimony" espoused in many modeling texts and guidelines. First, the dimensionality of the calibration problem is reduced to facilitate a tractable model (i.e., few enough parameters are used to ensure their unique estimability) given the dataset available for calibration. The parameters values are then estimated through implicitly or explicitly maximizing some goodness-of-fit criterion. When the fit is judged to be "sufficient" (usually through minimization of an objective function), the model is deemed to be "calibrated" and therefore suitable for the making of predictions – predictions that may lay the groundwork for performance assessment calculations.

If automatic parameter estimation software is used in the calibration process, some estimates of parameter uncertainty are available. Estimates of the uncertainty of key model predictions can then be made based on the dependence of these predictions on the estimated parameters and their uncertainties.

The objective of this appendix is to show that calibrating a model and exploring the potential error of model predictions based on the theory of mathematical regularization, used in portions of this report, are better than methods based on the traditional approach to model calibration and predictive error analysis based on the principle of parsimony, which is not always effective or accurate. This same theory of mathematical regularization is regularly applied in many other branches of science where the analysis of costly and important data demands that maximum information be extracted (e.g., geophysical exploration and medical imaging). For example, a kidney is not defined prior to processing the data contained within a medical image; instead the location of the kidney "emerges" as a natural part of the data interpretation process. The same process should be used in groundwater data interpretation (which is what model calibration is) now that software that implements these methods efficiently in the groundwater modeling context are available. Public domain software that implements modern calibration and predictive uncertainty analysis based on regularized inversion is now available through the PEST package and its supporting utilities (Doherty 2003 [DIRS 178642], 2004 [DIRS 178643], 2006 [DIRS 178613]; PEST 2002 [DIRS 161564]). The groundwater industry will have to cross the same threshold that has been crossed in other industries, through application of regularized inversion as a methodology for model calibration and uncertainty analysis as a matter of course.

I1 THEORY – OVER DETERMINED CASE

This appendix is included to provide further background to the reader for the analysis conducted in Section 6.7.2, which is based on the theory presented below. Specifically, once a model is calibrated, the selected prediction made by that model can be maximized (or minimized) while maintaining a nominally calibrated model (e.g., the objective function must remain within 5% of its calibrated minimum). Changes in a model's prediction are made by varying parameters in the null space only (hence the ability of the model to remain calibrated). To the extent that the prediction depends on the null space parameters, its range can be estimated while maintaining calibration. This is a significantly more defensible way of presenting a confidence interval, because it eliminates the assumption that 95% confidence intervals are linearly dependent upon calibration parameters.

Vecchia and Cooley (1987 [DIRS 178577]) present a method for exploration of the confidence interval of a prediction made by a calibrated model, which accommodates the fact that the relationships between model outputs and parameters may not be linear. The methodology is based on a constrained optimization technique. The prediction of interest is maximized or minimized while parameters are constrained such that the model remains in a calibrated state at a certain confidence level. This confidence level is then equated to the confidence level of the prediction. Confidence is assessed in terms of the rise in the objective function that is incurred through maximizing or minimizing the prediction (and thereby incurring alterations to parameter values such that they no longer minimize that function). The relationship between objective function rise and parameter/predictive confidence interval is assessed in terms of the stochastic distribution that is assumed to pertain to measurement noise, together with a multiplier for this distribution (the so-called "reference variance") that is estimated through the calibration process.

Figure I-1 shows this process schematically. The dashed lines show contours of a prediction as a function of two parameters; let it be supposed that the value of the prediction increases to the upper right of this figure. The full line is a single contour of the objective function. The minimum of this objective function (which defines the values of parameters which calibrate the model) is within this contour. The contour itself defines the value of the objective function at which the model is no longer calibrated at a certain confidence level. The "critical points" A and B define locations in parameter space (and hence parameter values) at which the prediction of interest is minimized and maximized respectively at the same confidence level as that which applies to the contour. The difference between the corresponding model predictions defines the confidence interval of the prediction.

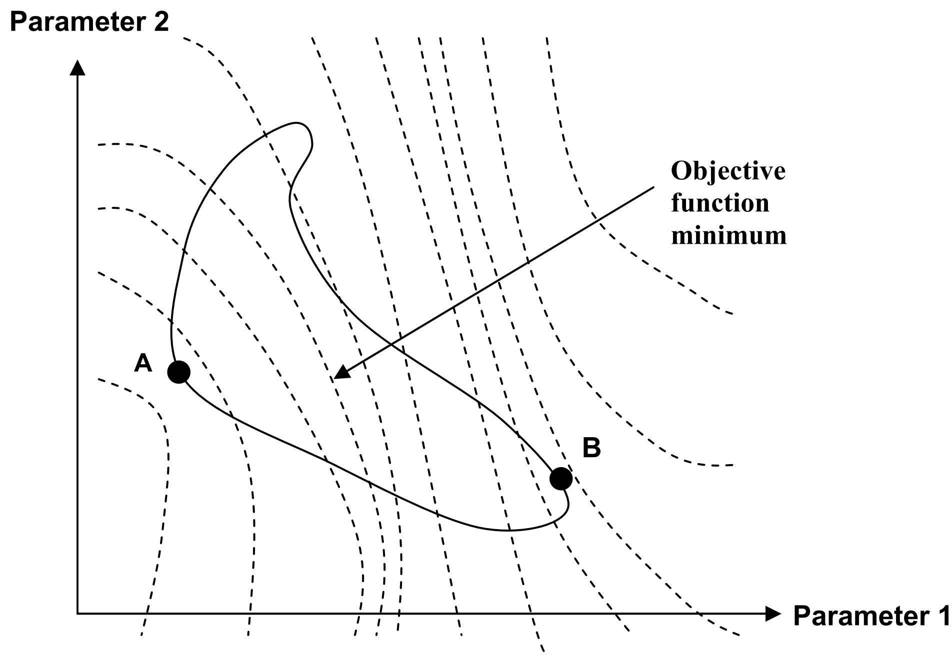


Figure I-1. Points in Parameter Space Corresponding to Maximum/Minimum Values of a Prediction at a Certain Confidence Level

Note that solution of the calibration problem through which parameters corresponding to Φ_{min} are computed, is achieved through an equation of somewhat similar form to Equation I-5, viz.:

$$\mathbf{p} = \left(\mathbf{X}^T\mathbf{Q}\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{Q}\mathbf{h}. \quad \text{(Eq. I-31)}$$

When predictive analysis is carried out for a nonlinear model, the same equations are used. However in this case, **X** is replaced by the model Jacobian matrix, **J**, and a parameter upgrade vector is calculated instead of a solution vector. The solution process is then an iterative one in which the true solution is approached by repeated calculation of an upgrade vector based on repeated linearization of the problem through determination of a Jacobian matrix that is updated every iteration. For further details see Vecchia and Cooley (1987 [DIRS 178577]).

I2 UNDER-DETERMINED CASE

Use of the above theory assumes that the inverse problem of model calibration is unique; that is, it assumes that all contours about the minimum of the objective function are closed. Unfortunately, this is not the case for the SZ flow model, where the same objective function can be obtained using many different sets of parameters.

Fortunately, as Doherty (2006 [DIRS 178613]) and Moore (2005 [DIRS 178788]) show, the theory can be extended to the case of under-determined parameter estimation without too much difficulty.

For underdetermined parameter estimation there is no unique solution to Equation I-7. Hence, some form of regularisation must be introduced to the inverse problem. This often takes the form of a subspace method such as truncated singular value decomposition, or a Tikhonov method in which an optimal parameter set is defined as that which departs minimally from a preferred parameter condition. In either case, an optimised parameter set $\underline{\mathbf{p}}$ is computed as:

$$\underline{\mathbf{p}} = \mathbf{G}\mathbf{h}. \quad \text{(Eq. I-32)}$$

Now if the action of the model can be replaced by its linear matrix approximation, **X**, then (assuming zero offsets for simplicity):

$$\mathbf{h} = \mathbf{X}\mathbf{p} + \boldsymbol{\varepsilon}, \quad \text{(Eq. I-33)}$$

where **p** in Equation I-9 signifies the set of "real" system parameter values (can never be known), and **h** is, once again, the calibration dataset.

Thus:

$$\underline{\mathbf{p}} = \mathbf{R}\mathbf{p} + \mathbf{G}\boldsymbol{\varepsilon}, \quad \text{(Eq. I-34)}$$

where **R** is the "resolution matrix." Where noise is zero or minimal, each row of this matrix represents averaging weights through which calibrated parameter values contained in $\underline{\mathbf{p}}$ are obtained as functions of real parameter values contained in **p**. For under-determined inversion, **R** is always a rank-diminished matrix. Its null space defines the subspace of parameter space

2. The magnitude of structural noise associated with the calibration dataset (whether this be parsimonization-induced or a result of other model inadequacies) is normally assessed through the calibration process using a "reference variance" term. However, the estimation of this quantity has uncertainty associated with it. It is shown in most textbooks on parameter estimation that, even if measurement noise possesses a Gaussian distribution, parameter and predictive probabilities acquire a Student-*t* distribution for their characterization because of this. This will apply to the first term of Equation I-15, but not the second. Thus, use of the square of a normal variate for the total objective function as a means of assessing confidence will be somewhat in error.

I3 CONCLUSION

Overall, it is reiterated that the non-linear predictive error variance analysis developed in this appendix can be used to more accurately specify the range in a calibrated model prediction. That is, 95% confidence intervals are established for a model prediction while calibration is maintained and the assumption that model predictions are linearly dependent upon calibration is no longer required . While this does not ensure physical reasonableness of a prediction from a calibrated model, it demonstrates variability in a prediction based only on variation of parameters in the null space.