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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

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Page: 1 of 68

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
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CONTENTS

	Page
ACRONYMS	9
1. PURPOSE	11
2. QUALITY ASSURANCE	13
3. COMPUTER SOFTWARE AND MODEL USAGE	15
4. INPUTS	17
4.1 DATA AND PARAMETERS	17
4.2 CRITERIA	22
4.3 CODES AND STANDARDS	23
5. ASSUMPTIONS	25
5.1 ASSUMPTIONS REGARDING PHYSICAL CONDITIONS EXTERIOR TO THE MODELING PROCESS	25
5.2 ASSUMPTIONS REGARDING NUMERICAL GRID CONSTRUCTION	26
6. ANALYSIS/MODEL	29
6.1 NUMERICAL GRID DEVELOPMENT - OVERVIEW AND APPROACH	29
6.2 BOUNDARIES AND CALIBRATION FEATURES	31
6.3 UZ MODEL LAYERS AND FAULT GEOMETRIES	36
6.4 EXTRACTION OF GFM3.1 AND ISM3.0 DATA	41
6.4.1 Isochores	41
6.4.2 Reference Horizons, and Top and Bottom UZ Model Boundaries	43
6.5 2-D GRID GENERATION	44
6.6 3-D GRID GENERATION	45
6.6.1 Faults	46
6.6.2 Repository	48
6.6.3 Vitric/Zeolitic Boundaries	48
6.7 DUAL-PERMEABILITY GRID GENERATION	52
6.8 MODEL VALIDATION	56
7. CONCLUSIONS	59
7.1 LIMITATIONS AND UNCERTAINTIES	59
7.2 RESTRICTIONS FOR SUBSEQUENT USE	61
7.3 IMPACT OF DATA AND SOFTWARE QUALIFICATION	61
8. INPUTS AND REFERENCES	63
8.1 DOCUMENTS CITED	63
8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES	65
8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER	65
8.4 AMR OUTPUT DATA LISTED BY DATA TRACKING NUMBER	66

CONTENTS (CONTINUED)

	Page
9. ATTACHMENTS	67
ATTACHMENT I - DOCUMENT INPUT REFERENCE SHEETS	
ATTACHMENT II - ELECTRONIC GFM3.1 AND ISM3.0 DATA FILES USED TO DEVELOP UZ MODEL NUMERICAL GRIDS	
ATTACHMENT III - DEVELOPMENT OF NUMERICAL GRIDS FOR 1-D HYDROGEOLOGIC PROPERTY SET INVERSIONS	
ATTACHMENT IV - DEVELOPMENT OF CROSS-SECTIONAL GRIDS FOR FAULT HYDROGEOLOGIC PROPERTY CALIBRATIONS	
ATTACHMENT V - DEVELOPMENT OF A 3-D NUMERICAL GRID FOR UZ MODEL CALIBRATION	
ATTACHMENT VI - DEVELOPMENT OF A 3-D NUMERICAL GRID FOR CALCULATION OF FLOW FIELDS FOR PA	

FIGURES

	Page
1. Plan-View Schematic Showing the UZ Model Boundary, the Repository Outline, Major Fault Locations Derived from GFM3.1, Selected Boreholes, the ESF, and the ECRB.....	33
2. Schematic Illustration of Fault-Related Gridblocks in Map View and in Cross Section	47
3. Percent Zeolite Distribution from ISM3.0 Mineralogy Model, Upper 1/4 of Layer Tac (UZ Model layer "ch2")	50
4. Distribution of Ksat from ISM3.0 Rock Properties Model, Upper Tac.....	51
5. Extent of Vitric Region in FY 99 UZ Model Layers (a) ch1, (b) ch2, (c) ch3, (d) ch4, and (e) ch5	53

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TABLES

	Page
1. Computer Software Used in Numerical Grid Development.....	15
2. Summary of Input Data Used and Considered in Numerical Grid Development.....	17
3. Repository Boundary Coordinates Used for UZ Model Grids	18
4. Water Levels in Selected Boreholes	19
5. Fracture Hydrogeologic Properties	21
6. Summary of Grids Developed for FY 99 UZ Modeling Activities	29
7. YMP Scientific Notebooks Used for FY 99 Numerical Grid Development and Grid Resolution Sensitivity Analyses	30
8. UZ Model Areal Boundary Coordinates.....	32
9. Location of Boreholes, Alcoves, and Niches in the UZ Inversion and Calibration Models	35
10. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation	36
11. Faults Within the UZ Model Domain	39
12. Results of GFM3.1 Fault-Slope Analysis	40

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ACRONYMS

ACC	Accession Number
AMR	Analysis/Model Report
AP	Administrative Procedure (DOE)
CFR	Code of Federal Regulations
CFu	Crater Flat undifferentiated unit
CHn	Calico Hills nonwelded unit
CRWMS	Civilian Radioactive Waste Management System
DOE	Department of Energy
DTN	Data Tracking Number
ECM	Effective Continuum Method
ECRB	Enhanced Characterization of Repository Block
ESF	Exploratory Studies Facility
FY	Fiscal Year
GFM	Geologic Framework Model
HGU	Hydrogeologic Unit
IFD	Integral Finite Difference
ISM	Integrated Site Model
ITN	Input Tracking Number
Ksat	Saturated hydraulic conductivity
LBNL	Lawrence Berkeley National Laboratory
M&O	Management and Operating Contractor
NSP	Nevada State Planar
OCRWM	Office of Civilian Radioactive Waste Management
PA	Performance Assessment
PTn	Paintbrush nonwelded unit
QAP	Quality Administrative Procedure (M&O)
QARD	Quality Assurance Requirements and Description
QIP	Quality Implementing Procedure
RIB	Reference Information Base
RIS	Records Information System
STN	Software Tracking Number

ACRONYMS (CONTINUED)

TBV	To Be Verified
TCw	Tiva Canyon welded unit
TDMS	Technical Data Management System
TSw	Topopah Spring welded unit
USGS	United States Geological Survey
UZ	Unsaturated Zone
YMP	Yucca Mountain Site Characterization Project

1. PURPOSE

This Analysis/Model Report (AMR) describes the methods used to develop numerical grids of the unsaturated hydrogeologic system beneath Yucca Mountain. Numerical grid generation is an integral part of the development of a complex, three-dimensional (3-D) model, such as the Unsaturated-Zone Flow and Transport Model (UZ Model) of Yucca Mountain. The resulting numerical grids, developed using current geologic, hydrogeologic, and mineralogic data, provide the necessary framework to: (1) develop calibrated hydrogeologic property sets and flow fields, (2) test conceptual hypotheses of flow and transport, and (3) predict flow and transport behavior under a variety of climatic and thermal loading conditions. The work described herein follows the planning and work direction outlined in the "AMR Development Plan for U0000 Development of Numerical Grids for UZ Flow and Transport Modeling, Rev 00" (CRWMS M&O 1999c).

The steps involved in numerical grid development include: (1) defining the location of important calibration features, (2) determining model grid layers and fault geometry based on the Geologic Framework Model (GFM), the Integrated Site Model (ISM), and definition of hydrogeologic units (HGUs), (3) analyzing and extracting GFM and ISM data pertaining to layer contacts and property distributions, (4) discretizing and refining the two-dimensional (2-D), plan-view numerical grid, (5) generating the 3-D grid with finer resolution at the repository horizon and within the Calico Hills nonwelded (CHn) hydrogeologic unit, and (6) formulating the dual-permeability mesh. The products of grid development include a set of one-dimensional (1-D) vertical columns of gridblocks for hydrogeologic property set inversions, a 2-D UZ Model vertical cross-sectional grid for fault hydrogeologic property calibrations, a 3-D UZ Model grid for additional model calibrations, and a 3-D UZ Model grid for generating flow fields for Performance Assessment (PA).

Numerical grid generation is an iterative process that must achieve a proper balance between desired numerical accuracy in terms of gridblock size and computational time controlled by the total number of gridblocks. Gridblock size should reflect the scale of the process to be modeled. For example, in order to capture flow and transport phenomena along individual waste emplacement drifts, gridblock thickness and width should not exceed the drift diameter or the drift spacing. For large models, such as the site-scale UZ Model of Yucca Mountain, flow and transport phenomena occurring on scales of less than a few meters cannot be captured. Rather, the model is intended to provide an overview of key unsaturated-zone characteristics and processes potentially affecting repository performance.

Grids must also be adapted to the particular needs of the processes to be modeled because sharp gradients may occur in different domains for different flow processes. At Yucca Mountain, the heterogeneous, variably fractured layers are best represented by a dual-continua (matrix and fracture) model, rather than a single-continuum approach. Once developed, the UZ Model numerical grids are evaluated for appropriate resolution, representation of important features, and proper gridblock connections.

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2. QUALITY ASSURANCE

This AMR was developed in accordance with AP-3.10Q, *Analyses and Models*. Other applicable Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) Administrative Procedures (APs) and YMP-LBNL Quality Implementing Procedures (QIPs) are identified in the "AMR Development Plan for U0000 Development of Numerical Grids for UZ Flow and Transport Modeling, Rev 00" (CRWMS M&O 1999c).

This analysis was evaluated with other related activities in accordance with QAP-2-0, *Conduct of Activities*, and determined to be quality affecting and subject to the requirements of the QARD, *Quality Assurance Requirements and Description* (DOE 1998). This evaluation is documented in *Activity Evaluation of M&O Site Investigations* (CRWMS M&O 1999a, b).

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3. COMPUTER SOFTWARE AND MODEL USAGE

The software used in this study, listed in Table 1, was obtained from software configuration management (as discussed in the following paragraphs), was appropriate for the intended application, and was used only within the range of validation in accordance with applicable software procedures. The Q-status of each of these codes is given in Attachment I.

Table 1. Computer Software Used in Numerical Grid Development

Software Name	Version	Software Tracking Number (STN)	Computer Type
EARTHVISION	4.0	30035 V4.0	UNIX
ESF4_XYZ V.03.XLS	3.0	30092 V.03	PC
WinGridder ¹	1.0	10024-1.0-00	PC
Macros:			
DKMgenerator ³	1.0	ACC: MOL.19990909.0315	DOS or UNIX
ExportProp ³	1.0	ACC: MOL.19990910.0238	UNIX

NOTES: ¹ Previously referred to as WinGrid.

² See discussion below.

³ Software macro qualified per AP-SI.1Q.

EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0) is used to evaluate and to extract data from the GFM3.1 and ISM3.0 files listed in Attachment II. The software program "ESF4_XYZ V.03.XLS" (ESF4_XYZ V.03.XLS V3.0, STN: 30092 V.03, Version 3.0) is used to calculate easting and northing coordinates for alcoves and niches within the Exploratory Studies Facility (ESF), given their linear distance in meters from the North Portal. The WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) software program is used to generate 1-, 2-, and 3-D gridblock element and connection information in a TOUGH2 format (the primary mesh is an "effective-continuum," or "ECM," mesh). The software macro DKMgenerator (DKMgenerator V1.0, ACC: MOL.19990909.0315) generates a dual-permeability mesh from a primary (ECM) mesh. Initial code development of DKMgenerator V1.0 is described in Scientific Notebook YMP-LBNL-GSB-1.3 (pp. 42-45). Additional source code information and macro qualification are described in YMP-LBNL-YSW-2 (pp. 18-20, 129-132). The software macro ExportProp (ExportProp V1.0, ACC: MOL.19990910.0238) exports rock property information from ISM3.0. Development and qualification of this macro is discussed in Scientific Notebook YMP-LBNL-YSW-JH-2A (pp. 163-166).

EARTHVISION V4.0 and ESF4_XYZ V.03.XLS are qualified under *AP-SI.1Q, Software Management*. WinGridder V1.0 has been baselined and is currently being qualified under *AP-SI.1Q*.

Models used in the development of the UZ Model numerical grids include the Geologic Framework Model, Version 3.1 (GFM3.1) (DTN: MO9901MWDGFM31.000), and the Integrated Site Model, Version 3.0 (ISM3.0) [DTN: MO9901MWDISMRP.000 (Rock Properties Model)]. Data from the Mineralogic Model of ISM3.0 (DTN: MO9901MWDISMMM.000) were evaluated during grid development, but were not directly incorporated into the UZ Model grids (discussed in Section 6.6.3).

4. INPUTS

The initial stage of grid development begins with the definition of lateral domain and repository boundaries, along with the location of important calibration features [e.g., boreholes, the ESF, and the Enhanced Characterization of the Repository Block (ECRB)]. In order to generate a 3-D grid, WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) requires specification of three reference horizons: an upper and lower model boundary (usually the bedrock surface and water table, respectively) and a structural reference horizon that defines layer displacement along fault traces and sets the elevation of the remaining layer interfaces. These files consist of regularly spaced x, y, and elevation data. Isochore (borehole thickness) maps, consisting of regularly spaced x, y, and thickness data for each model layer, are then stacked above or below the structural reference horizon in order to build the vertical component of the UZ Model.

4.1 DATA AND PARAMETERS

The input data used and considered in numerical grid development are summarized in Table 2. The Q-status of each of these DTNs is provided in Attachment I.

Table 2. Summary of Input Data Used and Considered in Numerical Grid Development

Description	DTN or ACC
Geologic Framework Model, GFM3.1	MO9901MWDGFM31.000
Hydrogeologic Unit Definitions	MOL.19980429.0512 ¹
Integrated Site Model, ISM3.0	MO9901MWDISMRP.000 MO9901MWDISMMM.000 MO9804MWDGFM03.001
Repository Layout Configuration	MOL.19990409.0100 ²
Water Table Elevations	MO9609RIB00038.000 ³
Perched Water Elevations	GS980508312313.001
Fracture Data for Hydrogeologic Units	LB990501233129.001

NOTES: ¹ Hydrogeologic unit definitions (Flint 1998) used qualitatively; individual sample data not used.

² Data retrieved from the Records Information System (RISweb).

³ Data retrieved from the Reference Information Base (RIB).

The primary data feed for UZ Model grids is the Geologic Framework Model, GFM3.1 (DTN: MO9901MWDGFM31.000). The GFM is a representation of lithostratigraphic layering and major fault geometry in the Yucca Mountain area. The model contains information about layer thickness and layer contact elevation, and defines major fault orientation and displacement. The data for each layer and each fault within GFM3.1 are available on a regular horizontal grid spacing of 200 × 200 feet over the model's domain. A total of 48 geologic units and 42 faults are represented in GFM3.1. Approximately 40 of these units and 18 faults (those that lie within the UZ Model domain) are incorporated into the 3-D UZ Model grids. Alternate geologic models are

not available for use in the UZ Model, nor were they developed. Alternative geologic interpretations have been considered in the development of GFM3.1, and the resulting geologic interpretation it represents is the Yucca Mountain Site Characterization Project's (YMP) geologic model to be used in site-scale process models. GFM3.1 files used in UZ Model grid development are listed in Attachment II.

Geologic data alone cannot adequately capture all important features that affect flow and transport in the unsaturated zone at Yucca Mountain. Hydrogeologic rock-property data must also be considered. Based on analyses of several thousand rock samples performed by the U. S. Geological Survey (USGS), 30 hydrogeologic units (HGUs) have been identified based on "limited ranges where a discrete volume of rock contains similar hydrogeologic properties" (Flint 1998, pp. 1, 3-4). Since the hydrogeologic property sets to be calculated with the UZ Model grid use, to a large extent, the matrix properties data collected and analyzed by Flint (1998), layering within the numerical grid was chosen to correspond as closely as possible to HGUs, in order to facilitate data usage. The boundaries of HGUs are not defined by regularly spaced data, but are more qualitative in nature. The qualitative descriptions given in Flint (1998, pp. 21-32), when correlated with GFM3.1 data, are used to develop a set of hydrogeologic layers (whose thickness and elevation are described by regularly spaced data) for the UZ Model.

Because of the importance of mineral (especially zeolitic) alteration on flow and transport calculations, boundaries between vitric and zeolitic areas are defined within certain UZ Model grid layers below the repository horizon. Alteration to zeolites has been shown to greatly reduce permeability (Flint 1998, p. 32; Loeven 1993, p. 18-19, 22) and may increase the rock's ability to adsorb radionuclides. Data used in numerical grid development for defining low-permeability, zeolitic volumes of rock are obtained from the ISM3.0 Rock Properties Model (DTN: MO9901MWDISMRP.000). ISM3.0 files used in UZ Model grid development are listed in Attachment II.

The repository layout configuration (CRWMS 1999d) is used during numerical grid generation to locate areas of enhanced numerical resolution. The areal boundary coordinates for and elevations (in meters above sea level, masl) of the repository are summarized in Table 3.

Table 3. Repository Boundary Coordinates Used for UZ Model Grids

Easting (m)	Northing (m)	Elevation (masl)
170311.019	231086.867	1111.02
170893.964	230897.466	1111.02
171124.528	231435.342	1101.02
171343.408	235611.814	1044.70
170427.845	235909.300	1044.66
170354.437	234508.665	1063.59
170205.807	234147.767	1069.13
170055.118	232749.315	1088.40

ACC: MOL.19990409.0100

The lower UZ Model boundary is defined by the most recent water table elevations given in DTN: MO9609RIB00038.000 (Table 1, column labeled 1993). Average water table elevations from boreholes, used to develop a potentiometric surface for the UZ Model grids, are listed in Table 4. Not included in Table 4 are perched water elevations for boreholes USW G-2 and USW WT-24 (DTN: GS980508312313.001), to be discussed in Section 5. This DTN has been superseded; however, the change has no impact on the work described in this AMR. Only approximate water levels in boreholes G-2 and WT-24 are considered here, and these approximations are not explicitly used to develop the numerical grids.

Table 4. Water Levels in Selected Boreholes

Borehole ID ¹	Water Table Elevation (masl)
USW G-3 ²	730.54
USW H-1 ²	730.96
USW H-3 ²	731.20
USW H-4 ²	730.46
USW H-5 ²	775.55
USW H-6 ²	776.03
USW WT-1 ²	729.96
USW WT-2 ²	730.70
UE-25 WT#3	729.68
UE-25 WT#4 ²	730.37
UE-25 WT#6 ²	1034.14
USW WT-7 ²	775.86
USW WT-10	776.08
USW WT-11	730.65

From Figure 1 of DTN: MO9609RIB00038.000

NOTES: ¹ For simplicity, the borehole names used throughout the remainder of this document drop the USW and UE-25 prefixes.

² These boreholes lie within or along UZ Model boundaries.

Table 4. Water Levels in Selected Boreholes (Cont.)

Borehole ID ¹	Water Table Elevation (masl)
UE-25 WT#12	729.24
UE-25 WT#13	729.06
UE-25 WT#14	729.57
UE-25 WT#15	729.02
UE-25 WT#16	738.22
UE-25 WT#17	729.45
UE-25 WT#18 ²	730.72
UE-25 J#13	728.46
UE-25 b#1 ²	730.68
UE-25 c#2	729.98
UE-25 c#3	730.21

From Figure 1 of DTN: MO9609RIB00038.000

NOTES: ¹ For simplicity, the borehole names used throughout the remainder of this document drop the USW and UE-25 prefixes.

² These boreholes lie within or along UZ Model boundaries.

Fracture hydrogeologic properties (DTN: LB990501233129.001) describing UZ Model layers are used to formulate the dual-permeability (dual-k) meshes for 1-D hydrogeologic property set inversions, for 2-D fault property calibration, for 3-D UZ Model calibration, and for generating 3-D flow fields for PA. Fracture hydrogeologic properties used for dual-k grid generation are listed in Table 5. The development of these fracture properties are documented in a separate AMR.

Table 5. Fracture Hydrogeologic Properties

Model Layer	Fracture Porosity* (m ³ /m ³)	Fracture Aperture (m)	Fracture Frequency (m ⁻¹)	Fracture Interface Area (m ² /m ³)
tcw11	2.8E-02	7.3E-04	9.2E-01	1.6E+00
tcw12	2.0E-02	3.2E-04	1.9E+00	1.3E+01
tcw13	1.5E-02	2.7E-04	2.8E+00	3.8E+00
ptn21	1.1E-02	3.9E-04	6.7E-01	1.0E+00
ptn22	1.2E-02	2.0E-04	4.6E-01	1.4E+00
ptn23	2.5E-03	1.8E-04	5.7E-01	1.8E+00
ptn24	1.2E-02	4.3E-04	4.6E-01	3.4E-01
ptn25	6.2E-03	1.6E-04	5.2E-01	1.1E+00
ptn26	3.6E-03	1.4E-04	9.7E-01	3.6E+00
tsw31	5.5E-03	1.5E-04	2.2E+00	3.9E+00
tsw32	9.5E-03	2.0E-04	1.1E+00	3.2E+00
tsw33	6.6E-03	2.3E-04	8.1E-01	4.4E+00
tsw34	1.0E-02	9.8E-05	4.3E+00	1.4E+01
tsw35	1.1E-02	1.5E-04	3.2E+00	9.7E+00
tsw36	1.5E-02	1.6E-04	4.0E+00	1.2E+01
tsw37	1.5E-02	1.6E-04	4.0E+00	1.2E+01
tsw38	1.2E-02	1.2E-04	4.4E+00	1.3E+01
tsw39	4.6E-03	2.0E-04	9.6E-01	3.0E+00
ch1VI	6.9E-04	3.0E-04	1.0E-01	3.0E-01
ch2VI	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch3VI	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch4VI	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch5VI	8.9E-04	2.6E-04	1.4E-01	4.3E-01

DTN: LB990501233129.001

NOTES: *These fracture porosities are used to develop all UZ Model dual-k grids except the 1-D, dual-k, calibration grids "1doldtrans.mesh" and "1doldstdyst.mesh" (DTN: LB990501233129.002), which were developed previously and for which porosity was scaled using an alternative permeability value for UZ Model layer "tsw34." The relationship between these two fracture porosities is as follows:

$$\Phi_{f,1D,cal} = \Phi_f \left[\frac{k_{tsw34}}{k_{tsw34,alt}} \right]^{1/3}$$

where $\Phi_{f,1D,cal}$ is the fracture porosity for the 1-D calibration, Φ_f is the fracture porosity as listed in the second column of Table 5, k_{tsw34} is the permeability of model layer "tsw34" (equal to 3.4E-13 m²), and $k_{tsw34,alt}$ is the alternative permeability of model layer "tsw34" (equal to 1.6E-13 m²) (DTN: LB990501233129.001).

Table 5. Fracture Hydrogeologic Properties (Cont.)

Model Layer	Fracture Porosity* (m ³ /m ³)	Fracture Aperture (m)	Fracture Frequency (m ⁻¹)	Fracture Interface Area (m ² /m ³)
ch1Ze	1.7E-04	2.0E-04	4.0E-02	1.1E-01
ch2Ze	4.3E-04	1.3E-04	1.4E-01	4.3E-01
ch3Ze	4.3E-04	1.3E-04	1.4E-01	4.3E-01
ch4Ze	4.3E-04	1.3E-04	1.4E-01	4.3E-01
ch5Ze	4.3E-04	1.3E-04	1.4E-01	4.3E-01
ch6Ze	1.7E-04	2.0E-04	4.0E-02	1.1E-01
pp4	4.3E-04	1.3E-04	1.4E-01	4.3E-01
pp3	1.1E-03	2.4E-04	2.0E-01	6.1E-01
pp2	1.1E-03	2.4E-04	2.0E-01	6.1E-01
pp1	4.3E-04	1.3E-04	1.4E-01	4.3E-01
bf3	1.1E-03	2.4E-04	2.0E-01	6.1E-01
bf2	4.3E-04	1.3E-04	1.4E-01	4.3E-01
tr3	1.1E-03	2.4E-04	2.0E-01	6.1E-01
tr2	4.3E-04	1.3E-04	1.4E-01	4.3E-01
tcwfl	4.4E-02	5.5E-04	1.9E+00	1.3E+01
ptnfl	1.6E-02	4.0E-04	5.4E-01	1.3E+00
tswfl	3.6E-02	4.7E-04	1.7E+00	8.6E+00
chnfl	1.6E-03	3.3E-04	1.3E-01	4.7E-01

DTN: LB990501233129.001

NOTES: *These fracture porosities are used to develop all UZ Model dual-k grids except the 1-D, dual-k, calibration grids "1doldtrans.mesh" and "1doldstdyst.mesh" (DTN: LB990501233129.002), which were developed previously and for which porosity was scaled using an alternative permeability value for UZ Model layer "tsw34." The relationship between these two fracture porosities is as follows:

$$\phi_{f,1D,cal} = \phi_f \left[\frac{k_{tsw34}}{k_{tsw34,alt}} \right]^{1/3}$$

where $\phi_{f,1D,cal}$ is the fracture porosity for the 1-D calibration, ϕ_f is the fracture porosity as listed in the second column of Table 5, k_{tsw34} is the permeability of model layer "tsw34" (equal to $3.4E-13$ m²), and $k_{tsw34,alt}$ is the alternative permeability of model layer "tsw34" (equal to $1.6E-13$ m²) (DTN: LB990501233129.001).

4.2 CRITERIA

At this time, no specific criteria (e.g., System Description Documents) have been identified as applying to this analysis and modeling activity in project requirements documents. However, this AMR provides information required in specific subparts of the proposed U.S. Nuclear Regulatory Commission rule 10 CFR 63 (see Federal Register for February 22, 1999, 64 FR 8640). It supports the site characterization of Yucca Mountain, (Subpart B, Section 15), the compilation of

information regarding the hydrology of the site in support of the License Application (Subpart B, Section 21(c)(1) (ii)), and the definition of hydrologic parameters used in performance assessment (Section 114(a)).

4.3 CODES AND STANDARDS

No specific formally established codes or standards have been identified as applying to this analysis and models activity.

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5. ASSUMPTIONS

The assumptions presented below are necessary to develop the UZ Model numerical grids. This section presents the rationale and supporting data for the assumptions, and references the section of this AMR in which an assumption is used.

Assumptions used in the development of the numerical grids are of two kinds: assumptions made about the physical world, and assumptions made about the effects of certain features of the grid upon the results of model calculations. Assumptions about the physical world are needed when existing data are incomplete, and can in principle be verified by obtaining additional data. For this AMR, it is not anticipated that additional data will be forthcoming to verify any of the following assumptions.

Certain features of the grid are simplifications that are known to be different from the physical prototype. These simplifications are necessary in order for calculations to be done with existing computers and qualified software. Assumptions about the effects of such simplifications upon the results of model calculations can be verified through sensitivity analyses; that is, by running simulations with the assumptions as stated and with alternative assumptions. Sensitivity studies addressing the effects of numerical grid resolution and the simplified representation of faults on flow and transport model simulation results are not within the scope of this AMR and will be documented in a future AMR.

5.1 ASSUMPTIONS REGARDING PHYSICAL CONDITIONS EXTERIOR TO THE MODELING PROCESS

The following three assumptions pertain to the elevation of the water table, which defines the lower UZ Model boundary.

1. It is assumed that the water table is flat at 730 meters above sea level (masl) east of the Solitario Canyon fault and flat at 776 masl west of the Solitario Canyon fault (Section 6.2).

This assumption is based on data collected from 25 wells in the Yucca Mountain area (13 of which lie within or along the UZ Model boundary). Water elevations in these wells are summarized in Table 4. The data indicate that water levels in 19 out of the 21 wells that lie east of the Solitario Canyon fault vary by only 2.74 m (from 728.46 masl to 731.20 masl). As indicated in Table 4, wells H-6, WT-7, WT-10, and H-5, which are all west of the Solitario Canyon fault (except for H-5, which lies west of a splay of the Solitario Canyon fault), have water levels ranging from 775.55 masl to 776.08 masl, which is approximately 46 m higher than the water levels east of the Solitario Canyon fault (except in WT#6, see discussion below for Assumption 3). Thus, it appears that the Solitario Canyon fault creates an elevation discontinuity in an otherwise uniform water table.

2. The Solitario Canyon fault is assumed to act as a barrier to lateral flow at the water table (Section 6.2).

This assumption provides the mechanism to explain the observed 46-meter difference in water table elevation discussed in the paragraph above. This large-displacement, normal fault may act as a barrier to lateral flow because of the formation of low-permeability fault gouge, or because it juxtaposes layers with contrasting hydrogeologic properties.

3. It is assumed that the observed water levels in boreholes WT#6, G-2, and WT-24 represent perched water (Section 6.2).

Observed water levels in these three boreholes from northern Yucca Mountain (located east of the Solitario Canyon fault) are much higher than 730 masl. In borehole WT#6, water levels measure about 1,034 masl. In boreholes USW G-2 and USW WT-24, not included in Table 4, water levels are approximately 1,020 masl and 986 masl, respectively (DTN: GS980508312313.001). These data indicate that existing data are inadequate to define precisely the water table altitude beneath northern Yucca Mountain. The perched water assumption enables the UZ Model to simulate and calibrate to perched water data under northern Yucca Mountain.

5.2 ASSUMPTIONS REGARDING NUMERICAL GRID CONSTRUCTION

The following two assumptions relate to the definition of low-permeability, zeolitic regions within certain UZ Model layers. Within UZ Model layers ch1, ch2, ch3, ch4, and ch5, the tuff has been altered from vitric to zeolitic in some areas. For the purposes of flow and transport modeling, the principal differences between these two types of tuff are the adsorptive properties and the saturated hydraulic conductivity. Each gridblock in these UZ Model layers must be assigned to either the vitric or zeolitic material.

4. It is assumed that saturated hydraulic conductivity (K_{sat}) data can be used as a surrogate for assigning gridblocks within certain layers of the Calico Hills nonwelded (CHn) hydrogeologic unit either vitric or zeolitic material names (and thus, separate hydrogeologic properties) (Section 6.6.3).

There are two main reasons why K_{sat} data are used as a surrogate to assign gridblocks either vitric or zeolitic material names. First, existing data show that the K_{sat} of vitric tuff is orders of magnitude greater than that of zeolitic tuff (Flint 1998, p. 44). Also, there are much more available data on K_{sat} values than on mineralogic alteration (i.e., % zeolite).

5. It is assumed that, in UZ Model layers ch1, ch2, ch3, ch4, and ch5, tuff is vitric where K_{sat} is greater than 10^{-10} m/s and zeolitic where K_{sat} is less than 10^{-10} m/s (Section 6.6.3).

Results from analyses by Flint (1998, p. 44) indicate that vitric K_{sat} values are on the order of 10^{-7} m/s, while zeolitic K_{sat} values are on the order of 10^{-10} to 10^{-11} m/s. No definitive K_{sat} cutoff value exists by which to distinguish vitric material from zeolitic material, as this transition occurs over about three orders of magnitude. The K_{sat} -value cutoff of 10^{-10} m/s is somewhat arbitrarily chosen; however, the sensitivity of the 10^{-10} m/s cutoff is not expected to be significant compared to using a 10^{-9} m/s or 10^{-8} m/s cutoff, since these contours are closely spaced in the repository footprint within the ISM3.0 Rock Properties Model (see Figure 4).

The final assumption pertains to the representation of faults within the UZ Model grids.

6. It is assumed that the simplification of representing steeply dipping faults as vertical in the UZ Model grids will not significantly affect model calculations (Section 6.3).

This assumption is supported by sensitivity studies, to be reported in a separate AMR, that indicate that flow through faults is much more sensitive to the rock properties assigned to fault zones than to slight variations in fault dip.

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6. ANALYSIS/MODEL

6.1 NUMERICAL GRID DEVELOPMENT -- OVERVIEW & APPROACH

Numerical grids of the unsaturated zone beneath Yucca Mountain are used to develop calibrated hydrogeologic property sets and flow fields, to test conceptual hypotheses of flow and transport, and to predict flow and transport behavior under a variety of climatic and thermal loading conditions. This report describes the development of four different sets of grids. The purpose and general characteristics of each grid set are summarized in Table 6. A description of the steps involved in the generation of these grids is provided in the following sections and in scientific notebooks. Key scientific notebooks used for numerical grid generation activities described in this AMR, along with relevant page numbers and accession numbers, are listed in Table 7.

Table 6. Summary of Grids Developed for FY 99 UZ Modeling Activities

DTN (filename)	Purpose	Grid Description
LB990501233129.002 (primary.mesh) ¹ (1doldtrans.mesh) ² (1doldstdyst.mesh) ² (1dtrans.mesh) ³ (1dstdyst.mesh) ³	1-D hydrogeologic property set inversions and calibrations	Consists of 1-D columns centered at borehole locations. Enforces borehole contact elevation picks (except for UZ-14) based on the GFM3.1 file "pix99el.dat" (DTN: MO9901MWDGFM31.000) and HGU boundaries defined by Flint (1998). UZ-14 layer-contact elevations were extracted from a 3-D grid generated using GFM3.1 isochore and elevation data provided on a regular grid spacing of 61 × 61 m. ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Boreholes used in the 1-D meshes include: SD-6, SD-7, SD-9, SD-12, NRG#5, NRG-6, NRG-7a, UZ#4, UZ-14, UZ#16, and WT#24. <i>See Attachment III for additional details.</i>
LB990501233129.003 (primary.mesh) ¹ (2d2ktrans.mesh) ³ (2d2kstdyst.mesh) ³	Fault hydrogeologic property calibration	East-west, cross-sectional grid through borehole UZ-7a. Grid columns are generated using GFM3.1 isochore and elevation data provided on a regular grid spacing of 61 × 61 m (DTN: MO9901MWDGFM31.000). ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Uses fracture hydrogeologic data in Table 5 to generate the dual-permeability meshes. <i>See Attachment IV for additional details.</i>
LB990501233129.004 (primary.mesh) ¹ (3d2kcalib_pc1.mesh) ⁴ (3d2kcalib_pc2.mesh) ⁵	3-D UZ Model calibration	Consists of a plan-view grid with discretization along major faults, the ESF, and the ECRB. Also contains columns of grid-blocks centered at borehole locations. The 3-D grids are generated using GFM3.1 isochore and elevation data provided on a regular grid spacing of 61 × 61 m (DTN: MO9901MWDGFM31.000). ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Uses fracture hydrogeologic data in Table 5 to generate the dual-permeability meshes. <i>See Attachment V for additional details.</i>

- NOTES: ¹ The primary mesh represents matrix blocks only; also referred to as an ECM grid.
² Dual-k mesh generated with previously developed fracture porosities (see footnote to Table 5).
³ Dual-k mesh generated with fracture properties from Table 5.
⁴ Dual-k mesh generated with fracture properties from Table 5, with perched water conceptual model #1 (flow through zeolites) modifications.
⁵ Dual-k mesh generated with fracture properties from Table 5, with perched water conceptual model #2 (reduced fracture flow through zeolites) modifications.

Table 6. Summary of Grids Developed for FY 99 UZ Modeling Activities (Cont.)

DTN (filename)	Purpose	Grid Description
LB990701233129.001 (primary.mesh) ¹ (3d2kpa.mesh) ³ (3d2kpa_pc1.mesh) ⁴ (3d2kpa_pc2.mesh) ⁵	To generate 3-D flow fields for PA	Consists of a plan-view grid with repository refinement, but no ESF or ECRB discretization. The 3-D grids are generated using GFM3.1 isochore and elevation data provided on a regular grid spacing of 61 × 61 m (DTN: MO9901MWDGFM31.000). ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Uses fracture hydrogeologic data in Table 5 to generate the dual-permeability meshes. See Attachment VI for additional details.

- NOTES: ¹ The primary mesh represents matrix blocks only; also referred to as an ECM grid.
² Dual-k mesh generated with previously developed fracture porosities (see footnote to Table 5).
³ Dual-k mesh generated with fracture properties from Table 5.
⁴ Dual-k mesh generated with fracture properties from Table 5, with perched water conceptual model #1 (flow through zeolites) modifications.
⁵ Dual-k mesh generated with fracture properties from Table 5, with perched water conceptual model #2 (reduced fracture flow through zeolites) modifications.

Table 7. YMP Scientific Notebooks Used for FY 99 Numerical Grid Development and Grid Resolution Sensitivity Analyses

LBNL Scientific Notebook ID	M&O Scientific Notebook ID	Relevant Pages	ACC#
YMP-LBNL-YSW-JH-2 (YMP-LBNL-YSW-JH-2A)	SN-LBNL-SCI-143-VI	3-37, 39-45, 45-57 (27-168 of ref binder)	MOL.19990720.0199
YMP-LBNL-GSB-LP-2	SN-LBNL-SCI-103-VI	38-46, 49-68, 72-75	MOL.19990720.0200
YMP-LBNL-GSB-1.1.2 (and reference binder)	SN-LBNL-SCI-003-VI	85-89, 97, 106, 112-116 (4-8, 12, 108 of ref binder)	MOL.19990720.0203
YMP-LBNL-GSB-1.3	SN-LBNL-SCI-071-VI	42-45	MOL.19990720.0204
YMP-LBNL-YSW-2	SN-LBNL-SCI-120-VI	18-20, 129-132	MOL.19990720.0201
YMP-LBNL-YSW-WZ-1	SN-LBNL-SCI-115-VI	52-56, 66-72	MOL.19990720.0202

Data extracted from GFM3.1 and ISM3.0 form the basis for numerical grid development. With these data, an initial 2-D (plan-view) grid is developed defining borehole, fault, ESF, ECRB, and repository column locations, where appropriate. Using the 2-D grid as the basis for column locations, a 3-D (ECM) grid is constructed using layer horizon and thickness data from GFM3.1. Initial grid generation is followed by an iterative process of grid evaluation and modification in order to achieve appropriate spatial resolution and representation of important features and to ensure proper connections between the various elements of the grid. Revisions are made accordingly until these criteria are met. Next, the 3-D (ECM) grid is modified to allow for dual-continua processes (matrix and fracture flow) using a dual-permeability (dual-k) mesh maker, DKMgenerator V1.0 (ACC: MOL.19990909.0315). The DKMgenerator V1.0 incorporates information (i.e., fracture porosity, spacing, aperture, and fracture-matrix interaction area) from fracture data analyses (see Table 5) into the grids.

The computer code WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) is used to generate 1-, 2- and 3-D integral finite difference (IFD) grids for the UZ Model domain. The type

of grid generated by WinGridder V1.0 is consistent with the computational requirements of the TOUGH2 numerical code simulator (Pruess 1991, pp. 27-30, 41-42). TOUGH2 and the inverse modeling code ITOUGH2 use cells, or gridblocks, and connections between those gridblocks to represent the flow system without requiring the global location of each gridblock or connection. This approach provides great flexibility in describing complex flow geometry and relationships between individual objects within the system.

Unlike other gridding software, WinGridder V1.0 has the capability of designing complex, irregular grids with large numbers of cells and connections, and it can handle incorporation of nonvertical faults and other embedded refinements, such as waste emplacement drift spacing within the potential repository area at Yucca Mountain.

Described in this report are the methods used to develop numerical grids for hydrogeologic-property set inversions, for model calibration, and for calculation of 3-D, unsaturated-zone flow fields for PA. The stages of grid development include the following:

1. Establish domain boundaries and location of important calibration features such as boreholes, alcoves, niches, ESF, and ECRB. (Section 6.2)
2. Determine UZ Model layers and fault geometries based on GFM3.1, ISM3.0, and correlation with Flint's (1998) HGUs. (Section 6.3)
3. Extract and format GFM3.1 and ISM3.0 data for incorporation into 3-D grids. (Section 6.4)
4. Generate 2-D grid, incorporating information from Steps 1 and 2, and refine as needed to capture spatial variability in USGS infiltration data. (Section 6.5)
5. Generate 3-D (ECM) grid, based on the column locations established in the 2-D grid and data from Step 3. (Section 6.6)
6. Combine the results of fracture analyses with the ECM grid from Step 5 to generate a dual-permeability mesh. (Section 6.7)

The process of verifying that appropriate gridblock material names, gridblock volumes and locations, connection lengths and interface areas between gridblocks, and direction of absolute permeability are used in the UZ Model numerical grids is documented in Section 6.8 and in Attachments III through VI. Section 6.8 also summarizes results from corroborative studies that support the use of fairly coarse numerical grid resolution to model flow and transport processes.

6.2 BOUNDARIES AND CALIBRATION FEATURES

The areal domain of the UZ Model encompasses approximately 40 km² of the Yucca Mountain area. Yucca Wash marks the northern model boundary, while the approximate latitude of borehole G-3 defines the southern boundary. The eastern model boundary coincides with the Exile Hill, "Toe," and Bow Ridge faults, and the western boundary lies approximately 1 km west of the Solitario Canyon fault. These boundaries encompass many of the existing hydrology wells for

which extensive moisture tension data are used as calibration points for determining layer properties. One important objective of selecting these boundaries was to minimize potential boundary effects on numerical simulation results within the repository footprint. Table 8 lists the Nevada State Planar (NSP) coordinates for the domain boundary, while Figure 1 shows a map view of the model domain, including the repository boundary, the paths of the ESF and ECRB, major faults defined in GFM3.1, and selected boreholes.

Table 8. UZ Model Areal Boundary Coordinates

Easting (m)	Northing (m)
168100.0	229500.0
172687.1	229494.6
172890.1	229953.3
173077.1	230704.2
173075.5	230754.3
173063.1	231405.1
173083.6	231855.7
173091.1	232106.0
173105.9	232957.1
173152.9	233658.0
173152.5	233708.1
173030.3	234308.9
173027.9	234959.7
173226.6	235860.9
173222.6	236061.1
173225.0	236161.2
173294.4	237012.3
172914.9	237813.4
172857.0	238213.9
169600.0	239000.0

DTN: LB990051233129.001

The upper boundary of the UZ Model is the bedrock surface (topography minus alluvium), which is defined by the GFM3.1 file "s31bedrockRWC.2grd." The lower boundary is the water table, or potentiometric surface, derived from water level elevation data in the RIB (DTN: MO9609RIB00038.000). Borehole water level elevations beneath northern Yucca Mountain suggest a "large hydraulic gradient," as seen in the GFM3.0 file "potentiometric.2grd" (DTN: MO9804MWDGFM03.001), with water levels rising from about 730 masl in the repository area to over 1,000 m only a few kilometers north of the repository area. One alternative explanation for the apparent 300-m water level difference is the occurrence of perched or semi-perched water under northern Yucca Mountain (DTN: GS980508312313.001; Ervin et al. 1994, p. 15; Czarnecki et al. 1994; Czarnecki et al. 1995). For the purpose of developing UZ Model grids,

water table elevations beneath northern Yucca Mountain are assumed to represent perched water, as stated in Section 5, Assumption 3.

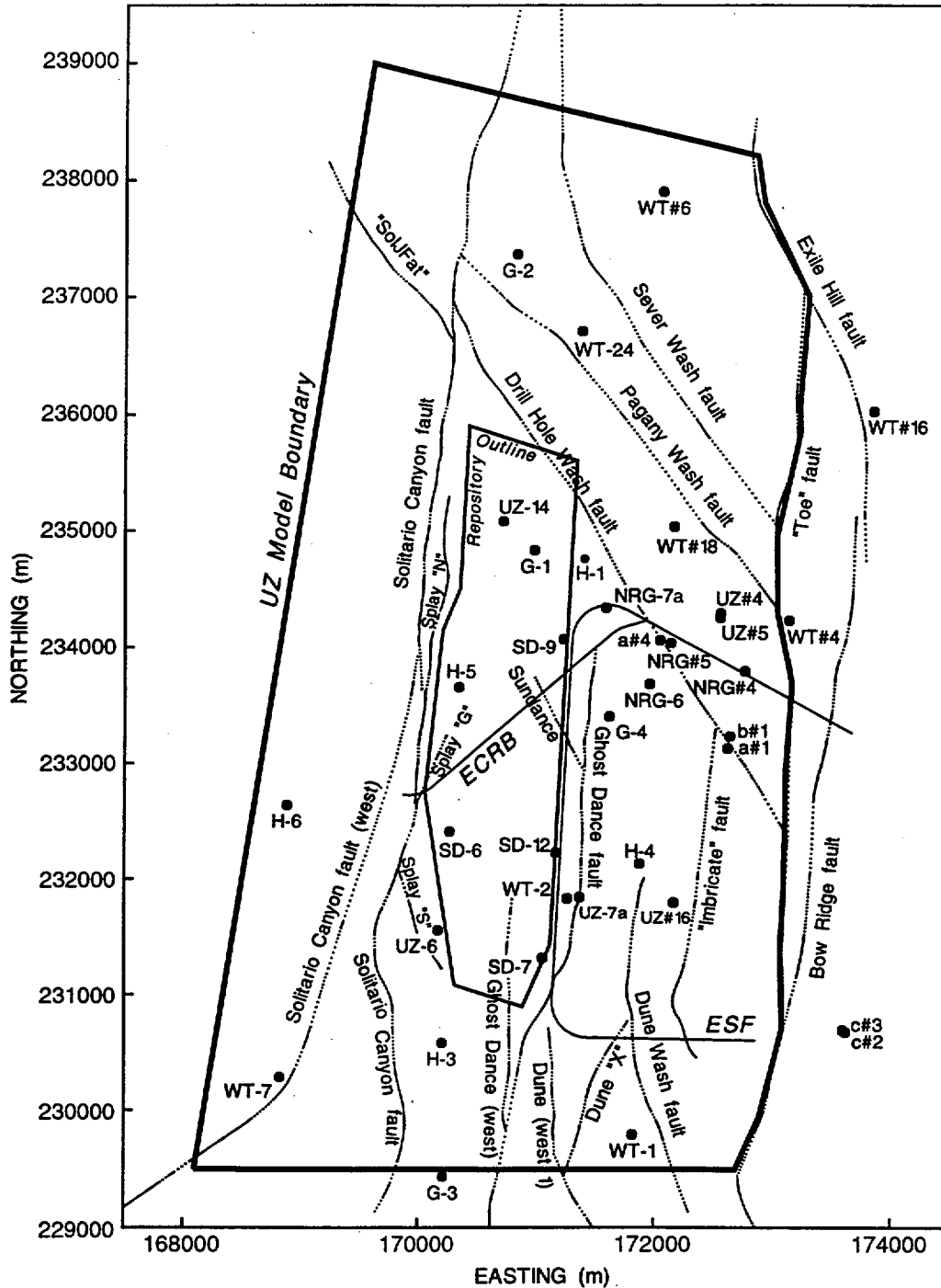


Figure 1. Plan-View Schematic Showing the UZ Model Boundary, the Repository Outline, Major Fault Locations Derived from GFM3.1, Selected Boreholes, the ESF, and the ECRB

UZ Model calibration features represented as column centers in the 1-D inversion and 3-D calibration grids include:

1. Vertical boreholes USW SD-6, USW SD-7, USW SD-9, USW SD-12, UE-25 UZ#4, USW UZ-14, UE-25 UZ#16, USW UZ-6, USW UZ-7a, UE-25 NRG#4, UE-25 NRG#5, USW NRG-6, USW NRG-7a, USW WT-24, UE-25 WT#6, USW G-1, USW G-2, USW G-4, USW H-5, and UE-25 a#4. [For simplicity, the borehole names used throughout the remainder of this document drop the USW and UE-25 prefixes.]
2. ESF Alcoves 3, 5, 6, and 7 (Alcove 4 and borehole NRG#4 are only approximately 16 m apart and are represented by one column centered on NRG#4).
3. ESF Niches "3107," "3566," "3650," and "4788."
4. ESF and ECRB centerline locations in plan view.

Boreholes, alcoves, niches, the ESF, and the ECRB are important for hydrogeologic property set inversions and calibration because these are the locations from which data have been collected, and because their locations determine the upper boundary condition (surface infiltration rate).

The GFM3.1 file "boreholepaths.dat" (in DTN: MO9901MWDGFM31.000) is used to define the location of boreholes that will serve as column centers within the various UZ Model grids. Since the coordinates contained within this file are listed in feet, rather than meters (which is the desired unit of measure in the UZ Model), a simple unit conversion is performed (1 ft = 0.304785 m). The GFM3.1 file "boreholepaths.dat" is also used to define the location of the ESF and ECRB.

The Microsoft Excel Worksheet "ESF4_XYZ V.03.XLS" (ESF4_XYZ V.03.XLS V3.0, STN: 30092 V.03, Version 3.0) is used to determine ESF alcove and niche locations. (With this worksheet, the user supplies the ESF Station in meters from the North Portal, and the worksheet calculates the NSP coordinates in meters.)

Alcoves 5, 6, and 7 have lengths in excess of 120 m. Column centers in the 2-D grid are placed at the approximate location of the midpoint (along the length) of these alcoves rather than at their intersection point with the ESF centerline. The locations of boreholes, alcoves, and niches are summarized in Table 9. Derivation of these coordinates is documented in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 11-13).

The spatial relationship between boreholes, alcoves, niches, faults (determination of fault locations in the 2-D grid is described below), and ESF/ECRB locations is such that these features may intersect or lie within 30 meters of each other (which is typically less than the desired lateral resolution of the grid). As a result, the location of certain features (i.e., column centers) is prioritized. For example, Alcove 4 and borehole NRG#4 are about 16 meters apart and are represented by one column centered on NRG#4. In general, the following hierarchy is enforced: boreholes (highest priority), alcoves and niches, faults, ESF, ECRB, other domain nodes (lowest priority).

Table 9. Location of Boreholes, Alcoves, and Niches in the UZ Inversion and Calibration Models

Easting (m)	Northing (m)	Feature
170985	234837	G-1
170833	237374	G-2
171619	233407	G-4
170347	233659	H-5
172758	233795	NRG#4
172133	234041	NRG#5
171956	233687	NRG-6
171589	234343	NRG-7a
171169	232233	SD-12
171058	231317	SD-7
170268	232413	SD-6
171234	234074	SD-9
170723	235087	UZ-14
172160	231800	UZ#16
172551	234293	UZ#4
170169	231555	UZ-6
171371	231848	UZ-7a
171382	236718	WT-24
172058	237908	WT#6
172042	234066	a#4
171273.9	233327.1	Niche3566
171269.5	233243.2	Niche3650
171297.9	233785.5	Niche3107
171210.0	232106.8	Niche4788
173019.7	233644.4	Alcove3 ¹
171373.5	234045.3	Alcove5 ²
171355.0	233156.3	Alcove6 ²
171295.5	231831.2	Alcove7 ²

DTN: MO9901MWDGFM31.000

NOTES: ¹ Coordinates calculated with "ESF4_XYZ V.03.XLS" using ESF station location given in Barr et al. (1996, p. 122).

² Coordinates calculated with "ESF4_XYZ V.03.XLS" using ESF station locations given in Albin et al. (1997, p. 8).

6.3 UZ MODEL LAYERS AND FAULT GEOMETRIES

As discussed previously in Section 4, layering within the UZ Model grid is chosen to correspond as closely as possible to HGUs, in order to facilitate usage of rock properties data. Table 10 provides a correlation between major hydrogeologic units, GFM3.1 lithostratigraphic units, UZ Model layers, and Flint's (1998) HGUs. In many cases, HGUs correlate 1-to-1 with, or are simple combinations of, GFM3.1 layers. In a few instances, multiple HGUs can be present within one GFM3.1 layer, such as within the Yucca Mountain Tuff (Tpy), the lower nonlithophysal zone of the Topopah Spring Tuff (Tptpln), or the Calico Hills Formation (Tac). Using Table 10 as a basis for UZ Model layering, GFM3.1 layer-thickness (isochore) grid files are combined or subdivided, as appropriate (see Section 6.4.1), to correspond to Flint's (1998) HGUs.

Table 10. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation

Major Unit (Modified from Montazer and Wilson 1984)	GFM3.1 Lithostratigraphic Nomenclature*	FY 99 UZ Model Layer	Hydrogeologic Unit (Flint 1998, pp. 3-4)
Tiva Canyon welded (TCw)	Tiva_Rainier	tcw11	CCR, CUC
	Tpcp	tcw12	CUL, CW
	TpclD		
	Tpcpv3	tcw13	CMW
	Tpcpv2		
Paintbrush nonwelded (PTn)	Tpcpv1	ptn21	CNW
	Tpbt4	ptn22	BT4
	Tpy (Yucca)		
		ptn23	TPY
		ptn24	BT3
	Tpbt3		
	Tpp (Pah)	ptn25	TPP
	Tpbt2	ptn26	BT2
	Tptrv3		
Tptrv2			

NOTE: * Buesch et al. (1996) define the units in the Paintbrush Group (layers beginning with "Tp"). Buesch and Spengler (1999) describe the symbols for the Crater Flat Tuffs. GFM3.1 nomenclature uses the symbols that are included parenthetically below layer Tpbt1.

Table 10. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation (Cont.)

Major Unit (Modified from Montazer and Wilson 1984)	GFM3.1 Lithostratigraphic Nomenclature*	FY 99 UZ Model Layer	Hydrogeologic Unit (Flint 1998, pp. 3-4)
Topopah Spring welded (TSw)	Tptrv1	tsw31	TC
	Tptrn		
		tsw32	TR
	Tptrl, Tptf	tsw33	TUL
	Tptpul		
	Tptpmn	tsw34	TMN
	Tptpll	tsw35	TLL
	Tptpln	tsw36	TM2 (upper 2/3 of Tptpln)
		tsw37	TM1 (lower 1/3 of Tptpln)
	Tptpv3	tsw38	PV3
Tptpv2	tsw39	PV2	
Calico Hills nonwelded (CHn)	Tptpv1	ch1 (vit, zeo)	BT1 or BT1a (altered)
	Tpbtl		
	Tac (Calico)	ch2 (vit, zeo)	CHV (vitric) or CHZ (zeolitic)
		ch3 (vit, zeo)	
		ch4 (vit, zeo)	
		ch5 (vit, zeo)	
	Tacbt (Calicobt)	ch6	BT
	Tcpuv (Prowuv)	pp4	PP4 (zeolitic)
	Tcpuc (Prowuc)	pp3	PP3 (devitrified)
	Tcpm (Prowmd)	pp2	PP2 (devitrified)
	Tcplc (Prowlc)		
	Tcplv (Prowlv)		
Tcpbt (Prowbt)	pp1	PP1 (zeolitic)	
Tcbuv (Bullfroguv)			

NOTE: * Buesch et al. (1996) define the units in the Paintbrush Group (layers beginning with "Tp"). Buesch and Spengler (1999) describe the symbols for the Crater Flat Tuffs. GFM3.1 nomenclature uses the symbols that are included parenthetically below layer Tpbtl.

Table 10. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation (Cont.)

Major Unit (Modified from Montazer and Wilson 1984)	GFM3.1 Lithostratigraphic Nomenclature*	FY 99 UZ Model Layer	Hydrogeologic Unit (Flint 1998, pp. 3-4)
Crater Flat undifferentiated (CFu)	Tcbuc (Bullfroguc)	bf3	BF3 (welded)
	Tcbm (Bullfrogmd)		
	Tcblc (Bullfroglc)		
	Tcblv (Bullfroglv)	bf2	BF2 (nonwelded)
	Tcbbt (Bullfrogbt)		
	Tctuv (Tramuv)		
	Tctuc (Tramuc)	tr3	Not Available
	Tctm (Trammd)		
	Tctlc (Tramlc)		
	Tctlv (Tramlv)	tr2	Not Available
	Tctbt (Trambt)		

NOTE: * Buesch et al. (1996) define the units in the Paintbrush Group (layers beginning with "Tp"). Buesch and Spengler (1999) describe the symbols for the Crater Flat Tuffs. GFM3.1 nomenclature uses the symbols that are included parenthetically below layer Tpbt1.

Faults are important features to include in the UZ Model grids since they may provide fast pathways for flow or may serve as barriers to flow. A fault can be a surface with arbitrary shape in the 3-D UZ Model domain and is represented as a surface (defined by a set of x, y, z data on a regular grid spacing) in GFM3.1. In UZ Model grids, fault surfaces are represented by a series of connected columns of gridblocks. Faults can be represented in the grid as either vertical or nonvertical features. Many of the faults at Yucca Mountain are steeply dipping, particularly within the unsaturated zone. For UZ flow and transport modeling studies of Yucca Mountain, it is believed that flow through faults is much more sensitive to the rock properties assigned to fault zones rather than to slight variations in fault dip. Since large numbers of gridblocks are needed to discretize nonvertical fault zones (which adds significantly to the computational time of model calibration and forward simulations), certain criteria have been developed under Assumption 6 (Section 5) to reduce the total number of gridblocks along faults in order to simplify the UZ Model grids. Faults are modeled as vertical if they meet any of the following criteria: (a) their average dip exceeds 85 degrees, (b) their average dip exceeds 80 degrees and they lie sufficiently far (>1 km) from the repository layout area so as not to significantly affect flow and transport calculations, (c) they lie west of the Solitario Canyon fault, or (d) they coincide with UZ Model boundaries. Table 11 lists the GFM3.1 faults that lie within or along UZ Model boundaries.

Table 11. Faults Within the UZ Model Domain

Fault Name	GFM3.1 File Name
Solitario Canyon	f31sol.2grd
Solitario Canyon (west)	f31solwest.2grd
Unnamed – joins Solitario Canyon & Fatigue Wash faults	f31soljfat.2grd
Splay "G"	f31splayg.2grd
Splay "N" (north)	f31splayn.2grd
Splay "S" (south)	f31splays.2grd
Sundance	f31sundance.2grd
"Toe"	f31toe.2grd
Sever Wash	f31sever.2grd
Pagany Wash	f31pagany.2grd
Drill Hole Wash	f31drill.2grd
Ghost Dance	f31ghost.2grd
Ghost Dance (west)	f31ghostw.2grd
Dune Wash	f31dune.2grd
Dune Wash "X"	f31dunex.2grd
Dune Wash (west 1)	f31dunew1.2grd
"Imbricate"	f31imb.2grd
Exile Hill (or Bow Ridge east)	f31exile.2grd

DTN: MO9901MWDGFM31.000

The average slope of each fault is evaluated in order to determine which faults can be reasonably approximated by vertical columns of gridblocks in UZ Model grids. This task involves the calculation of slope along each fault (as it transects the unsaturated zone) using the Slope Grid Calculation utility in EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0). Refer to YMP Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 15-16) for details regarding this calculation. The results are summarized in Table 12.

Table 12. Results of GFM3.1 Fault-Slope Analysis

Fault Name	Slope Range (average)	Minimum Dip	Maximum Dip	Average Dip
Solitario Canyon	2.0 – 6.7 (3.6) north	63.4	81.5	74.5
	1.0 – 2.6 (1.7) south	45.0	69.0	59.5
Solitario Canyon (west)	5.3 – 10.1 (6.2)	79.3	84.3	80.8
"Soljfat"	3.6 – 4.3 (3.8)	74.5	76.9	75.3
Splay "G"	1.7 – 2.3 (2.1)	59.5	66.5	64.5
Splay "N"	1.4 – 2.4 (1.8)	54.5	67.4	60.9
Splay "S"	1.6 – 2.0 (1.8)	58.0	63.4	60.9
Sundance	9.3 – 12.3 (11.6)	83.9	85.4	85.1
"Toe"	3.6 – 5.1 (4.1)	74.5	78.9	76.3
Sever Wash	5.6 – 8.3 (6.8)	79.9	83.1	81.6
Pagany Wash	11.2 – 12.5 (11.6)	84.9	85.4	85.1
Drill Hole Wash	11.4 – 13.1 (11.8)	85.0	85.6	85.2
Ghost Dance	10.2 – 13.8 (11.7)	84.4	85.9	85.1
Ghost Dance (west)	11.3 – 11.9 (11.5)	84.9	85.2	85.0
Dune Wash	1.6 – 3.1 (2.0)	58.0	72.1	63.4
Dune Wash "X"	3.8 – 4.5 (4.1)	75.3	77.5	76.3
Dune Wash (west1)	3.7 – 4.3 (4.0)	74.9	76.9	76.0
"Imbricate"	11.5 – 12.5 (12.1)	85.0	85.4	85.3
Exile Hill	5.5 – 6.6 (6.1)	79.7	81.4	80.7

DTN: LB990051233129.001

In accordance with Assumption 6, the following faults are represented by vertical columns of gridblocks (i.e., are assumed to be vertical) in the UZ Model grids: Solitario Canyon (west), "Soljfat," Sundance, "Toe," Sever Wash, Pagany Wash, Drill Hole Wash, Ghost Dance, Ghost Dance (west), Imbricate, and Exile Hill faults. The remaining faults [Solitario Canyon, Splay "S," Dune Wash, Dune Wash "X," and Dune Wash (west1)] are represented by nonvertical columns of gridblocks in the 3-D grids. Splay faults "N" and "G" lie close to the Solitario Canyon fault and intersect it at a relatively shallow depth. This presents complications when generating the 3-D grids because of the preferred numerical grid resolution and fault representation method (described in Section 6.6.1). Thus, these two splay faults are considered part of the Solitario Canyon fault zone and are not explicitly defined; however, after grid generation, fault properties can be assigned to the gridblocks closest to the location of these faults, as needed.

Preparation of GFM3.1 fault data for incorporation into UZ Model grids first involves a simple unit conversion from feet to meters. The spatial position of the faults is then determined by intersecting each fault surface (*.2grd) with one or more horizontal planes, producing data files describing fault-trace locations at prescribed elevations. Faults represented as vertical features in the UZ grids use fault-trace information at an arbitrary elevation of 1,100 meters above mean sea level. During grid generation, vertical columns of gridblocks are assigned along each fault trace.

Faults represented as nonvertical features (i.e., by nonvertical columns of gridblocks) use fault-trace information at three elevations (one near the land surface, one near the water table, and one located approximately midway between the other two) in order to capture variations in dip. The UZ Model gridding process interpolates the location of each nonvertical fault using data points at the three prescribed elevations. With this approach, the dip of a fault within a given fault column is uniform in the upper interval between the highest and middle elevations, and is again uniform in the lower interval between the middle and lowest elevations. This allows the dip in the upper interval to be different from the dip in the lower interval (which may occur if the fault surface is curved, rather than planar). Furthermore, dip angles within the same vertical interval can be different in different columns (i.e., laterally along a fault). Thus, even a fault with variable dip along its trace can be represented with this method. For specific details regarding manipulation of fault data, refer to Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 14-20).

6.4 EXTRACTION OF GFM3.1 AND ISM3.0 DATA

6.4.1 Isochores

Geologic layers are correlated with Flint (1998) hydrogeologic units (HGUs) in Table 10, and UZ Model layers are determined based on this correlation. Because of its large thickness beneath northern Yucca Mountain, layer Tac is vertically subdivided equally into four layers throughout the UZ Model domain. Based on the relationships provided in Table 10, certain GFM3.1 layers (represented by isochore grids) are combined, while others were subdivided, to create hydrogeologic model layers for the UZ grids.

GFM3.1 isochore grids used in FY 99 UZ grid development include those lying between the upper Tpcpv3 contact and the lower Trambt contact. Layers are combined if (1) they have similar hydraulic properties based on analyses by Flint (1998), (2) they are very thin across Yucca Mountain, or (3) property data are very limited for the rock units. GFM3.1 isochores are subdivided if rock property data exists that suggest two or more distinct hydrogeologic layers within a geologic unit.

For specific details describing the manipulation and formatting of GFM3.1 isochore files, refer to Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 24-28). Below is a brief summary of the steps taken.

GFM3.1 isochore files that are not combined or subdivided include:

- ia31cpv1RWC.2grd
- ia31tppRWC.2grd
- ia31tpmnRWC.2grd
- ia31tpllRWC.2grd
- ia31tpv3RWC.2grd
- ia31tpv2RWC.2grd
- ia31tacbRWC.2grd
- ia31prowuvRWC.2grd
- ia31prowucRWC.2grd

These grids, which contain regularly spaced (200 × 200 ft) data, require no manipulation other than simple formatting for incorporation into the UZ grids. EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0) is used to export the regularly spaced data and to convert the units (x, y, and thickness) from feet to meters. Since GFM3.1 data coverage extends well beyond the UZ Model boundaries, each data file is reduced to the approximate UZ Model domain using the EARTHVISION V4.0 Graphic Editor to remove data points lying south of N 229,000 m and east of E 174,300 m.

GFM3.1 isochore files that are combined include:

- ia31cpv3RWC.2grd + ia31cpv2RWC.2grd
- ia31bt4RWC.2grd + 1/3(ia31tpyRWC.2grd)
- ia31bt3RWC.2grd + 1/3(ia31tpyRWC.2grd)
- ia31bt2RWC.2grd + ia31trv3RWC.2grd + ia31trv2RWC.2grd
- ia31trv1RWC.2grd + ia31trmRWC.2grd
- ia31trltfRWC.2grd + ia31tpulRWC.2grd
- ia31tpv1RWC.2grd + ia31bt1RWC.2grd
- ia31prowmdRWC.2grd + ia31prowlcRWC.2grd
- ia31prowlvRWC.2grd + ia31prowbtRWC.2grd + ia31bulluvRWC.2grd
- ia31bullucRWC.2grd + ia31bullmdRWC.2grd + ia31bulllcRWC.2grd
- ia31bulllvRWC.2grd + ia31bullbtRWC.2grd + ia31tramuvRWC.2grd
- ia31tramucRWC.2grd + ia31trammdRWC.2grd + ia31tramlcRWC.2grd
- ia31tramlvRWC.2grd + ia31trambtRWC.2grd

The EARTHVISION V4.0 Formula Processor is used to add the *.2grd files as shown above. The resulting files are then formatted as previously described for uncombined isochores.

GFM3.1 isochore files that are subdivided are described below and include:

- ia31tpyRWC.2grd
- ia31trv1RWC.2grd + ia31trmRWC.2grd
- ia31tplnRWC.2grd
- ia31tacRWC.2grd

GFM3.1 layer Tpy (Yucca Mountain Tuff)- Based on the HGUs defined by Flint (1998), GFM3.1 layer Tpy is subdivided vertically into 3 layers of equal proportion (i.e., 1/3, 1/3, 1/3). These three layers have the following characteristics:

- The upper portion is typically nonwelded and has properties similar to Tpbt4; therefore, it is combined with layer Tpbt4 (GFM3.1 isochore file "ia31bt4RWC.2grd") and corresponds to HGU "BT4."
- The middle portion can become moderately welded to the north (porosity <30%). This middle portion corresponds to HGU "TPY."

- The lower portion is typically nonwelded and has properties similar to Tpbt4 and Tpbt3; thus, it is combined with layer Tpbt3 (GFM3.1 isochore file "ia31bt3RWC.2grd") and corresponds to HGU "BT3."

GFM3.1 layers Tptrv1 and Tptrn (upper Topopah Spring Tuff)- The densely welded Tptrv1 is relatively thin (0-2 m thick, typically <0.5 m) across Yucca Mountain (Flint 1998, p. 27). Given a minimum vertical resolution of 1.5 m for the UZ Model grids, this layer would be missing from UZ simulations across most of Yucca Mountain. In order to capture this potentially important flow unit at the PTn/TSw interface, GFM3.1 isochores for Tptrv1 and Tptrn were combined, then the upper 2 m of this combined unit were assigned a distinct model layer name corresponding to Flint's "TC" HGU. The remaining thickness of the combined unit (Tptrv1 + Tptrn - 2 m) corresponds to Flint's "TR" HGU.

GFM3.1 layer Tptpln (Topopah Spring, lower nonlithophysal)- Tptpln is characterized by HGUs "TM2" and "TM1." According to the proportions given in Flint (1998, p. 3), GFM3.1 layer Tptpln is vertically subdivided into an upper portion (with 2/3 the total thickness of Tptpln) and a lower portion (with 1/3 the total thickness of Tptpln) for incorporation into the UZ Model.

GFM3.1 layer Tac (Calico Hills Formation)- The Tac is subdivided vertically into four layers of equal proportion (1/4, 1/4, 1/4, 1/4) because of its large thickness beneath northern Yucca Mountain.

After the isochores have been subdivided according to the specified criteria/proportions, they are formatted using the same steps used to format the uncombined isochores.

6.4.2 Reference Horizons, and Top and Bottom UZ Model Boundaries

WinGridder V1.0 generates a numerical grid based on the elevations of three major horizons: (1) a top boundary (e.g., the topographic or bedrock surface), (2) a structural reference horizon, which identifies faults and their associated offsets, and (3) a bottom boundary (e.g., the water table). The reference horizon is a surface from which elevations of all hydrogeologic-unit interfaces are calculated by stacking layer thicknesses above or below it based on their stratigraphic position. All offsets resulting from faulting are described by the reference horizon data. Any portions of hydrogeologic units lying above the top boundary or below the bottom boundary after stacking are removed (clipped).

GFM3.1 horizons used:

- s31bedrockRWC.2grd (bedrock/present-day erosional surface; UZ Model top boundary)
- s31TpcpUNCUT.2grd (top of Tpcp; surface used in the absence of Tpcp isochore)
- s31Tpbt4EX.2grd (top of Tpbt4; primary structural reference horizon for UZ grids).

The top of layer Tpcp (the contact between the crystal-rich and crystal-poor tuffs of the Tiva Canyon, defined as a surface in GFM3.1) is used to separate UZ Model layers "tcw11" and "tcw12," since no GFM3.1 isochore grids exist for these layers.

As with the isochore grids, the horizon grids, which also contain regularly spaced (200 × 200 ft) data, require no manipulation other than simple formatting for incorporation into the UZ Model. EARTHVISION V4.0 is used to export the regularly spaced data and to convert the units (x, y, and elevation) from feet to meters. The complete details for formatting these GFM3.1 horizon grids are provided in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 31-33).

The lower model boundary (i.e., the water table) is discussed previously in Section 5 (Assumptions 1-3) and in Section 6.2.

6.5 2-D GRID GENERATION

Used by WinGridder V1.0 to organize grid information, the 2-D (map-view) grid defines the structure of columns and segments that provide the basis for projecting the 3-D grid. Each column is represented by a node in map-view indicating the column's position in the x-y plane. Additionally, the shape of each column is a polygon in the x-y plane whose boundaries consist of segments that are defined prior to 3-D grid generation.

Grid development begins with the assignment of nodes in map view for each object (e.g., domain nodes, fault nodes, repository nodes) with specified orientation and density. Based on the location of these nodes, a primary 2-D grid is generated using Voronoi tessellation techniques embedded in the WinGridder V1.0 numerical code. The 2-D grid is then improved systematically and interactively by deleting physically incorrect or unnecessary connections. A few iterations of these steps, including adding, moving, and deleting certain nodes, are necessary to create a final 2-D grid, or column scheme, that serves as the basis for generating the vertical component of the grid.

Two-dimensional grid generation for the UZ Model considers the location of domain and repository boundaries; borehole, alcove, and niche locations; and map-view traces of the ESF, ECRB, and major faults. Various subsets of these features are included in the different UZ Model grids depending on their intended use. Since the 1-D hydrogeologic property set inversions only consider rock property data from vertical boreholes, only borehole locations are relevant when generating this particular grid. The 3-D, UZ Model calibration grid, on the other hand, assigns nodes in 2-D to the location of all data sources (i.e., boreholes, alcoves, niches, ESF, and ECRB), as well as within domain and repository boundaries and along faults. The mesh designed for PA activities (to generate flow fields) is populated with calibrated data to perform mainly predictive studies and, thus, uses only repository and UZ Model domain boundaries, fault traces, and borehole locations to formulate the 2-D grid.

Another issue considered in 2-D grid generation is spatial resolution. Grid resolution (node spacing) is a compromise between computational efficiency and a need to capture spatial variability in rock properties and boundary conditions (such as infiltration rate). In the case of model calibration, the goal is to generate a 3-D grid that runs as efficiently as possible, while capturing the level of detail necessary to perform reasonably accurate calibrations. The result is a fairly coarse 2-D grid with refinement added only in the location of calibration features (e. g., boreholes, alcoves, niches, ESF, and ECRB) and along faults. In doing this, the grid captures the needed spatial variability in the infiltration rate at the bedrock surface. Unlike the calibration

grid, the grid for PA activities contains greater numerical resolution within the repository boundary, the area most important to predictive studies.

6.6 3-D GRID GENERATION

Once UZ Model grid nodes are assigned in plan view and polygons are generated representing the lateral extent of each grid column, model layer contact elevations are determined for each vertical column within the grid based on the value of the closest GFM3.1 isochore or surface horizon data point (recall that GFM3.1 data are on a regular spacing of 61×61 m). With this approach, no interpolation of GFM3.1 data to the exact location of a UZ Model node is performed. The estimated maximum error in layer contact elevations at UZ Model column centers associated with this "nearest value" approach is about 5 m, assuming that the hydrogeologic layers dip 10 degrees. This amount of potential error is considered insignificant to grid development and subsequent site-scale UZ Model simulation activities because lateral column dimensions almost always exceed 61×61 m (except along faults); thus, encompassing the nearest GFM3.1 data point.

The 3-D grid describes the location, rock material name, and connection information for each 3-D gridblock in the UZ Model domain. All 3-D gridblocks are generated column by column with WinGridder V1.0, based on the 2-D (plan-view) grid design, to ensure that each vertical connection occurs between adjacent gridblocks and that each gridblock has at least one vertical connection. Lateral connections are then generated segment by segment within a model layer, with each segment joining two neighboring columns. This ensures that only gridblocks in two adjacent columns have lateral connections and that no connections between two adjacent columns are missing.

For a given column, 3-D gridblocks are built for each hydrogeologic unit, first above the Tpb4 structural reference surface until reaching the bedrock surface, and then below this reference surface down to the water table. The interfaces of the generated gridblocks are located exactly at the interfaces of the corresponding hydrogeologic layers. Vertical connections within the column are generated after each gridblock is built. A dummy gridblock is added to the top and bottom of each column to enable assignment of model boundary conditions.

When building lateral connections, each pair of two adjacent columns are searched top-to-bottom. If gridblocks in the adjacent columns belong to the same layer, a lateral connection is built for them. The lateral interface area is determined by the lesser height of two gridblocks that are connected. If the layer is missing in one of the two neighboring columns (resulting from a layer pinching out), the gridblock representing the last occurrence of the pinch-out layer is laterally connected to the adjacent gridblock, now occupied by the next hydrogeologic layer. The height of that interface at the pinch-out margin is reduced to 0.15 m (10% of the minimum gridblock height). This value was arbitrarily chosen and assumes that the pinch-out layers are not just layer discontinuities.

The maximum thickness of any cell within the UZ grids is 60 m. If the thickness of a model layer within a column exceeds 60 m, the layer is subdivided equally into two layers. Minimum vertical grid resolution is 1.5 m; thus, if the thickness of a hydrogeologic layer is less than 1.5 m within a column, the layer is considered absent and no gridblock is generated for the layer at this location.

In order to conserve the total thickness of the unsaturated zone, layer thicknesses below this cutoff are added to the overlying layer if they lie above the structural reference horizon (i.e., top of Tpbt4), or are added to the underlying layer if they lie below the reference horizon. Still, this may lead to a significant discontinuity if many thin, adjacent layers exist. Within UZ Model boundaries, however, no more than two adjacent hydrogeologic layers occur (in a vertical column), each with a thickness less than 1.5 m, except for a few locations near the land surface where erosion has removed most of the crystal-poor Tiva Canyon Tuff (Tpcp), and the underlying Tpcpv units (model layers tcw13 and ptn21) are also less than 1.5 m thick. In this rare case, the small layer thicknesses are added to the underlying layer, ptn22.

Further vertical grid resolution is added within and below the repository horizon. The repository itself is represented by five grid layers, each 5 m thick. Below the highest elevation of the potential repository horizon (i.e., below 1,111 masl) and in the area lying south of N 236,000 m and east of E 170,000 m, model layers are subdivided if their thickness exceeds 20 m. The additional resolution is added to enhance modeling of flow and transport phenomena between the repository horizon and the water table, including any potential down-gradient areas outside of the repository footprint.

Material properties are assigned to gridblocks depending on the hydrogeologic layer to which the gridblock corresponds. For layers with multiple properties, such as the vitric and zeolitic zones within the Calico Hills, polygons defining the areal extent of these zones are created (see Section 6.6.3). Assignment of material properties (i.e., vitric or zeolitic) to model gridblocks is then confined to the appropriate polygon.

6.6.1 Faults

Although faults may occur as displacement surfaces only or as deformation zones of variable width, each fault within the current UZ Model domain is represented by columns of gridblocks having an arbitrary width of 30 m. Nevertheless, adjustments can be made within a grid to assign appropriate rock properties to each fault zone to handle various fault configurations. Conceptually, there are three important features of a fault that are conserved in the numerical grid. First, a fault is a separator that causes discontinuity of geological layers and may serve as a structural barrier to lateral flow. Second, a fault zone is continuous and may serve as a fast path for flow depending on its hydraulic properties. Third, a fault may or may not be vertical, and its angle of inclination may vary spatially. To implement these features in the UZ grids, three parallel rows of fault-related columns are built for each fault. Each section of a fault in map view consists of three connected columns, with the fault column located in the middle (Figure 2). Each fault column is connected to two side columns and two neighboring fault columns only. Columns on opposite sides of a fault are always separated by a fault column.

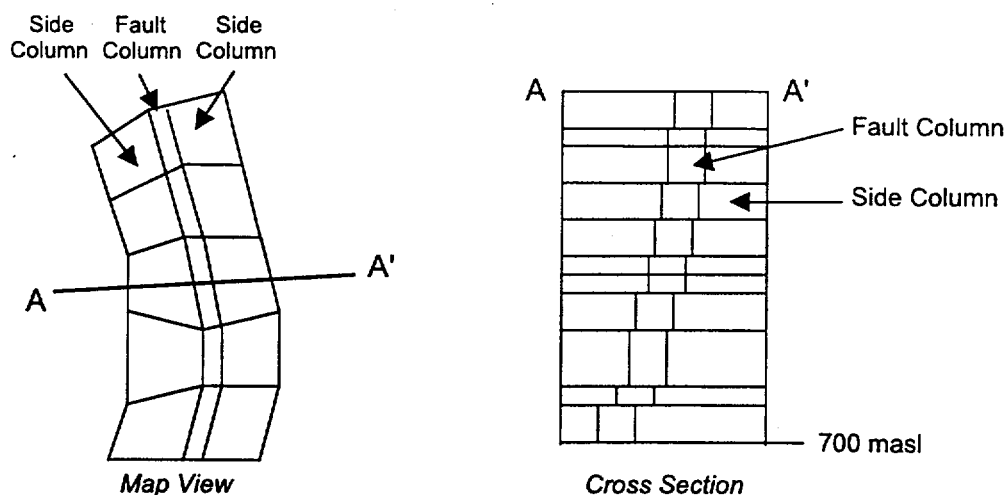


Figure 2. Schematic Illustration of Fault-Related Gridblocks in Map View and in Cross Section

The three fault-related columns (the fault column and its two side columns) are processed together to generate 3-D gridblocks representing the fault and layer offset. From the bedrock surface to the water table, the x, y location of fault gridblocks may shift according to the elevation and dip of the fault. Similarly, the volumes and the center (nodal point) location of the corresponding side cells are adjusted accordingly. As a result, the inclination of the fault is described by a series of connected gridblocks whose x, y locations vary with elevation. The fault-related gridblocks are connected vertically, if they belong to the same column, regardless of the fault angle. Columns of side cells are connected in a similar fashion regardless of the horizontal shifting of position and change in volume. To look at it from another perspective, each set of three fault-related columns (i.e., the fault column plus its two side columns) can be viewed collectively as one vertical column that is subdivided into three nonvertical columns to capture the angle of inclination along a fault. One limitation of this method is that intersecting faults cannot be represented.

This method of representing the three-dimensionality of faults requires that all fault gridblocks have the same elevation and thickness as the laterally adjacent gridblock in order to facilitate vertical displacement of geologic layers. Because Yucca Mountain is comprised of hydrogeologic layers with variable thickness, simply reassigning material properties from one row of gridblocks to another to establish offset along faults is insufficient for representing the true layer configurations. This approach removes certain layers from columns adjacent to fault columns and often misrepresents layer thicknesses. To avoid such error, additional vertical resolution is added to fault-related gridblocks based on the elevation of hydrogeologic layer contacts on both sides of the fault. Therefore, vertical grid discretization in each set of three fault-related columns is identical, and all interfaces between hydrogeologic units in both side columns correspond to the interfaces between gridblocks. The layer and rock properties of fault gridblocks are then assigned according to the stratigraphy of the fault column.

The assignment of lateral connections that involve fault-related gridblocks is different from the way lateral connections are assigned to normal (non-fault-related) gridblocks. Fault-related

lateral connections are of two types, fault-fault gridblock connections and fault-side cell connections. In these two cases, lateral connections occur between gridblocks that share the same interface. The interface area is determined exactly by the contact area between the two gridblocks.

6.6.2 Repository

For numerical gridding purposes, the repository is defined as a 3-D object that is subdivided into a regular mesh of gridblocks. Current repository design calls for a set of waste emplacement drifts to be constructed westward from the ESF Main Drift (MOL.19990409.0100). All repository columns are aligned along the direction of the emplacement drifts, as currently designed, and each column of gridblocks (except those corresponding to borehole locations) has four sides to facilitate the representation of a drift with a series of connected 3-D gridblocks.

Local refinement is added vertically at the repository horizon in the UZ Model grids for PA. For each repository column, a repository thickness of 25 m is assigned at the appropriate elevation. This thickness is then divided vertically into five layers, each 5 m thick. For the interfaces between repository gridblocks, lateral connections are established if two adjacent gridblocks belong to the same layer within the five-layer grid structure of the repository horizon. For interfaces between a repository gridblock and a nonrepository gridblock, the connection is built based on their hydrogeologic-layer similarity. The assignment of rock properties to repository gridblocks is determined by the elevation of the gridblock and the corresponding hydrogeologic layer present at that elevation.

6.6.3 Vitric/Zeolitic Boundaries

The ISM3.0 Rock Properties Model (DTN: MO9901MWDISMRP.000) is used to add resolution to UZ Model grids within the Calico Hills nonwelded unit (CHn). Of great importance to UZ flow and transport modeling is the distribution of low-permeability zeolites, because of their potential to significantly alter flowpaths and travel times and to retard radionuclides migrating from the repository horizon to the water table.

At high matrix saturations, groundwater flow within the CHn is believed to divert around zeolitic volumes of rock and preferentially flow through the less-altered, higher-permeability matrix. Consequently, only a low percentage of the total percolation flux is expected to travel through significantly zeolitized tuffs. This suggests that sorption within the slightly altered (mostly vitric) tuffs is of far greater importance. As such, high- and low-permeability regions are defined within certain UZ Model layers corresponding to the tuffs of the upper CHn (above lithostratigraphic unit Tacbt).

Lateral boundaries between high- and low-permeability tuffs within the CHn were determined using results from the geostatistical Rock Properties Model contained in ISM3.0. The details and results of this exercise and a comparison between the Rock Properties and Mineralogy Models from ISM3.0 are provided below. The net result is the subdivision of the lithostratigraphic unit Tac vertically into four grid layers, and laterally into vitric and zeolitic regions for which separate hydrogeologic and sorptive properties are assigned. The UZ Model layer ch1 (corresponding to the combined lithostratigraphic units Ttpv1 and Tpbt1) is also laterally subdivided into vitric and

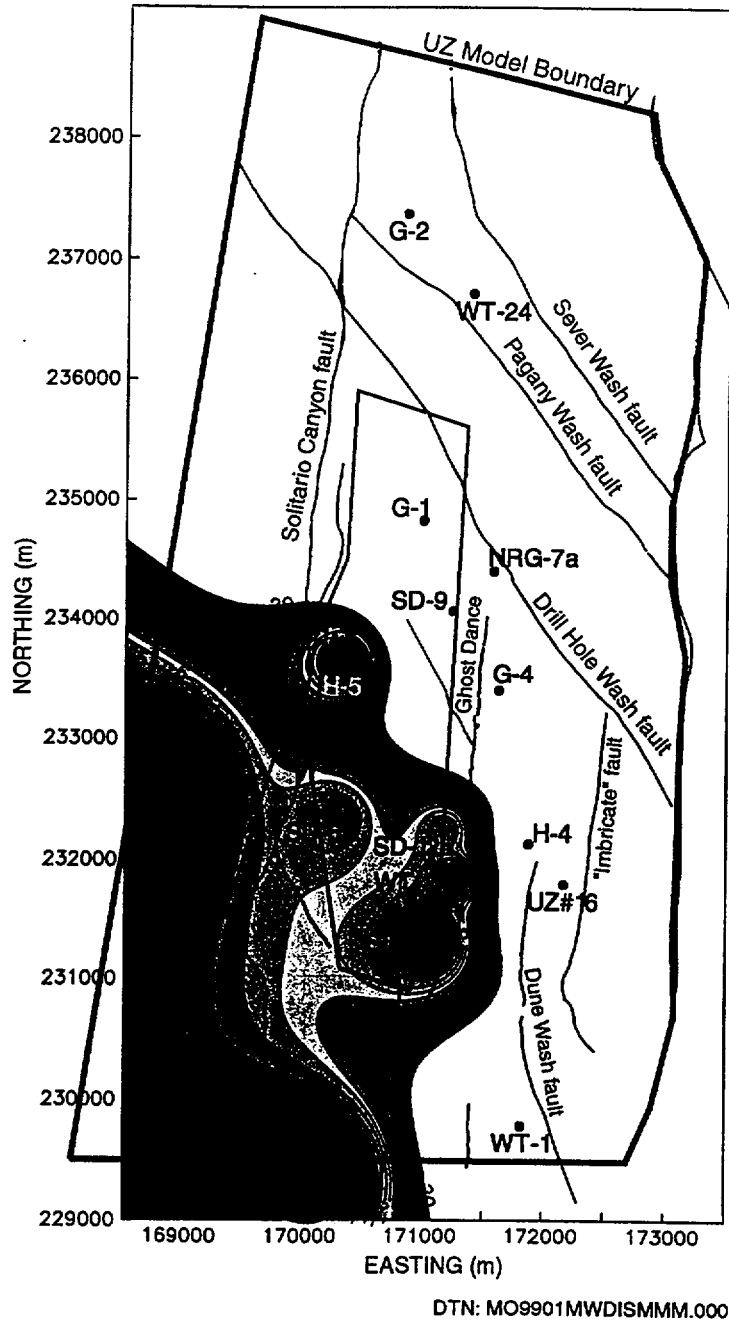
zeolitic regions. It should be noted that the horizontal and vertical resolution of the UZ Model grids is too coarse to capture meter-scale heterogeneity within the CHn. Small-scale heterogeneity is, however, observed within the CHn, and may have an impact on flow and transport calculations. Grid resolution and rock property heterogeneity below the repository are important Performance Assessment (PA) issues that are expected to be addressed through future sensitivity studies.

ISM3.0 Mineralogic and Rock Properties Models are analyzed in EARTHVISION V4.0 by generating map-view figures of percent-zeolite distribution and interpreted saturated hydraulic conductivity (Ksat) data. Percent-zeolite plots were made in EARTHVISION V4.0 by contouring (2-D minimum tension gridding) the regularly spaced (200 × 200 m) percent-zeolite data for the CHn contained in the ISM3.0 file "mineralsM.pdat." No averaging or significant interpolation of the data was done. In other words, the plots essentially represent the exact results of the Mineralogic Model. The plots show a general trend of increased zeolitic alteration to the north and east across the model area. Figure 3 is an example of one of these plots for the upper one-fourth of the Tac lithostratigraphic unit. This representation of zeolite distribution is not appropriate for use in defining vitric-zeolitic boundaries in the numerical grids discussed in this AMR because of the lack of mineralogic sample data and the interpolation technique used in the development of the Mineralogic Model.

Results from the Rock Properties Model of ISM3.0 are also examined. The Rock Properties Model uses porosity (data that are relatively abundant at Yucca Mountain) as a surrogate to predict Ksat values. The limitations of this correlation are discussed in Rautman and McKenna (1997, pp. 13-14). Ksat distributions within the CHn (represented with 24 grid layers in the rock properties model) are plotted in EARTHVISION V4.0 by contouring (2-D minimum tension gridding) the regularly spaced (200 × 200 m) Ksat data for each of the 24 rock-property grid layers. In the Rock Properties Model, the CHn consists of the volume of rock lying between the upper Tptpv1 contact and the lower Tacbt contact (in other words, geologic layers Tptpv1, Tpbt1, Tac, and Tacbt, shown in Table 10). The 24 rock-property grid layers are not stratabound; rather, they are equally thick at any given x, y coordinate. The plots were generated using the ISM3.0 rock property file "CHnEKsat.grid" and show Ksat data that range from approximately 10^{-5} to 10^{-12} m/sec. Figure 4 shows an example of one of these Ksat plots for the upper Tac lithostratigraphic unit (note that this figure cannot be directly correlated with Figure 3 because the distributions consider different thicknesses within the upper Tac; however, some general comparisons regarding interpolation techniques can be made).

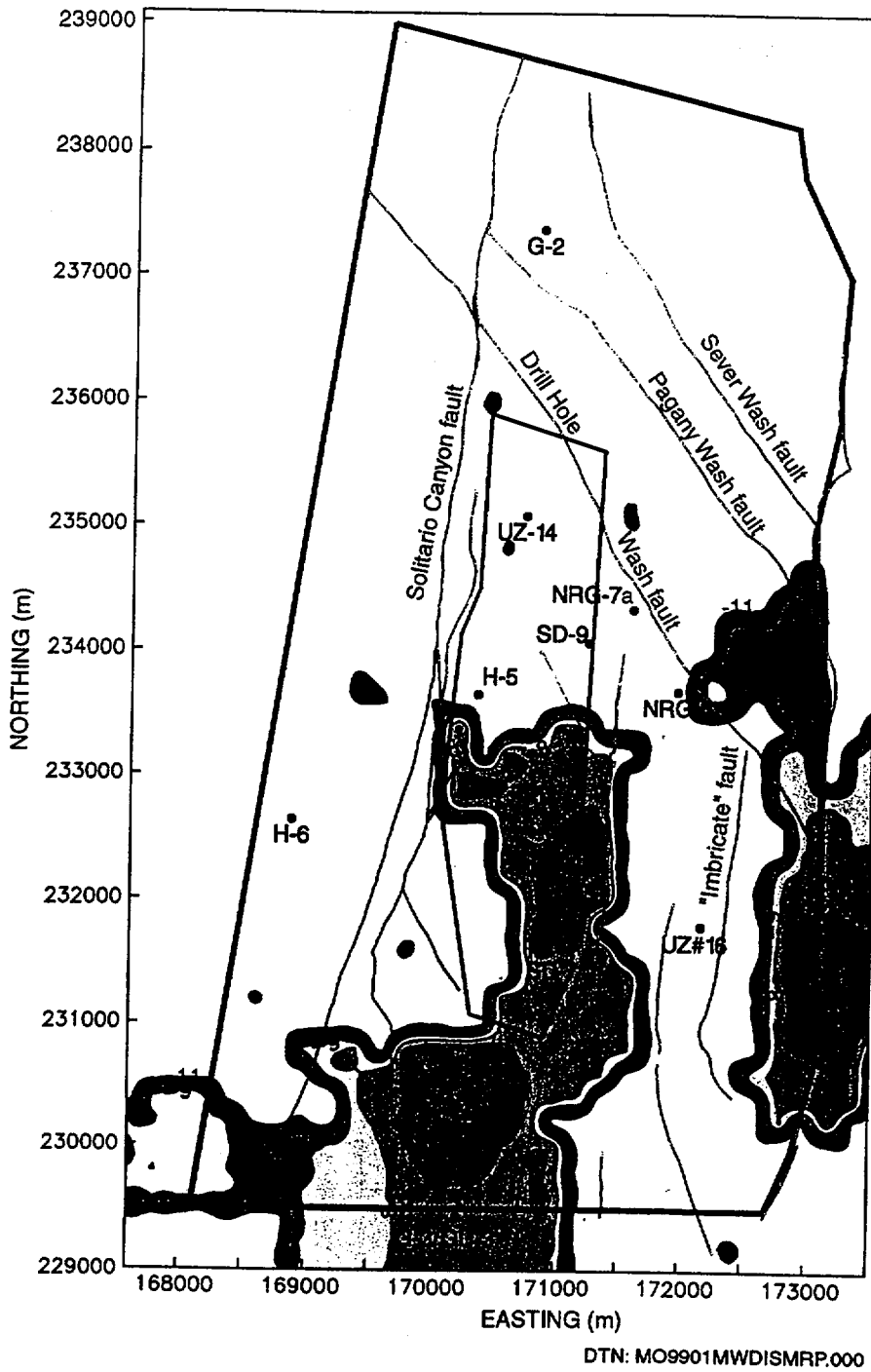
Distribution of Ksat typically shows a relatively sharp transition between high and low Ksat regions. This transition occurs over the Ksat range of about 10^{-8} to 10^{-11} m/s. As stated in Section 5, Assumption 5, we assume the 10^{-10} m/sec contour to be the boundary between high and low Ksat, and thus, to represent the vitric-zeolitic boundary. This yields a more continuous distribution of less altered (higher permeability) rock in each of the 24 rock-property grid layers, compared with the vitric distributions from the mineralogic model. Consequently, only the Rock Properties Model from ISM3.0 is used to define the vitric-zeolitic boundary in UZ Model layers ch1, ch2, ch3, ch4, and ch5 (ch6 consists entirely of low-permeability material using the results of the Rock Properties Model). It should be noted, however, that data from recently-drilled borehole SD-6 were not available for inclusion in the ISM3.0 Rock Properties Model. Liquid saturation

data from SD-6 have since indicated that the CHn tuffs in this area are largely vitric, rather than zeolitic.



NOTE: White areas indicate >20% zeolite. Repository and UZ model boundaries shown with heavy black lines.

Figure 3. Percent Zeolite Distribution from ISM3.0 Mineralogy Model, Upper 1/4 of Layer Tac (UZ Model layer "ch2")



NOTE: White areas indicate Ksat values $<10^{-11}$ m/s and are assumed to correlate with significant mineral alteration. Repository and UZ model boundaries shown with heavy black lines.

Figure 4. Distribution of Ksat from ISM3.0 Rock Properties Model, Upper Tac. Ksat Contour Units are "log₁₀" (m/s)

Details explaining the extraction of relevant ISM3.0 rock properties data used to define vitric boundaries within UZ model grid layers are provided in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 34-37). This process involves the execution of the single-user software macro ExportProp V1.0 (ACC: MOL.19990910.0238), whose qualification is documented in Scientific Notebooks YMP-LBNL-YSW-JH-2A (pp. 163-166) and YMP-LBNL-YSW-JH-2 (pp. 34-35). The extent of the vitric-zeolitic boundaries, shown in Figure 5 (a-e), are used in WinGridder V1.0 to assign material names to gridblocks (i.e., "vitric" or "zeolitic," for which associated rock properties will be assigned) within UZ Model layers ch1, ch2, ch3, ch4, and ch5.

6.7 DUAL-PERMEABILITY GRID GENERATION

The single-user software macro DKMgenerator V1.0 (ACC: MOL.19990909.0315), has been created to generate dual-permeability (dual-k) numerical grids for heterogeneous, fractured rocks. The code development and qualification of DKMgenerator V1.0, which contains executable file "2kgridv1," is described in Section 3 of this AMR. Written in Fortran 77, "2kgridv1" generates a dual-permeability grid using (a) a primary mesh of a single-continuum, or ECM grid, and (b) fracture properties for multiple hydrogeological units. The software macro DKMgenerator V1.0 is designed to handle three types of fractured media:

- A set of parallel, infinite fractures (Type #1) with uniform spacing within each hydrogeological unit.
- Two sets of parallel, infinite, orthogonal fractures (Type #2) with the same spacing within each hydrogeological unit.
- Three sets of parallel, infinite, orthogonal fractures (Type #3) with the same spacing within each hydrogeological unit.

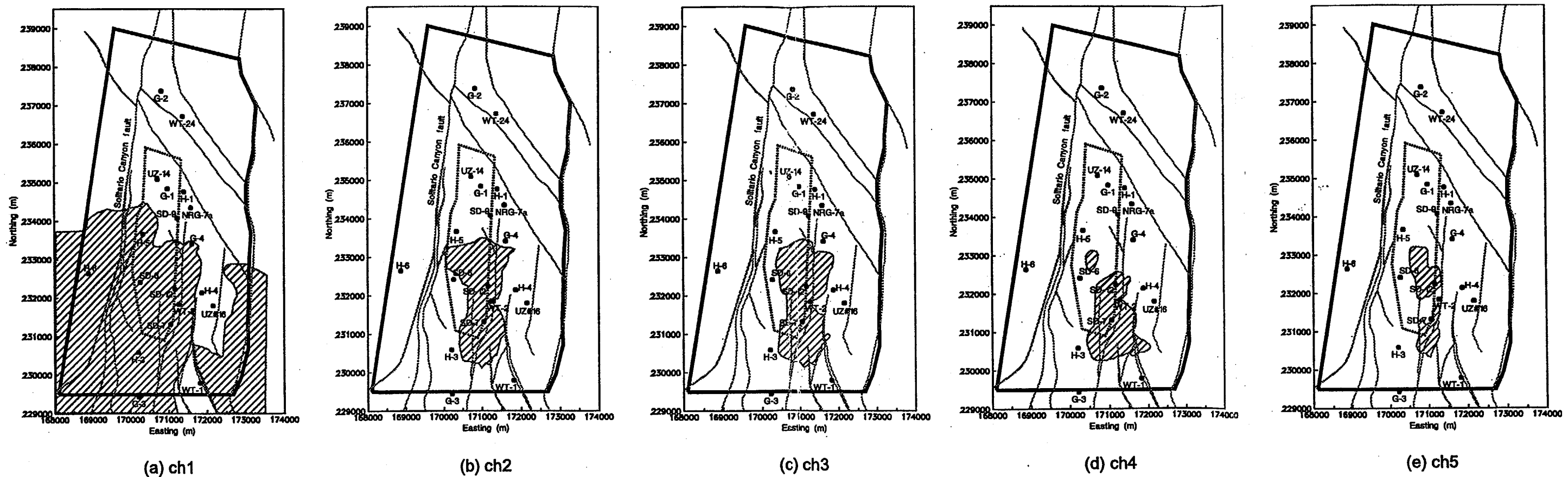
Volumes of fracture and matrix elements are computed with DKMgenerator V1.0 using the following formulas:

$$V_f = \phi_f V_n \quad (\text{Eq. 1})$$

and

$$V_m = (1 - \phi_f) V_n \quad (\text{Eq. 2})$$

where V_f and V_m are volumes of fracture and matrix elements, respectively, for the dual-permeability grid, and V_n is the volume of element n of the primary mesh, from which a dual-permeability grid is being generated. ϕ_f is the porosity or fractional volume of fractures within the bulk rock.



NOTE: White areas indicate "zeolitic" material.

Figure 5. Extent of Vitric Region (indicated by the blue diagonal lines) in FY 99 UZ Model Layers (a) ch1, (b) ch2, (c) ch3, (d) ch4, and (e) ch5.

The connection information in the dual-permeability grid is determined as follows:

- Global fracture-fracture and matrix-matrix connection data are kept the same as the connections in the primary mesh for the same/corresponding gridblocks. This implies that permeabilities used for both fracture and matrix systems are the “continuum” values for both, relative to the bulk-connecting areas.
- Inner-connection distances between fractures and matrix within a primary gridblock are calculated as:

$$D_f = 0 \quad (\text{Eq. 3})$$

$$D_m = \frac{D}{6} \quad \text{for Type \#1 fractures} \quad (\text{Eq. 4})$$

$$D_m = \frac{D}{8} \quad \text{for Type \#2 fractures} \quad (\text{Eq. 5})$$

$$D_m = \frac{D}{10} \quad \text{for Type \#3 fractures} \quad (\text{Eq. 6})$$

and

$$D = \frac{1}{F} \quad (\text{Eq. 7})$$

where D_f is the distance from the fracture center to the surface of a matrix block; D_m is the distance between the surface of a matrix block and the inner point of that matrix block, based on the quasi-steady state assumption (Warren and Root 1963); D is the fracture spacing; and F is the fracture frequency within the unit.

The interface area (A) between fractures and matrix blocks is estimated by:

$$A = A_{fm} V_n \quad (\text{Eq. 8})$$

where A_{fm} is a volume-area factor, which represents the total fracture-matrix interface area per unit volume of rock, determined from the site fracture characterization studies. Fracture analyses and determination of fracture properties for FY 99 UZ Model activities are documented in the AMR supporting DTN: LB99051233129.001.

Three input files are required to run the DKMgenerator V1.0 executable “2kgridv1.” These files are called “2kgrid.dat,” “connec.dat,” and “framtr.dat,” and contain the following information:

1. The “2kgrid.dat” file contains the two parts of ELEME and CONNE data blocks from the primary single-continuum mesh using the same formats.

2. The "connec.dat" file contains connection indexes from the primary single-continuum mesh using the same formats.
3. The "framtr.dat" file contains fracture properties (DTN: LB990501233129.001) with the following format and data:

Format (A5, 5X, 4E10.3)
ROCKS, PHIF, B, F, A_FM

ROCKS 5-character code name of rock unit
PHIF fracture porosity
B fracture aperture (m)
F fracture frequency (m^{-1})
A_FM interface areas between fractures and matrix blocks per unit bulk rock (m^2).

Execution of "2kgridv1" creates three output files:

1. The "2kgrid.out" file contains information from the primary mesh and new dual-permeability meshes for grid verification purposes.
2. The "eleme.dat" file contains "ELEM" data blocks for the new dual-permeability grid.
3. The "conne.dat" contains "CONNE" data blocks for the new dual-permeability grid.

6.8 MODEL VALIDATION

Numerical grids are fixed objects, or frameworks, that alone do not capture physical processes or phenomena occurring at Yucca Mountain. As such, the process of "model validation," in the usual sense, does not apply. The process of grid "verification"—an evaluation of how accurately the numerical grid represents the geologic and hydrogeologic input—does apply, however, and is discussed in this section.

The parameters generated for each numerical grid include gridblock material names, gridblock volumes and locations, connection lengths and interface areas between gridblocks, and direction of absolute permeability for each connection. Because of the number and size of the numerical grids developed for UZ Model activities, it is not practical to verify each parameter for each gridblock generated. Consequently, a subset of gridblocks from each mesh is taken, and the associated parameters are verified in order to ensure the accuracy and representativeness of the mesh. The criteria by which the numerical grids are evaluated are not as rigorous as, for example, those specified for engineering design. This is because of the simplified approximation and large uncertainty inherent in modeling studies, where variations in modeling results up to an order of magnitude may be considered acceptable.

For the 1-D numerical grids (DTN: LB990501233129.002), which consist of columns of gridblocks at borehole locations only, gridblock material names and elevations are verified through comparison with stratigraphic information from GFM3.1 (see Attachment III for details). For the 2-D cross-sectional grids through borehole UZ-7a (DTN: LB990501233129.003), gridblock material names and elevations are verified through visual comparison with stratigraphic and structural information from GFM3.1 exported surface horizons (see Attachment IV for details). For the 3-D UZ Model calibration grids (DTN: LB990501233129.004) and for the 3-D UZ Model grids for calculation of flow fields (DTN: LB990701233129.001), gridblock material names and elevations are verified through comparisons at borehole locations with the GFM3.1 file "pix99el.dat" and through visual comparison with stratigraphic and structural information from GFM3.1 exported surface horizons (see Attachments V and VI for details).

A spot check involving hand calculation of gridblock volumes, connections lengths, and interface areas between gridblocks showed consistency with calculated results for all UZ Model grids generated. A spot check of the direction of absolute permeability confirmed vertical permeabilities for all connections within gridblock columns and horizontal permeabilities for all connections between gridblock columns. These spot checks are documented in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 53-57).

Corroborative Studies

Documentation of sensitivity studies that examine the effect of grid resolution (i.e., gridblock size) on flow and transport simulation results using the aforementioned numerical grids are not within the scope of this AMR. Rather, these studies will be documented in a separate AMR supporting the Unsaturated Zone Flow and Transport PMR. Information from two previous sensitivity studies, however, is available (see summary below). Results from these previous grid resolution studies are from FY 97 and FY 98 UZ Models and their associated calibrated hydrogeologic property sets, which were developed with unqualified data; thus, these results can only be considered as corroborative material for this AMR.

FY 97 UZ Model Sensitivity Study- Both coarse and refined 2-D, cross-sectional grids of the unsaturated zone at Yucca Mountain were developed by Haukwa and Wu (1997, pp. 12-13) in order to address concerns over the use of appropriate numerical grid resolution in UZ moisture flow modeling. The cross sections were developed along a north-south (N-S) transect through the potential repository area, extending from borehole G-2 in the north to borehole G-3 in the south. The coarse grid used an average horizontal spacing of 50 m within the repository area and 100 m outside the repository area. The fine grid used a horizontal spacing as small as 6 m within the repository area and as high as 50 m outside the repository area. The coarse grid was comprised of 23 vertical layers, while the refined grid had 61 layers Haukwa et al. (1997, pp. 2-3). The same layer-averaged rock properties were used in both grids. From comparison of flow simulation results using the coarse and refined grids, it was concluded by Haukwa et al. (1997, p. 16) that the 100-m lateral grid resolution within the repository area, used in the 3-D UZ Model, was sufficient for ambient site-scale flow modeling purposes.

Results indicated that moisture flow is predominantly vertical (Haukwa et al. 1997, p. 4), except where zeolites are present, suggesting that modeling results are less sensitive to lateral gridblock dimensions than to vertical changes in grid resolution, unless a sudden change in rock

hydrogeologic properties occurs at a layer contact resulting in significant lateral diversion. Below the repository horizon, lateral diversion is most likely to occur above zeolites in the CHn. Calculated saturation and percolation flux distribution could be adequately resolved by adding a few grid layers at the PTn-TSw interface and at the vitric-zeolitic interfaces within the CHn, since these are transitional areas where rock properties change rapidly over short distances.

The current (FY 99) 3-D UZ Model is vertically resolved with about 44 layers in the repository footprint; about 15 of these layers are above the repository horizon, 5 layers are within the repository horizon, and about 24 layers lie between the repository horizon and the water table). The transitional areas at the PTn-TSw and vitric-zeolitic interfaces are generally captured by several thin layers.

FY 98 UZ Model Sensitivity Study- In this study, the influence of gridblock size on flow and transport simulation results was examined along an east-west (E-W) cross section through borehole SD-9. Four meshes, each with a different nominal gridblock size, were developed along the E-W transect (for details, refer to Scientific Notebook YMP-LBNL-YSW-WZ-1, pp. 52-56, 66-72). Three simulation scenarios were considered in this study. In the first simulation scenario (Scenario #1), no modifications are made to the calibrated FY 98 hydrogeologic property sets in order to create perched water. In the second simulation scenario (Scenario #2), FY 98 calibrated perched water hydrogeologic properties are used. In the third simulation scenario (Scenario #3), perched water properties are used, but fracture flow is ignored in zeolitic units (except in fault zones). Both conservative and reactive tracers are considered in the transport simulations for each of the three scenarios.

Under the conditions prescribed in Scenario #1 (no perched water), the effect of gridblock size is minimal. Results from the coarsest of the four cross-sectional grids (which has a nominal horizontal spacing of 112 m and a maximum layer thickness of 60 m), compared with the results from the finest of the four cross-sectional grids (which has a nominal horizontal spacing of 28 m and a maximum layer thickness of 15 m), show an approximate 20% difference in the time at which half of the tracer mass (both conservative and reactive) reaches the water table.

Under the conditions prescribed in Scenario #2 (perched water), model results for the coarsest mesh and finest mesh show differences of about 10% in the time at which half of the tracer mass reaches the water table for conservative tracers. For reactive tracers, results for the coarsest mesh differ from those for the finest mesh by a factor of two.

Under the conditions prescribed in Scenario #3 (perched water, no fractures in zeolites), the effect of gridblock size is once again minimal. Results from the coarsest of the four cross-sectional grids, compared with the results from the finest of the four cross-sectional grids, show an approximate 20% difference in the time at which half of the conservative tracer mass reaches the water table and an approximate 15% difference in the time at which half of the reactive tracer mass reaches the water table.

Because PA is interested in sensitivity studies that produce order of magnitude changes in dosage, the results of this FY 98 modeling study suggest that the numerical grid resolution used in the FY 99 site-scale UZ Model grids, at least within the potential repository area, is appropriate for capturing important flow and transport phenomena.

7. CONCLUSIONS

Integration of geologic and hydrogeologic data is required in the development of integral finite-difference numerical grids that represent the unsaturated zone beneath Yucca Mountain. Geologic layers from GFM3.1 can be correlated with hydrogeologic units defined by Flint (1998), and can be subdivided based on rock properties data contained in ISM3.0 in order to produce a layering scheme appropriate for unsaturated-zone flow and transport modeling.

Activities involving verification of appropriate gridblock material names, gridblock volumes and locations, connection lengths and interface areas between gridblocks, and direction of absolute permeability demonstrate the accuracy of the numerical grids developed and described in this AMR.

Corroborative sensitivity studies with previous UZ Model grids indicate that a fairly coarse mesh is sufficient to capture important ambient flow and transport phenomena. Grid resolution added to FY 99 UZ Model grids below the repository horizon and in down-gradient areas outside of the repository footprint is adequate to characterize flow and transport phenomena between the repository horizon and the water table.

Results from the development of numerical grids of the unsaturated zone at Yucca Mountain include:

- One primary mesh and four dual-k meshes consisting of 1-D columns at borehole locations (DTN: LB990501233129.002) used for developing calibrated hydrogeologic property sets for the unsaturated zone at Yucca Mountain.
- One primary mesh and two dual-k meshes comprising a 2-D cross section through borehole UZ-7a (DTN: LB990501233129.003) used to calibrate fault hydrogeologic properties in the unsaturated zone at Yucca Mountain.
- One primary mesh and two dual-k meshes (DTN: LB990501233129.004) used for 3-D UZ Model calibration.
- One primary mesh and three dual-k meshes (DTN: LB990701233129.001) used to generate 3-D, unsaturated-zone flow fields for Performance Assessment.

7.1 LIMITATIONS AND UNCERTAINTIES

A model of a complex system such as Yucca Mountain must be used with recognition of its limitations. For the site-scale UZ Model, a key limitation is imposed by numerical grid resolution. Since computational time rapidly increases with grid size (i.e., number of gridblocks and connections), the use of large refined grids is currently limited by both simulation time and computer space requirements. Refining an entire 3-D model with gridblocks having dimensions roughly equivalent to the expected drift spacing in the repository and using comparably refined vertical resolution would increase current grid sizes by more than an order of magnitude. Thus, it is not feasible at the mountain scale to characterize flow behavior on horizontal scales less than a few tens of meters. However, current lateral resolution (up to 300 m in areas outside the

repository boundary) can sometimes lead to high aspect ratios within very thin layers. This may lead to inaccuracies when trying to calculate lateral flow components; however, fracture spacing and orientation data suggest that groundwater flow is primarily downward, except within the altered tuffs.

The accuracy of UZ Model grids depends largely on the accuracy of the GFM3.1 and ISM3.0 input data. Both of these models, which are assumed to provide a representative picture of subsurface geology and rock properties, are constructed with limited data resources. GFM3.1 includes assumptions about the lateral continuity and thickness trends of layers at Yucca Mountain based on limited borehole data. The UZ Model numerical grids attempt to match this layered approach as closely as possible in order to constrain unsaturated-zone flow and transport processes. While the degree of lateral continuity of layers represented in GFM3.1 is a valid interpretation, the impact of more lateral discontinuity resulting from the inclusion of small faults on flow could be significant, especially in areas where little or no information has been collected. However, these areas typically lie too far from the repository area to have any significant impact on repository performance.

Within ISM3.0, the interpretation of saturated hydraulic conductivity (K_{sat}) distribution and mineral alteration at Yucca Mountain is also based on limited data and assumed correlations (e.g., using porosity as a surrogate for predicting K_{sat}). The spatial heterogeneity of low-permeability alteration products such as zeolites has a profound impact on UZ flow and transport modeling, yet the nature of their distribution is not fully understood. Though currently represented per hydrogeologic layer (i.e., UZ Model layers "ch1" to "ch5"), true mineral alteration and rock property variation may not strictly follow a layered model. As discussed previously, sensitivity studies to test the appropriateness of the layered modeling approach are not within the scope of this AMR.

Grid verification exercises show that UZ Model layer thicknesses and elevations are reasonable representations of the hydrogeologic input data. Using visual cross-sectional comparisons with GFM3.1, UZ Model layer contact elevations are shown to have some large (approximately 50-m) differences in areas immediately adjacent to inclined fault zones, reflecting the coarse lateral grid resolution used, as well as certain limitations of the gridding software. Given the large uncertainties associated with fault zone hydrogeologic characteristics, the effect of these differences along faults on modeling results has yet to be determined, but is likely limited in extent to the area immediately surrounding the fault zones. Additional hydrogeologic property data and analyses within fault zones would reduce uncertainty in this area.

Finally, the approximation of a flat water table beneath northern Yucca Mountain (Assumption 1 in Section 5) may not be representative of the true potentiometric surface, yet it provides flexibility for simulating and calibrating to perched-water data. The water table configuration in this area is uncertain given the paucity of data. However, within and down-gradient of the repository footprint, where the accuracy of calculated groundwater travel times from the repository horizon to the water table will be important, the flat water table assumption is consistent with water levels measured in several nearby boreholes.

7.2 RESTRICTIONS FOR SUBSEQUENT USE

The UZ Model numerical grids developed herein shall be used only for development of unsaturated-zone hydrogeologic property sets, for UZ Model calibration, and for development of UZ flow fields for Performance Assessment. These activities will involve the use of software from the TOUGH2 family of codes.

7.3 IMPACT OF DATA AND SOFTWARE QUALIFICATION

All data residing in the TDMS were designated as "To Be Verified (TBV)" until further verification and it is anticipated that those data previously considered Q will remain Q after the verification process. Of most concern, on the issue date of this report, are data that were previously designated NQ (i.e., GFM3.1 and ISM3.0) and the numerical gridding software, WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0), is currently undergoing software qualification under AP-SI.1Q. Once these data and software become qualified and verified, the UZ Model grids are considered to be Q.

The status of all the inputs for this AMR is available by referring to the DIRS database for the most recent version of the DIRS included in Attachment I.

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Software Code: ESF4_XYZ V.03.XLS (ESF4-XYZ Version 03), STN: 30092 V.03, Version 3.0.

Software Code: WinGridder V.1.0, STN: 10024-1.0-00, Version 1.0.

Macro/Routine: DKMgenerator V.1.0. ACC: MOL.19990909.0315.

Macro/Routine: ExportProp V.1.0. ACC: MOL.19990910.0238.

8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

64 FR (Federal Register) 8640. Disposal of High-Level Radioactive Waste in a Proposed Geologic Repository at Yucca Mountain. Proposed rule 10 CFR 63. Readily available.

AP-3.10Q. *Analyses and Models*. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990225.0335.

AP-SI.1Q. *Software Management*. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990520.0164.

DOE (U.S. Department of Energy) 1998. *Quality Assurance Requirements and Description*. DOE/RW-0333P, REV 8. Washington D.C.: DOE OCRWM. ACC: MOL.19980601.0022.

QAP-2-0, Rev. 5. *Conduct of Activities*. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.

8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

GS980508312313.001. Water-Level and Related Data Collected in Support of Perched-Water Testing in Borehole USW WT-24, September 10, 1997 through February 3, 1998. Submittal date: 05/07/1998.

LB990501233129.001. Fracture Properties for the UZ Model Grids and Uncalibrated Fracture and Matrix Properties for the UZ Model Layers. Submittal date: 08/25/1999.

MO9609RIB00038.000. Hydrologic Characteristics: Potentiometric Surface. Submittal date: 05/07/1997.

MO9804MWDGFM03.001. An Update to GFM 3.0; Corrected Horizon Grids for Four Fault Blocks. Submittal date: 04/14/1998.

MO9901MWDISMMM.000. ISM3.0 Mineralogic Models. Submittal date: 01/22/1999.

MO9901MWDISMRP.000. ISM3.0 Rock Properties Models. Submittal date: 01/22/1999.

MO9901MWDGFM31.000. Geologic Framework Model. Submittal date: 01/06/1999.

8.4 AMR OUTPUT DATA LISTED BY DATA TRACKING NUMBER

LB990051233129.001. Tables Supporting UZ Model Grid Development.

LB990501233129.002. Mesh Files for 1-D Hydrogeologic Property Set Inversions and Model Calibration.

LB990501233129.003. Mesh Files for 2-D Fault Hydrogeologic Property Calibration.

LB990501233129.004. Mesh Files for 3-D UZ Model Calibration.

LB990701233129.001. Mesh Files for Generating 3-D UZ Flow Fields.

9. ATTACHMENTS

Attachment I - Document Input Reference Sheets

Attachment II - Electronic GFM3.1 and ISM3.0 Data Files Used to Develop UZ Model Numerical Grids

Attachment III - Development of Numerical Grids for 1-D Hydrogeologic Property Set Inversions

Attachment IV - Development of Cross-Sectional Grids for Fault Hydrogeologic Property Calibrations

Attachment V - Development of a 3-D Numerical Grid for UZ Model Calibration

Attachment VI - Development of a 3-D Numerical Grid for Calculation of Flow Fields for PA

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DIRS as of the issue date of this AMR. Refer to the DIRS database for the current status of these inputs.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00		Change: N/A		Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed	
2a									
1.	DTN: GS980508312313.001. Water-Level and Related Data Collected in Support of Perched-Water Testing in Borehole USW WT-24, September 10, 1997 through February 3, 1998. Initial Use.	Entire	TBV-3310	4 5 6.2	Perched water elevations	1	N/A	N/A	✓
2.	DTN: LB990501233129.001. Fracture Properties for the UZ Model Grids and Uncalibrated Fracture and Matrix Properties for the UZ Model Layers.	Layer name, fracture porosity, fracture aperture, fracture frequency, fracture interface area	TBV-3168	4 6.7	Fracture data for hydrogeologic units. Fracture Properties	1	N/A	N/A	✓
3.	DTN: MO9609RIB00038.000. Hydrologic Characteristics: Potentiometric Surface.	Used 1993 average borehole water level elevation data only.	TBV-3057	4 6.2	Data used to define water table altitude (lower UZ Model Boundary).	1	N/A	N/A	✓

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
4.	DTN: MO9804MWDGFM03.00 1. An Update to GFM 3.0; Corrected Horizon Grids for Four Fault Blocks.	Considered file: "potentiometric.dat"	Reference only	4 6.2	Contains alternative potentio-metric surface (data are considered but not used in UZ Model development)	N/A	N/A	N/A	N/A
5.	DTN: MO9901MWDISMRP.00 0. ISM3.0 Rock Properties Models. Initial use.	Used files: "CHnKsatE type.out", "CHnEKsat .grid", and "ISM3.seq"	TBV-3060	3 4	Model results used for grid development. Data define low- permeability volumes of rocks in CHn. Data define low- permeability volumes of rocks in CHn.	1	✓	N/A	N/A
6.	DTN: MO9901MWDISMMM.00 00. ISM3.0 Mineralogic Models.	Considered file: "mineralsM .pdatt"	Reference only	3 4 6.6.3 Figure 3	Model results considered but not used in UZ Model grid development % zeolite distribution	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00		Change: N/A		Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed	
7.	DTN: MO9901MWDGFM31.00 0. Geologic Framework Model. Initial Use.	Used numerous files (see Attachment II).	TBV-3005	3, 4 6.2 (Table9) 6.3 (Table11) Att. III (Tables III-1,2,3) Att. IV (Fig IV-2) Att. V (Fig V-5, 6, 7, 8) Att. VI (Fig VI-5, 6)	Model results used for UZ Model grid development X, Y coordinates of boreholes. Fault orientation data files used. <hr/> Borehole stratigraphic picks, isochores, and surface grids	1	✓	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00		Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling						
Input Document		4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed	
8.	Albin, A.L.; Singleton, W.L.; Moyer, T.C.; Lee, A.C.; Lung, R.C.; Eatman, G.L.W.; and Barr, D.L. 1997. <i>Geology of the Main Drift—Station 28+00 to 55+00, Exploratory Studies Facility, Yucca Mountain Project, Yucca Mountain, Nevada.</i> Denver, Colorado: Bureau of Reclamation. ACC: MOL.19970804.0137.	p. 8	Reference only	6.2	Alcoves 5, 6, and 7 station locations	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00		Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling						
Input Document		4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed	
9.	Barr, D.L.; Moyer, T.C.; Singleton, W.L.; Albin, A.L.; Lung, R.C.; Lee, A.C.; Beason, S.C.; and Eatman, G.L.W. 1996. <i>Geology of the North Ramp—Stations 4+00 to 28+00, Exploratory Studies Facility, Yucca Mountain Project, Yucca Mountain, Nevada.</i> Denver, Colorado: Bureau of Reclamation. ACC: MOL.19970106.0496.	p. 122	Reference only	6.2	Alcove 3 station location	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET										
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling						
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un- confirm ed	
10.	Buesch, D.C.; Spengler, R.W.; Moyer, T.C.; and Geslin, J.K. 1996. <i>Proposed Stratigraphic Nomenclature and Macroscopic Identification of Lithostratigraphic Units of the Paintbrush Group Exposed at Yucca Mountain, Nevada.</i> Open File Report 94-469. Denver, Colorado: U.S. Geological Survey. TIC: 226214.		Entire	Reference only	6.3	Define units in Paintbrush Grp.	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	Unqual.						From Uncontrolled Source	Un-confirmed	
11.	Buesch, D.C. and Spengler, R.W. 1999. "Correlations of Lithostratigraphic Features with Hydrogeologic Properties, a Facies-Based Approach to Model Development in Volcanic Rocks at Yucca Mountain, Nevada". <i>Proceedings of Conference on Status of Geologic Research and Mapping, Death Valley National Park, Las Vegas, Nevada, April 9-11, 1999</i> , 62-64. U.S. Geological Survey Open File Report 99-153. Denver, Colorado: U.S. Geological Survey. TIC: 245245.	Entire	Reference only	6.3	Nomenclature/symbols	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	Unqual.						From Uncontrolled Source	Un-confirmed	
12.	CRWMS M&O 1999a. <i>M&O Site Investigations</i> -(Q). Activity Evaluation. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990317.0330.	Entire	Reference only	2	Regulations, standards, and codes	N/A	N/A	N/A	N/A
13.	CRWMS M&O 1999b. <i>M&O Site Investigations</i> -(Q). Activity Evaluation. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990928.0224.	Entire	Reference only	2	Regulations, standards, and codes	N/A	N/A	N/A	N/A
14.	CRWMS M&O 1999c. <i>Analysis & Modeling Development Plan (DP) for U0000 Development of Numerical Grids for UZ Flow and Transport Modeling, Rev.00.</i> "TDP-NBS-HS-000001. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990729.0221.	Entire	Reference Only	1, 2	Planning & work direction	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET										
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling						
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To			
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed	
15.	CRWMS M&O 1999d. Design Input Transmittal: Enhanced Design Alternative (EDA) II Repository Layout for 10 cm/s Ventilation Plan. Las Vegas, Nevada. ACC: MOL.19990409.0100. Initial use.		Figure 2	TBV-3008	4	Repository layout configuration	1	N/A	✓	N/A
16.	Czarniecki, J.B.; O'Brien, G.M.; and Nelson, P.H.; Sass, J.H.; Bullard, J.W.; and Flint, A.L. 1994. "Is There Perched Water under Yucca Mountain in Borehole USW G-2?" <i>EOS Transactions</i> , 75 (44), 249-250. TIC: 226992.		Entire	Reference only	6.2	Perched water alternative to "large hydraulic gradient" conceptual model (used as corroborative information)	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00		Change: N/A		Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Unconfirm ed
17.	Czamecki, J. B.; Nelson, P.H.; O'Brien, G.M.; Sass, J.H.; Thapa, B.; Matsumoto, Y.; and Murakami, O. 1995. "Testing in Borehole USW G-2 at Yucca Mountain: The Saga Continues." <i>EOS Transactions</i> , 76 (46), 191-192. TIC: 240933.	Entire	Reference only	6.2	Perched water alternative to "large hydraulic gradient" conceptual model (used as corroborative information)	N/A	N/A	N/A	N/A
18.	DKMgenerator V.1.0. ACC: MOL.19990909.0315.	Used macro/routine only	Q	3 Table 7 6.7	Macro to generate dual-permeability mesh	N/A	N/A	N/A	N/A
19.	EARTHVISION V.4.0, STN: 30035 V4.0.	Used software only	Q	3 6.3 6.4 6.6.3 Att. III Att. IV Att. V Att. VI	Software to evaluate and extract data from GFM3.1 and ISM3.0 files.	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
20.	ESF4_XYZ V.03.XLS (ESF4-XYZ Version 03). STN: 30092 v.03. DI: 30092-2999, Rev. 00. MI: 30092-M04-001. ACC: MOL.19990217.0166.	Used software only	Q	6.2	Calculates NSP coordinates	N/A	N/A	N/A	N/A
21.	Ervin, E.M.; Luckey, R.R.; and Burkhardt, D.J. 1994. <i>Revised Potentiometric-surface Map, Yucca Mountain and Vicinity, Nevada</i> . Water Resources Investigations Report 93-4000. Denver, Colorado: U.S. Geological Survey. ACC: NNA.19930212.0018.	p. 15	Reference only	6.2	Perched water alternative to "large hydraulic gradient" conceptual model (used as corroborative information)	N/A	N/A	N/A	N/A
22.	ExportProp V.1.0. ACC: MOL.19990910.0238.	Used macro/routine only	Q	3 6.6.3	Macro to export rock property information from ISM3.0.	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
23.	Flint, L.E. 1998. <i>Characterization of Hydrogeologic Units Using Matrix Properties, Yucca Mountain, Nevada.</i> Water Resources Investigations Report 97-4243. Denver, Colorado: U.S. Geological Survey. ACC: MOL.19980429.0512.	pp. 1, 3-4, 21-32, 44	N/A - Data do not affect the system's critical characteristics, scientific results, or conclusions- Corrabative evidence only.	4, 7 4 5 6.1 6.3 (Table 10) 6.4.1 Att. III	Definition of HGUs. Alteration to zeolites reduces permeability. Ksat of vitric tuff v. zeolitic tuff HGU boundaries HGU boundaries HGU boundaries	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
24.	Haukwa, C.; Wu, Y.; and Bodvarsson, G.S. 1997. "Modeling Study of Moisture Flow Using a Refined Grid Model." Chapter 12 of <i>The Site-Scale Unsaturated-Zone Model of Yucca Mountain, Nevada, for the Viability Assessment</i> . Bodvarsson, G.S.; Bandurraga, T.M. and Wu, Y.S. eds. Milestone Report SP24UFM4. Berkeley, California: Lawrence Berkeley National Laboratory. ACC: MOL.19971014.0232.	pp. 2-3, 4, 16	Reference only	6.8	Results from grid resolution sensitivity studies (used for corroborative purposes only)	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
25. Haukwa, C. and Wu, Y. 1997. "Grid Generation and Analysis." Chapter 4 of <i>The Site-Scale Unsaturated-Zone Model of Yucca Mountain, Nevada, for the Viability Assessment</i> . Bodvarsson, G.S.; Bandurraga, T.M. and Wu, Y.S. eds. Milestone Report SP24UFM4. Berkeley, California: Lawrence Berkeley National Laboratory. ACC: MOL.19971014.0232.	pp. 12-13	Reference only	6.8	FY97 UZ Model 2-D cross-sectional grids (used for corroborative purposes only)	N/A	N/A	N/A	N/A	

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
26.	Loeven, C. 1993. <i>A Summary and Discussion of Hydrologic Data from the Calico Hills Nonwelded Hydrogeologic Unit at Yucca Mountain, Nevada.</i> Report LA-12376-MS, UC-814. Los Alamos, New Mexico: Los Alamos National Laboratory. TIC: 205254.	pp. 18-19, 22	Reference only.	4	Alteration to zeolites reduces permeability (used as corroborative information)	N/A	N/A	N/A	N/A
27.	Montazer, P. and Wilson, W.E. 1984. <i>Conceptual Hydrologic Model of Flow in the Unsaturated Zone, Yucca Mountain, Nevada.</i> Water Resources Investigations Report 84-4345. Denver, Colorado: U.S. Geological Survey. TIC: 203223.	Entire	Reference only.	6.3	Major hydrogeologic units	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
28.	Moyer, T. C.; Geslin, J.K.; and Buesch, D. C. 1995. <i>Summary of Lithologic Logging of New and Existing Boreholes at Yucca Mountain, Nevada, July 1994 to November 1994</i> . (Q Logs for SD-9, SD-12, and UZ-N32). U.S. Geol. Surv. Open File Report 95-102. Denver, Colorado: U.S. Geological Survey. MOL.19960222.0335.	p. 6	N/A – Data do not affect the system's critical characteristics, scientific results, or conclusions- Corroborative evidence only.	Att. III	Define depth-to-layer-contacts in borehole UZ-14.	N/A	N/A	N/A	N/A
29.	Pruess K. 1991. <i>TOUGH2 – A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow</i> . Report LBL-29400, UC-251. Berkeley, California: Lawrence Berkeley National Laboratory. NNA.19940202.0088	pp. 27-30, 41-42	Reference only	6.1	TOUGH2 computational requirements	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version	3. Section	Unqual.					From Uncontrolled Source	Un-confirmed	
30.	Rousseau, J.P.; Kwicklis, E.M.; and Gillies, D.C., eds. 1999. <i>Hydrogeology of the Unsaturated Zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, Nevada</i> . Water Resources Investigations Report 98-4050. Denver, Colorado: U.S. Geological Survey. ACC: MOL.19990419.0335.	Pg. 1	Reference only	Attachment s V & VI	Predominance of fracture flow in the TCw	N/A	N/A	N/A	N/A
31.	Rautman, C.A. and McKenna, S.A. 1997. <i>Three-Dimensional Hydrological and Thermal Property Models of Yucca Mountain, Nevada</i> . SAND97-1730. Albuquerque, New Mexico: Sandia National Laboratories. MOL.19980311.0317.	pp. 13-14	Reference only	6.6.3	Limitations of using porosity as a surrogate to predict K_{sat} values	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT DOCUMENT INPUT REFERENCE SHEET									
1. Document Identifier No./Rev.: ANL-NBS-HS-000015/Rev. 00			Change: N/A	Title: Development of Numerical Grids for UZ Flow and Transport Modeling					
Input Document		3. Section	4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version							Unqual.	From Uncontrolled Source	Un-confirmed
32.	Warren, J.E. and Root, P.J. 1963. "The Behavior of Naturally Fractured Reservoirs." <i>Society of Petroleum Engineers Journal</i> , 228, 245-255. Dallas, Texas: Society of Petroleum Engineers. TIC: 233671.	Entire	Reference only	6.7	quasi-steady state assumption	N/A	N/A	N/A	N/A
33.	WinGridder V.1.0, STN: 10024-1.0-00.	Used software routine only	TBV-3478.	6.1 6.6.3 Att. IV Att. V Att. VI	Computer code to generate 1-, 2- and 3-D integral finite difference grids	1	✓	N/A	N/A

AP-3.15Q.1

Rev. 06/30/1999

ATTACHMENT II.

Electronic GFM3.1 and ISM3.0 Data Files Used to Develop UZ Model Numerical Grids.

GFM3.1 Files: (DTN: MO9901MWDGFM31.000)

Isochores:

ia31cpv3RWC.2grd
 ia31cpv2RWC.2grd
 ia31cpv1RWC.2grd
 ia31bt4RWC.2grd
 ia31tpyRWC.2grd
 ia31bt3RWC.2grd
 ia31tppRWC.2grd
 ia31bt2RWC.2grd
 ia31trv3RWC.2grd
 ia31trv2RWC.2grd
 ia31trv1RWC.2grd
 ia31trnRWC.2grd
 ia31trltfRWC.2grd
 ia31tpulRWC.2grd
 ia31tpmnRWC.2grd
 ia31tpllRWC.2grd
 ia31tplnRWC.2grd
 ia31tpv3RWC.2grd
 ia31tpv2RWC.2grd
 ia31tpv1RWC.2grd
 ia31bt1RWC.2grd
 ia31tacRWC.2grd
 ia31tacbtRWC.2grd
 ia31prowuvRWC.2grd
 ia31prowucRWC.2grd
 ia31prowmdRWC.2grd
 ia31prowlcRWC.2grd
 ia31prowlvRWC.2grd
 ia31prowbtRWC.2grd
 ia31bulluvRWC.2grd
 ia31bullucRWC.2grd
 ia31bullmdRWC.2grd
 ia31bulllcRWC.2grd
 ia31bulllvRWC.2grd
 ia31bullbtRWC.2grd
 ia31tramuvRWC.2grd
 ia31tramucRWC.2grd
 ia31trammdRWC.2grd
 ia31tramlcRWC.2grd
 ia31tramlvRWC.2grd
 ia31trambtRWC.2grd

Faults & Fault Polygons:

f31sol.2grd
 f31solwest.2grd
 f31soljfat.2grd
 f31splayg.2grd
 f31splayn.2grd
 f31splays.2grd
 f31sundance.2grd
 f31toe.2grd
 f31sever.2grd
 f31pagany.2grd
 f31drill.2grd
 f31ghost.2grd
 f31ghostw.2grd
 f31dune.2grd
 f31dunex.2grd
 f31dunew1.2grd
 f31imb.2grd
 f31exile.2grd
 f31drill.ply
 f31dune.ply
 f31dunew1.ply
 f31dunex.ply
 f31ghost.ply
 f31ghostw.ply
 f31imb.ply
 f31pagany.ply
 f31sever.ply
 f31soljfat.ply
 f31splays.ply
 f31splayn.ply
 f31splayg.ply
 f31sundance.ply

Surface Horizons:

s31bedrockRWC.2grd
 s31Tpbt4EX.2grd
 s31Ttpv1EX.2grd
 s31ProwuvEX.2grd

Other:

boreholepaths.dat pix99el.dat

ISM3.0 Files:	mineralsM.pdat*	(DTN: MO9901MWDISMMM.000)
	CHnKsatEtype.out	(DTN: MO9901MWDISMRP.000)
	CHnEKsat.grid	(DTN: MO9901MWDISMRP.000)
	ISM3.seq	(DTN: MO9901MWDISMRP.000)
	potentiometric.dat*	(DTN: MO9804MWDGFM03.001)

*Data considered but not used.

ATTACHMENT III.

Development of Numerical Grids for 1-D Hydrogeologic Property Set Inversions.

UZ Model numerical grids developed for the FY 99 1-D hydrogeologic property set inversions are comprised of several 1-D columns centered at borehole coordinates. Layer subdivision within these 1-D columns (except at UZ-14) is based on a combination of borehole stratigraphic picks identified in the GFM3.1 file "pix99el.dat" (DTN: MO9901MWDGFM31.000) and HGU boundaries defined by Flint (1998). Borehole UZ-14 layer contact elevations used in the 1-D inversions are from a 3-D UZ Model grid.

The mesh files identified by DTN: **LB990501233129.002** and created for use in 1-D hydrogeologic property set inversions and calibration for the UZ Model include:

- The primary (ECM) mesh, "**primary.mesh.**"
- The dual-k mesh "**1doldtrans.mesh**" for transient (pneumatic) simulations based on the old fracture porosity values (see footnote to Table 5).
- The dual-k mesh "**1doldstdyst.mesh**" for steady-state simulations based on the old fracture porosity values (see footnote to Table 5).
- The dual-k mesh "**1dtrans.mesh**" for transient (pneumatic) simulations based on the fracture values given in Table 5.
- The dual-k mesh "**1dstdyst.mesh**" for steady-state simulations based on the fracture values given in Table 5.

The detailed steps describing the generation of these files are documented in Scientific Notebook YMP-LBNL-YSW-JH-2A (pp. 95-99).

Table III-1 summarizes the layer contact elevation input to the 1-D inversion grids based on the GFM3.1 file "pix99el.dat." Note that the GFM3.1 borehole elevations, which have been converted from feet to meters, are adjusted in the same manner as described in Section 6.4.1 of this AMR in order to correspond with Flint's (1998) HGUs. Values in italics were not available from the GFM3.1 borehole picks file. Instead, these elevations were determined by back interpolating from GFM3.1 surface grids using EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0). The 1-D inversion grids match these data within 0.1 m in boreholes NRG#5, NRG-6, SD-7, and SD-9, and within 0.2 m in boreholes NRG-7a, SD-12, UZ#4, UZ#16, and WT-24. Contact elevations within the SD-6 grid column match within 0.3 m, except for the upper contact of layer tsw36 (corresponding to the upper 2/3 of Tptpln), which is 1.4 m too high. Given an overall thickness for this layer of 30.6 m, it is not anticipated that the 1.4-m difference will have a significant impact on the inversion results.

Table III-1. Borehole Layer Upper Contact Elevations from GFM3.1. Units Have Been Converted to Meters.
(from DTN: MO9901MWDGFM31.000)

UZ Model	GFM3.1	HGU	NRG-6	NRG-7a	SD-6	SD-7	SD-9	SD-12	UZ-14	UZ#16	UZ#4	WT-24	NRG#5
tcw11	Tpcr	CCR, CUC	1240.9	1277.0	1496.2	1347.7	1286.0	1322.1	<i>1343.1</i>	1207.0	1189.0	1494.1	1251.8
tcw12	Tpcp	CUL, CW	1240.9	1277.0	1470.0	1347.7	1286.0	1322.1	<i>1343.1</i>	1207.0	1189.0	1468.9	1251.8
tcw13	Tpcpv3,2	CMW	1205.9	1261.0	1369.8	1270.0	1284.9	1250.7	<i>1343.1</i>	1176.2	1179.1	1428.5	1209.1
ptn21	Tpcpv1	CNW	1200.9	1258.1	1365.4	1266.7	1279.0	1245.7	<i>1343.1</i>	1172.5	1177.1	1416.3	1204.8
ptn22	Tpbt4+upper 1/3 Tpy	BT4	1198.8	1251.1	1361.4	1263.7	1274.5	1243.3	<i>1341.2</i>	1170.2	1170.7	1409.1	1202.1
ptn23	middle 1/3 Tpy	TPY	1197.6	1244.8	1354.1	1262.2	1268.5	1242.6	<i>1335.8</i>	1166.3	1163.9	1399.7	1194.8
ptn24	lower 1/3 Tpy+Tpbt3	BT3	1197.6	1239.7	1354.1	1262.2	1264.0	1242.6	<i>1331.9</i>	1166.3	1159.3	1391.3	1194.8
ptn25	Tpp	TPP	1193.9	1229.8	1349.9	1258.5	1255.0	1238.9	<i>1319.8</i>	1161.6	1147.9	1349.6	1186.2
ptn26	Tpbt2+Tptrv3,2	BT2	1179.9	1203.4	1347.2	1254.5	1233.3	1234.9	<i>1277.6</i>	1161.6	1107.9	1293.1	1164.0
tsw31	Tptrv1	TC	1168.0	1192.0	1336.0	1245.3	1220.5	1224.8	<i>1264.6</i>	1149.2	1095.7	1281.6	1151.2
tsw32	Tptrn	TR	1166.0	1190.0	1334.0	1243.3	1218.5	1222.8	<i>1262.6</i>	1147.2	1093.7	1279.6	1149.2
tsw33	Tptrl+Tptf+Tptpul	TUL	1116.4	1136.5	1303.6	1216.7	1165.2	1190.7	<i>1218.8</i>	1110.1	<i>1039.5</i>	1231.6	1094.2
tsw34	Tptpmn	TMN	1029.9	1056.7	1236.2	1155.0	1079.9	1121.4	<i>1133.2</i>	1053.0	<i>984.8</i>	1143.0	1017.1
tsw35	Tptpll	TLL	1000.3	1014.8	1192.9	1118.2	1044.6	1083.8	<i>1098.6</i>	1015.2	<i>954.5</i>	1109.5	977.0
tsw36	Tptpln (upper 2/3)	TM2	<i>896.1</i>	903.4	1098.4	1052.1	942.1	998.9	<i>976.8</i>	934.2	<i>857.5</i>	998.8	876.9
tsw37*	Tptpln (lower 1/3)	TM1	862.9	868.5	1067.8	1019.2	906.3	955.7	961.2	899.1	856.7	987.6	854.4
tsw38	Tptpv3	PV3	<i>846.3</i>	851.0	1052.4	1002.7	888.4	934.1	<i>953.4</i>	881.6	<i>856.3</i>	982.0	<i>843.1</i>
tsw39	Tptpv2	PV2	<i>835.6</i>	838.2	1038.1	971.3	870.0	925.0	934.8	864.0	<i>844.1</i>	969.6	<i>831.2</i>
ch1	Tptpv1+Tpbt1	BT1, BT1a	<i>832.0</i>	832.8	1032.9	964.3	867.8	916.0	927.2	860.1	<i>837.6</i>	966.7	<i>825.4</i>
ch2	upper 1/4 Tac	CHV or CHZ	<i>821.6</i>	825.7	1020.4	934.6	851.3	893.5	915.8	854.3	<i>834.6</i>	955.0	<i>820.8</i>
ch3*	middle 1/4 Tac	CHV or CHZ	793.7	801.1	1012.6	922.3	829.6	879.2	895.0	834.6	797.0	900.5	789.9
ch4*	middle 1/4 Tac	CHV or CHZ	765.9	776.7	1004.7	910.0	808.0	864.9	874.1	815.0	759.5	846.0	759.0
ch5*	lower 1/4 Tac	CHV or CHZ	738.0	752.3	996.9	897.6	786.3	850.5	853.3	795.3	721.9	791.5	728.1
ch6	Tacbt	BT	<i>710.2</i>	<i>727.9</i>	989.0	885.3	764.6	836.2	832.4	775.6		<i>737.0</i>	<i>697.1</i>
pp4	Prowuv	PP4			973.5	868.8	747.4	821.3	815.2	766.5		705.5	
pp3	Prowuc	PP3			965.9	861.2	732.8	812.6	795.5	762.7			
pp2	Prowmd+Prowlc	PP2			925.6	825.1	711.5	779.0	784.8	740.3			
pp1	Prowlv+Prowbt+Bulluv	PP1			914.7	792.4		755.3	769.9	710.4			
bf3	Bulluc+Bullmd+Bulllc	BF3			849.3	697.4		660.5	667.5				
bf2	Bulllv+Bullbt+Tramuv	BF2			732.4								

Elevations in italics are back interpolated from GFM3.1 surface elevation grids using EARTHVISION V4.0.

Notes on GFM3.1 nomenclature: Tpcr is equivalent to "Tiva_Rainier," Tpy is equivalent to "Yucca," Tpp is equivalent to "Pah," Tac is equivalent to "Calico."

*UZ Model layers tsw37, ch3, ch4, and ch5 are subdivisions of larger GFM3.1 layers; thus, their elevations are determined based on the thickness proportion (defined in column 2)

Layer contacts within the UZ-14 grid column match the values in Table III-1 within 0.5 m above model layer tsw36. The elevations of UZ Model layers tsw36 and below, however, are consistently off by approximately 27 m in the UZ-14 grid column. This discrepancy was examined by comparing data from GFM3.1 isochore and surface grids. Using the EARTHVISION V4.0 Formula Processor, layer thicknesses for UZ-14 were back interpolated from selected GFM3.1 isochore files as summarized in Table III-2.

Table III-2. UZ-14 Back-Interpolated Layer Thickness From GFM3.1 Isochores.
(from DTN: MO9901MWDGFM31.000)

GFM3.1 Isochore File	Layer	Thickness (m)
ia31tpllRWC.2grd	Tptpll	95.43
ia31tplinRWC.2grd	Tptplin	23.48
ia31tpv3RWC.2grd	Tptpv3	17.75
ia31tpv2RWC.2grd	Tptpv2	7.63

Next, layer contact elevations for UZ-14 were back interpolated from selected GFM3.1 surface grid (ExportGrid) files. The results are summarized in Table III-3.

Table III-3. UZ-14 Back-Interpolated Contact Elevations From GFM3.1 Surface Grids.
(from DTN: MO9901MWDGFM31.000).

GFM3.1 ExportGrid File	Layer	Top Elev (m)	Thickness* (m)
s31TptpllEX.2grd	Tptpll	1098.60	121.76
s31TptplinEX.2grd	Tptplin	976.84	23.48
s31Tptpv3EX.2grd	Tptpv3	953.36	17.75
s31Tptpv2EX.2grd	Tptpv2	935.61	7.63
s31Tptpv1EX.2grd	Tptpv1	927.98	--

*Thickness here is calculated by subtracting elevations in the third column.

The apparent discrepancy in thickness for GFM3.1 layer Tptpll in borehole UZ-14 is attributed to two factors: the lack of a complete geophysical record (absent above layer Tptpv2) for this borehole, and the method used to develop GFM3.1. This geologic model is generated, in essence, by stacking isochores above and below a primary reference horizon, which for GFM3.1 is the structural surface of the top of layer Tpb4. A secondary reference horizon is located at the top of the Calico Hills Formation (Tac). This structural horizon provides additional geological constraint in order to minimize potential propagation errors (resulting from limited data) when stacking isochores. Simply stacking GFM3.1 isochores below the Tpb4 horizon yields an elevation for the top of layer Tac, at the location of borehole UZ-14, that is approximately 27 m higher than the Tac lithostratigraphic pick for UZ-14. This mismatch is treated in GRM3.1 by moving the lower contact of layer Tptpll down approximately 27 m in the vicinity of UZ-14. Layer Tptpll was chosen to accommodate this adjustment because it is relatively thick across Yucca Mountain; thus, the overall percent change in its total thickness would be a relatively minor compared with other layers. However, this adjustment is not reflected in the GFM3.1 isochore file "ia31tpllRWC.2grd" for layer Tptpll.

Since UZ Model grids are developed using only one structural reference horizon (Tpbt4), with the elevation of the remaining layers determined by hanging isochores from this reference horizon according to their stratigraphic position, the 27-m adjustment to layer Tptpl is not captured. However, analyses of hydrogeologic properties data (Flint 1998, p. 28) and other stratigraphic analyses of borehole UZ-14 seem to suggest layer Tptpln should be adjusted rather than layer Tptpl, as is done in GFM3.1.

Data presented in Moyer et al. (1995, p. 6) define depth-to-layer-contacts in borehole UZ-14 above layer Tptpv2. These data suggest a Tptpln thickness of 43 m, rather than 23.5 m, and a Tptpl thickness of 94.5 m. This corroborative information supports the decision to modify the thickness of UZ Model layers tsw36 and tsw37 in the 3-D grids for model calibration and for developing flow fields for PA (i.e., grids identified by DTNs: LB990501233129.004 and LB990701233129.001, respectively) by adding a maximum thickness of 27 m to Tptpln, in the area immediately surrounding UZ-14. In order to meet deliverable deadlines, this modification was not implemented into the 1-D grids identified by DTN: LB990501233129.002.

ATTACHMENT IV.

Development of Cross-Sectional Grids for Fault Hydrogeologic Property Calibrations.

An east-west cross section through borehole UZ-7a was chosen for UZ Model fault calibration because UZ-7a intersects the Ghost Dance fault and because pneumatic data are available describing fracture/fault hydrogeologic characteristics. The UZ-7a cross section, along a Nevada State Planar northing of about N 231,860 m, extends from west of the Solitario Canyon fault to east of the "Imbricate" fault. Columns of gridblocks assigned along this cross section are about 100 m wide in the north-south direction and have a nominal horizontal spacing of 150 m. Grid columns are generated using formatted GFM3.1 fault data (as discussed in Section 6.3 of this AMR) and layer isochore and elevation data (as discussed in Sections 6.4.1 and 6.4.2).

The mesh files identified by DTN: **LB990501233129.003** and created for use in 2-D (cross-sectional) fault hydrogeologic property calibrations for the UZ Model include:

- The primary (ECM) mesh, "**primary.mesh.**"
- The dual-k mesh "**2d2ktrans.mesh**" for transient (pneumatic) simulations based on the fracture values given in Table 5.
- The dual-k mesh "**2d2kstdyst.mesh**" for steady-state simulations based on the fracture values given in Table 5.

The detailed steps describing the generation of these files are documented in Scientific Notebook YMP-LBNL-YSW-JH-2A (pp. 100-104).

Final dual-permeability grid statistics for the UZ-7a cross-sectional mesh are summarized in Table IV-1.

Table IV-1. Statistics for the UZ-7a Cross-Sectional Grids (describing DTN: LB990501233129.003).

	Primary (ECM) Mesh	Dual-k Meshes
# of Columns	40	40
# of Gridblocks	1,652	3,224
# of Connections	3,254	8,080

Figures

The UZ-7a cross-sectional grid is shown in Figure IV-1.

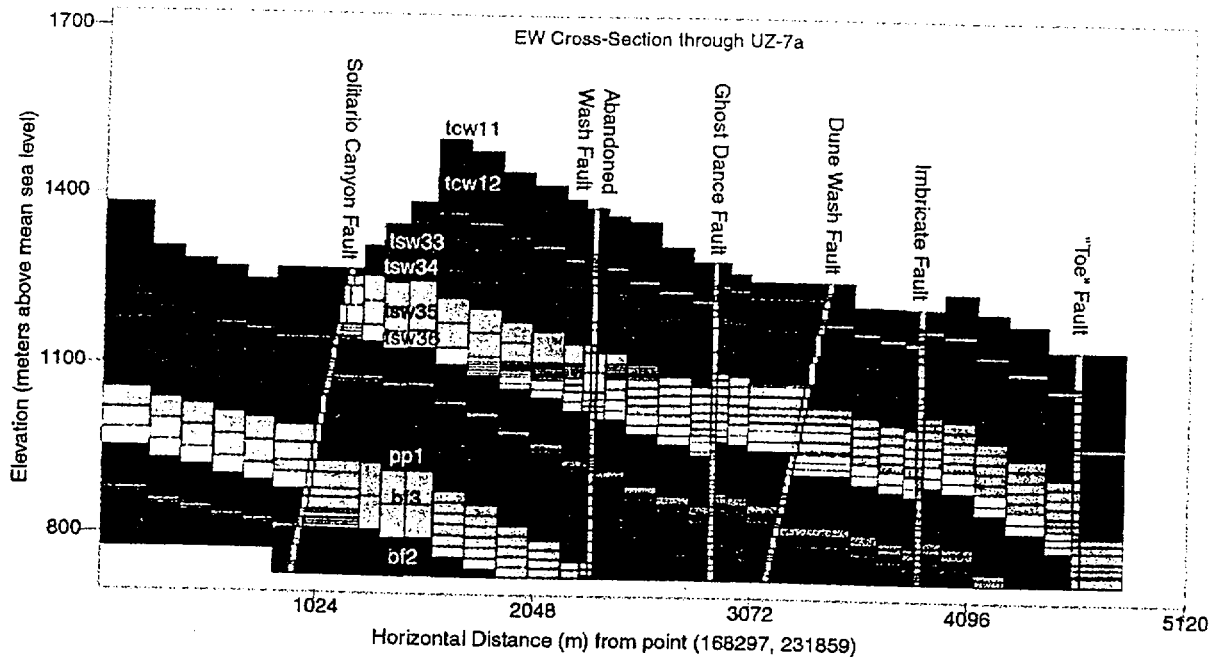


Figure IV-1. UZ-7a Cross-Sectional Grid (from DTN: LB990501233129.003).

Grid Verification

Grid verification involves a visual cross-section comparison between GFM3.1 and columns of gridblocks from the UZ-7a cross section. Figure IV-2 compares the two models. EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0) was used to extract cross-sectional data (layer contact elevations and fault locations) from GFM3.1 that are then used to develop the base map. In order to simplify the comparison, certain GFM3.1 layers are combined into single layers if they were grouped together in the UZ Model (e.g., Tpr1, Tptf, and Tptpul are combined into one layer equivalent to "tsw33"). Overlain on the base map are columns depicting the UZ Model representation of these layers along the same cross section. Data defining the top and bottom elevations of each hydrogeologic layer in the UZ Model were obtained as output directly from WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) after grid generation (actual grid resolution within hydrogeologic layers is not shown in the comparison plot; for this, refer to Figure IV-1). UZ Model gridblocks are color coded in each figure to match the corresponding GFM3.1 layer (or combination of layers, in certain cases). Note that the column width shown is not to scale and that all grid layer interfaces in the UZ Model are horizontal, rather than tilted as shown along faults.

Overall, the layer thickness and elevation match is acceptable between the UZ Model cross-sectional grid and GFM3.1. Layer offset along the Solitario Canyon fault is off somewhat in the UZ Model compared with GFM3.1 because the western splay of the Solitario Canyon fault (GFM3.1 fault file: "f31solwest.2grd") is not represented in this UZ Model cross section. Given that this western splay is about 2 km west of the calibration fault (i.e., the Ghost Dance fault), this simplification in the UZ grid is expected to have no significant impact of the calibration results. The offset shown in the UZ grid represents the combined offset of both the Solitario Canyon fault and the western splay. For simplification, another splay of the Solitario Canyon

fault, called Splay "S" in GFM3.1 and located just east of the Solitario Canyon fault in Figure IV-2, is not represented in the UZ Model cross-sectional grid. This simplification is also expected to have no significant impact on the calibration results since the splay is located about 1.5 km west of the Ghost Dance fault. Layer offset along the Dune Wash fault in the UZ Model cross-sectional grid is up to about 50 m greater than in GFM3.1. For the intended use of the model, this discrepancy is not considered significant.

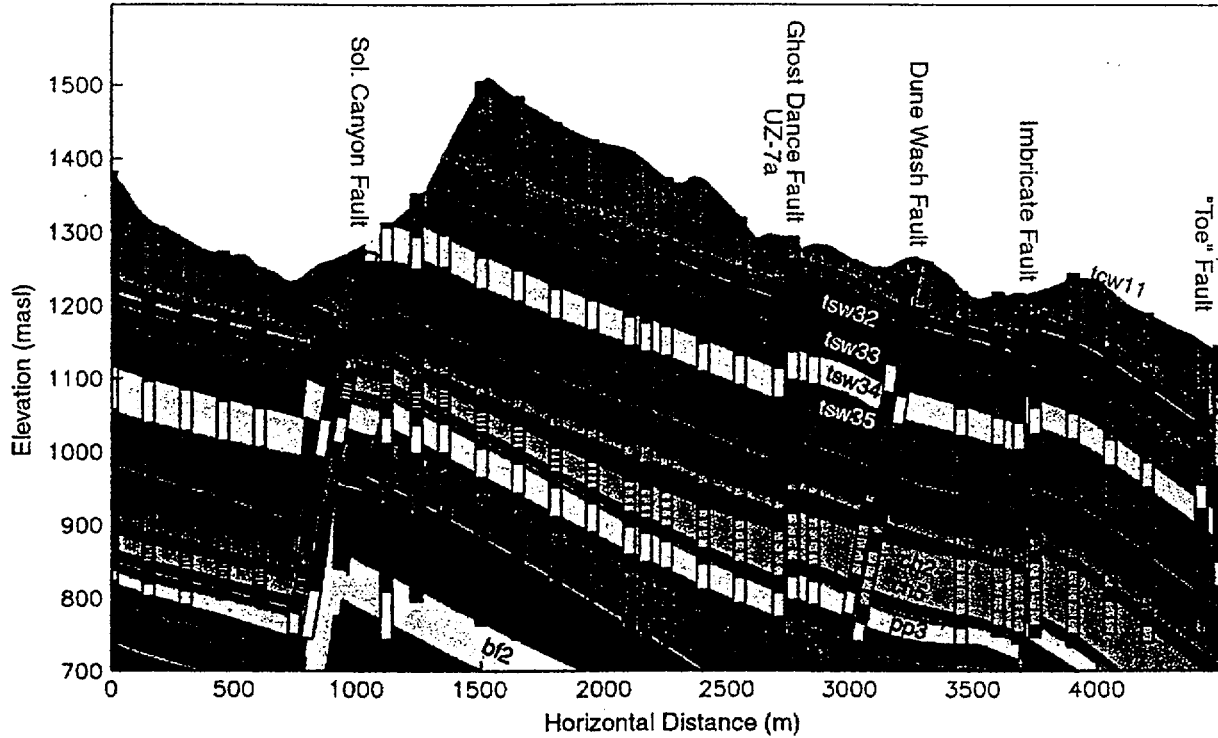


Figure IV-2. Comparison Between GFM3.1 (DTN: MO9901MWDGFM31.000) and Columns from the UZ-7a Cross-Sectional Grid (DTN: LB990501233129.003).

ATTACHMENT V.

Development of a 3-D Numerical Grid for UZ Model Calibration.

The 3-D numerical grids developed for FY 99 UZ Model calibration consist of a relatively coarse plan-view grid (see Table V-1) with nodes centered at borehole locations and with discretization along major faults, the ESF, and the ECRB. The primary 3-D grid is generated using formatted GFM3.1 fault data (as discussed in Section 6.3 of this AMR) and layer isochore and elevation data (as discussed in Sections 6.4.1 and 6.4.2). Vitric and zeolitic material names are assigned to gridblocks in UZ Model layers ch1, ch2, ch3, ch4, and ch5 based on the location of the vitric-zeolitic boundary (see Section 6.6.3, Figure 5). Dual-permeability meshes are generated from the primary mesh using fracture data presented in Table 5.

The mesh files identified by DTN: **LB990501233129.004** and created for use in 3-D UZ Model calibrations include:

- The primary (ECM) mesh, “**primary.mesh**.”
- The dual-k mesh “**3d2kcalib_pc1.mesh**” for perched-water conceptual model #1.
- The dual-k mesh “**3d2kcalib_pc2.mesh**” for perched-water conceptual model #2.

The two dual-k meshes contain identical numerical values. The only difference between the two is that certain material names have been modified (e.g., “tswM8” changed to “pcM38,” corresponding to the matrix gridblocks for UZ Model layer “tsw38”) so that special rock properties can be assigned in the TOUGH2 input card ROCKS in order to represent the different perched-water conceptual models (#1: flow-through, #2: reduced fracture permeability in zeolites).

The detailed steps describing the generation of the mesh files are documented in Scientific Notebook YMP-LBNL-YSW-JH-2A (pp. 105-112).

Primary and dual-permeability grid statistics are summarized in Table V-1.

Table V-1. Statistics for 3-D UZ Model Grids for Calibration (from DTN: LB990501233129.004).

	Primary (ECM) Mesh	Dual-k Meshes
# of Columns	1,434	1,434
# of Gridblocks	53,512	104,156
# of Connections	185,245	421,134

Figures

The 2-D (plan-view) grid for 3-D UZ Model calibration is shown in Figure V-1. Selected cross sections from the 3-D grid (along transects A-A', B-B', and C-C' as indicated in Figure V-1) are shown in Figures V-2 through V-4. Note that there is 5-m vertical resolution at the repository horizon and 20-m maximum vertical resolution below the repository horizon in the cross-sectional figures.

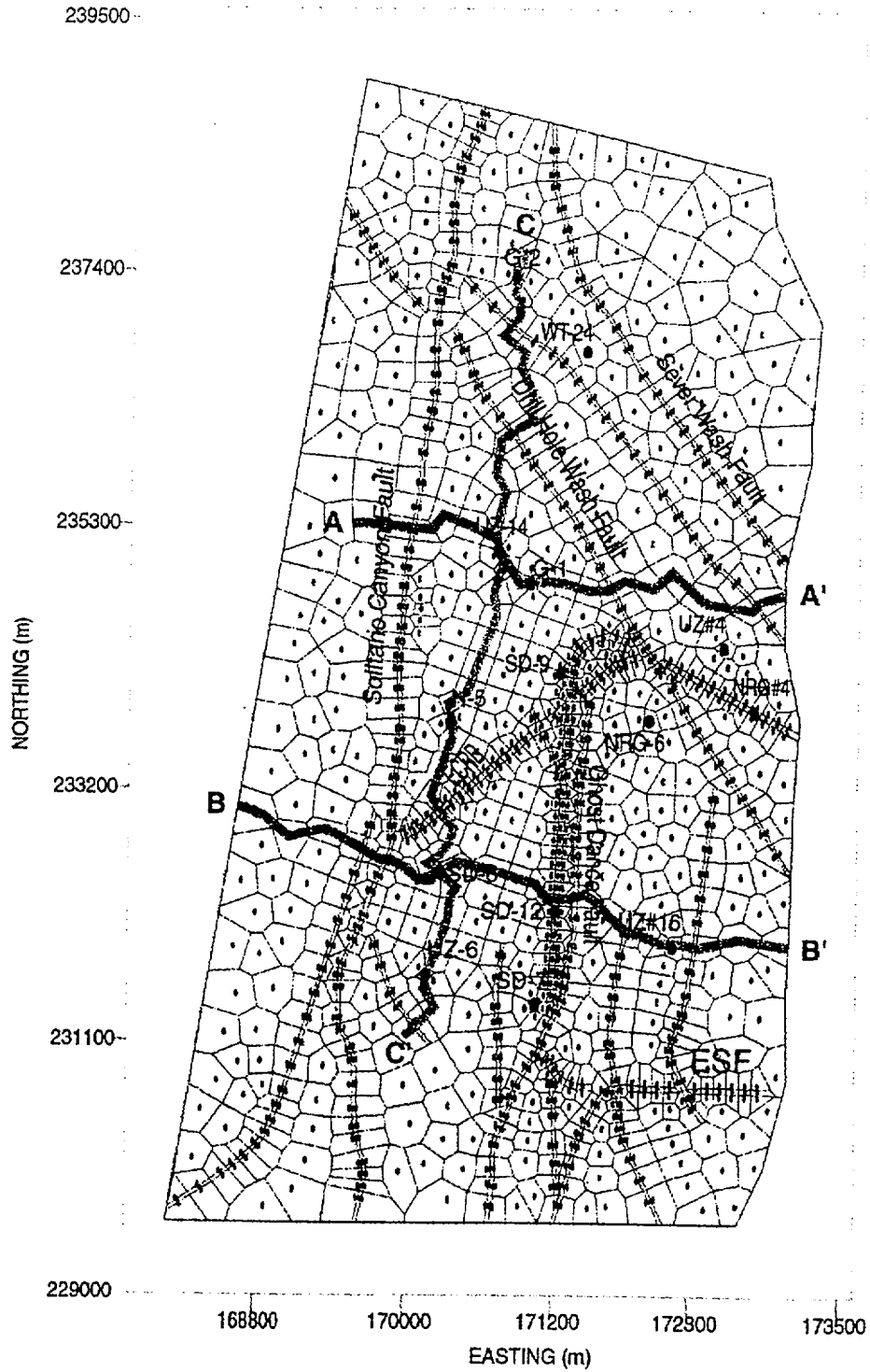


Figure V-1. 2-D (Plan-View) Grid Design for FY99 UZ Model Calibration (from DTN: LB990501233129.004).

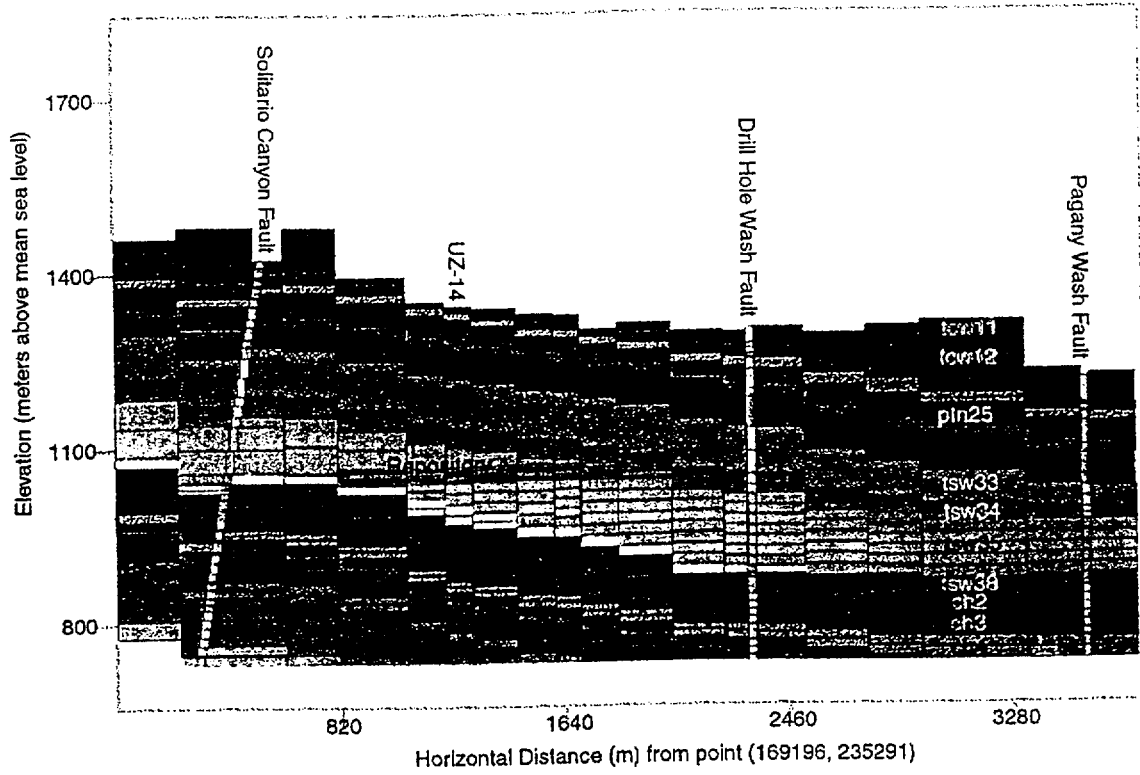


Figure V-2. East-West Cross Section A-A' from the 3-D UZ Model Calibration Grid (from DTN: LB990501233129.004).

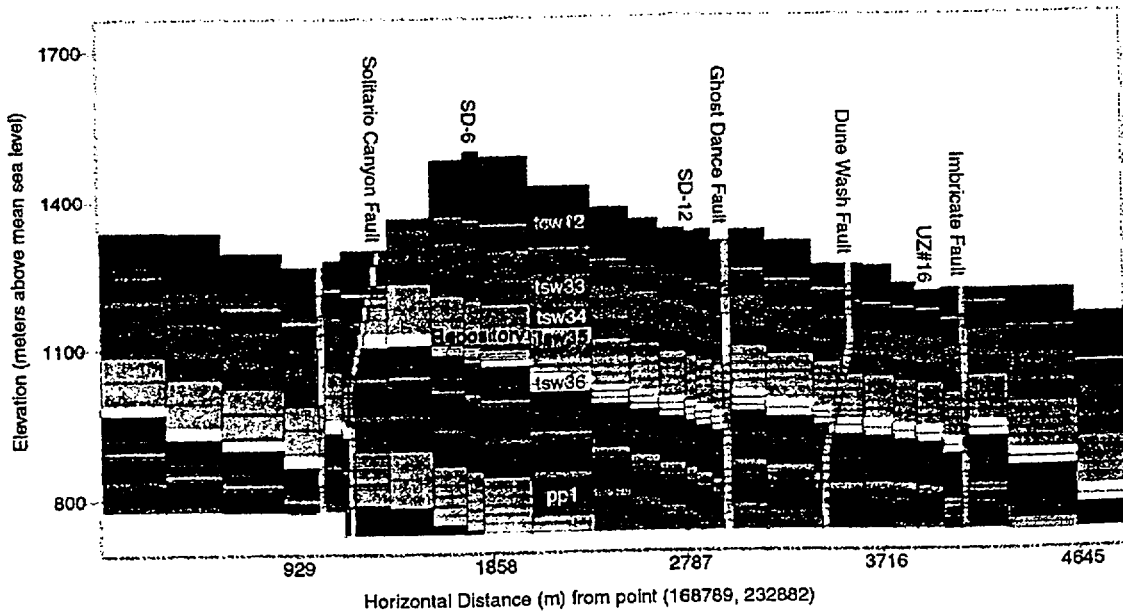


Figure V-3. East-West Cross Section B-B' from the 3-D UZ Model Calibration Grid (from DTN: LB990501233129.004).

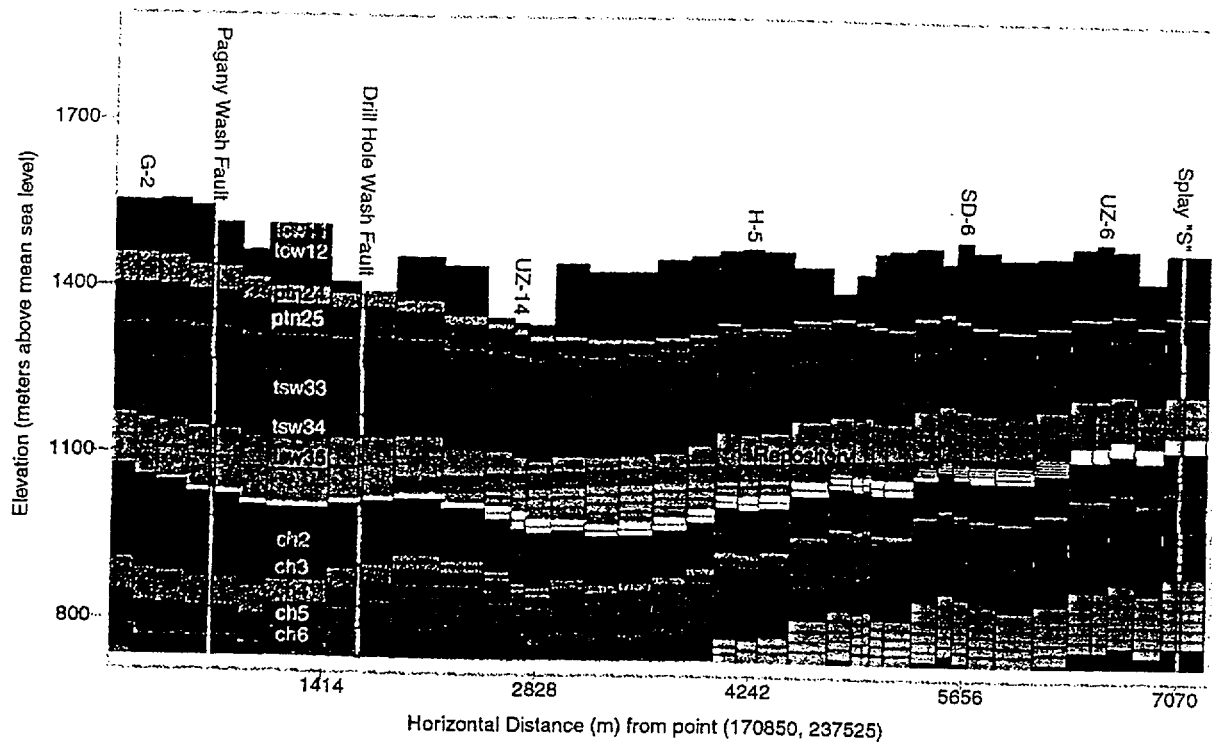


Figure V-4. North-South Cross Section C-C' from the 3-D UZ Model Calibration Grid (from DTN: LB990501233129.004).

Grid Verification

1. Gridblock Volume, Connection Length, and Interface Area Verification

Because the total number of gridblocks within the 3-D UZ Model calibration grids is so large, a subset of gridblocks from the model is evaluated to ensure the accuracy of the calculated gridblock volumes, connection lengths, and interface areas. Additional spot checks are performed that involve plotting simulated saturation contours along UZ Model cross sections in order to detect missing gridblock connections. These verification activities are described in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 53-57).

2. Borehole Verification

Model layer contact elevations for eleven grid columns corresponding to borehole locations were compared against the observed stratigraphic contact elevations contained in the GFM3.1 file "pix99el.dat" (where contact elevations were absent from this file, values were back interpolated from GFM3.1 surface elevation grids). Given an estimated maximum error in layer contact elevations at column centers of about 5 m (see first paragraph of Section 6.6), a grid validation criterion of plus-or-minus 5 m for layer contact elevations in grid columns corresponding to borehole locations was established. Differences in layer contact elevations (values from UZ Model calibration grid subtracted from values from "pix99el.dat") are plotted in Figure V-5 for

the eleven boreholes. Line discontinuities indicate missing, or pinched out, layers for that particular borehole.

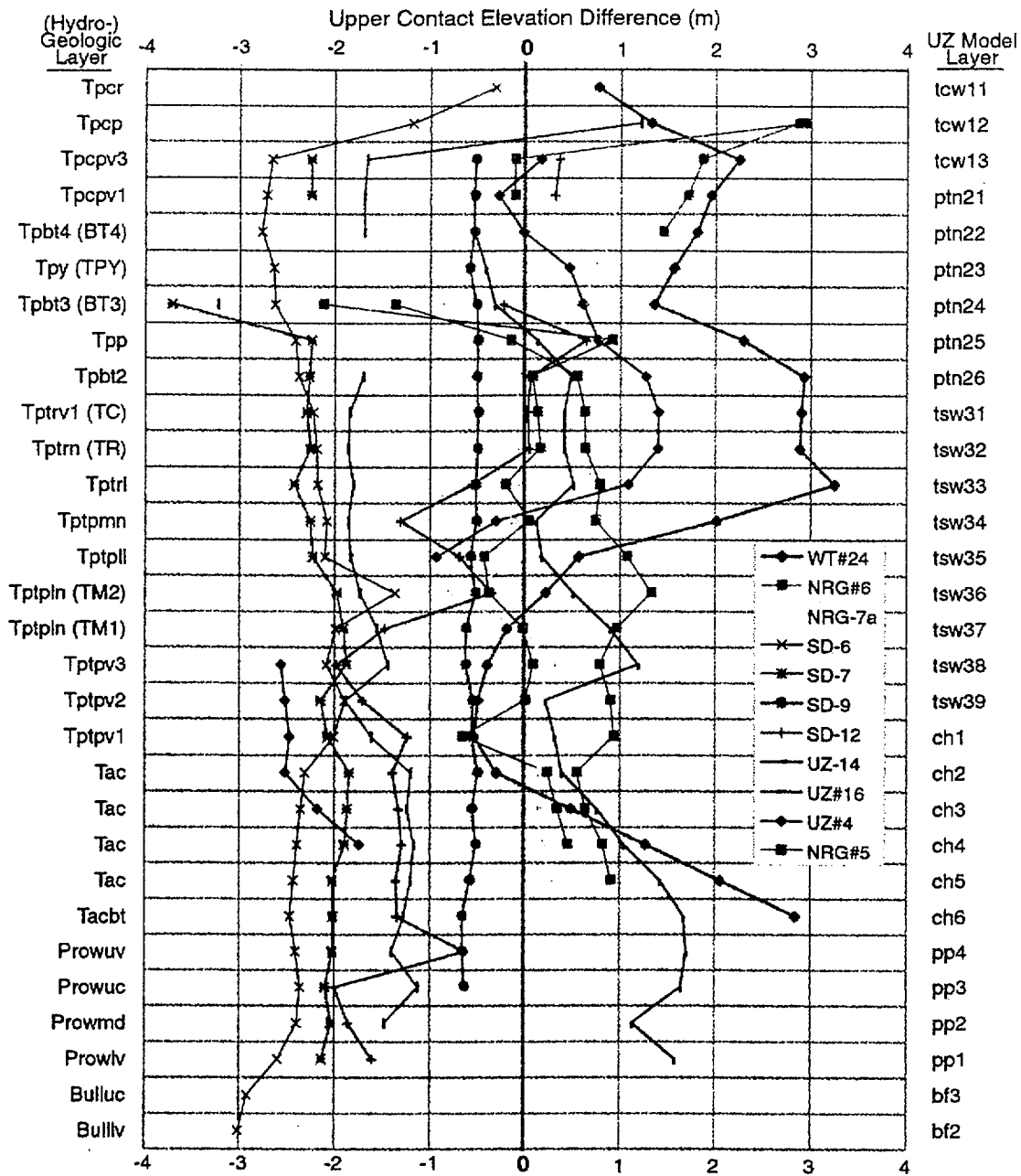


Figure V-5. Upper Contact Elevation Differences: GFM3.1 "pix99el.dat" (DTN: MO9901MWDGFM31.000) Minus 3-D UZ Model (Calibration) Grid (from DTN: LB990501233129.004) at Selected Borehole Locations. [A negative value means the UZ Model layer contact elevation is higher than the stratigraphic pick.]

Figure V-5 shows that the accuracy of the 3-D UZ Model calibration grid is typically within about 3 m for these borehole locations. Differences in the bedrock surface elevations for

boreholes NRG-7a, SD-7, SD-9, SD-12, and UZ#4 are not shown in this figure because they range from about 7 to 19 m. These large differences at the bedrock surface arise from fairly steep channel erosion that produces a surface with highly varying slope. Though the nearest GFM3.1 data point may be only meters to a few tens of meters away, irregularities in the bedrock surface may cause an elevation change of tens of meters over that distance. Given that fracture flow is predominant in the welded Tiva Canyon Tuff (as suggested by pneumatic and geochemical signals) (Rousseau et al. 1999, p. 1), the overestimate of layer Tpcp elevation in the UZ Model grid is believed to have an insignificant impact on modeling results.

3. Cross Section Verification

This type of verification involves visual, cross-section comparisons between GFM3.1 and columns of gridblocks from the UZ Model in order to ensure that gridblock material names and elevations are correct. One of the goals of this activity is to evaluate the UZ Model representation of stratigraphy immediately adjacent to fault planes—an area in which gridding can become extremely complex.

Figures V-6 through V-8 compare the two models. EARTHVISION (EARTHVISION V4.0, STN: 30035 V4.0, Version 4.0) was used to extract cross-sectional data (layer contact elevations and fault locations) from GFM3.1. These data are used to develop the base map in each figure. Three GFM3.1 cross sections, corresponding to the traverses highlighted in the plan-view grid diagram (Figure V-1), were extracted. In order to simplify the comparison, certain GFM3.1 layers are combined into single layers if they were grouped together in the UZ Model (e.g., Tptrl, Tptf, and Tptpul are combined into one layer equivalent to "tsw33"). Overlain on each base map are columns indicating the UZ Model representation of these layers along the same traverse. Data defining the top and bottom elevations of each hydrogeologic layer in the UZ Model were obtained as output directly from WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) after grid generation (actual grid resolution within hydrogeologic layers is not shown in these comparison plots). UZ Model gridblocks are color coded in each figure to match the corresponding GFM3.1 layer (or combination of layers, in certain cases). Note that the column width shown is not to scale and that all grid layer interfaces in the UZ Model are horizontal, rather than tilted as shown along faults.

Figure V-6 is an east-west cross section along transect A-A', which intersects Solitario Canyon, Drill Hole Wash, and Pagany Wash faults. Overall, the layer thickness and elevation match is good between the UZ Model grid and GFM3.1. Vertical displacement along the Solitario Canyon fault appears to be about 20 m less in the UZ Model than is seen in GFM3.1 along this cross section; however, this is only an artifact of the plotting technique. Recall that the column width shown in these cross-sectional comparison figures is not to scale. Gridblocks adjacent to nonvertical fault zones may be a few hundreds of meters wide (as is the case along the Solitario Canyon fault in this cross section). Thus, the elevations of the gridblocks shown in Figure V-6 are actually average elevations over larger lateral distances than suggested by the column width shown. With this in mind, it can be concluded that the elevation of UZ Model gridblocks are in reasonable agreement with GFM3.1 data along this cross section.

The only other apparent discrepancy is in the UZ-14 grid column and its adjacent columns. In this location, the UZ Model assumes a thickness for geologic layer Tptpln (corresponding to

model layers “tsw36” and “tsw37”) that is approximately twice the thickness from GFM3.1 (for justification, see discussion beginning on p. III-3).

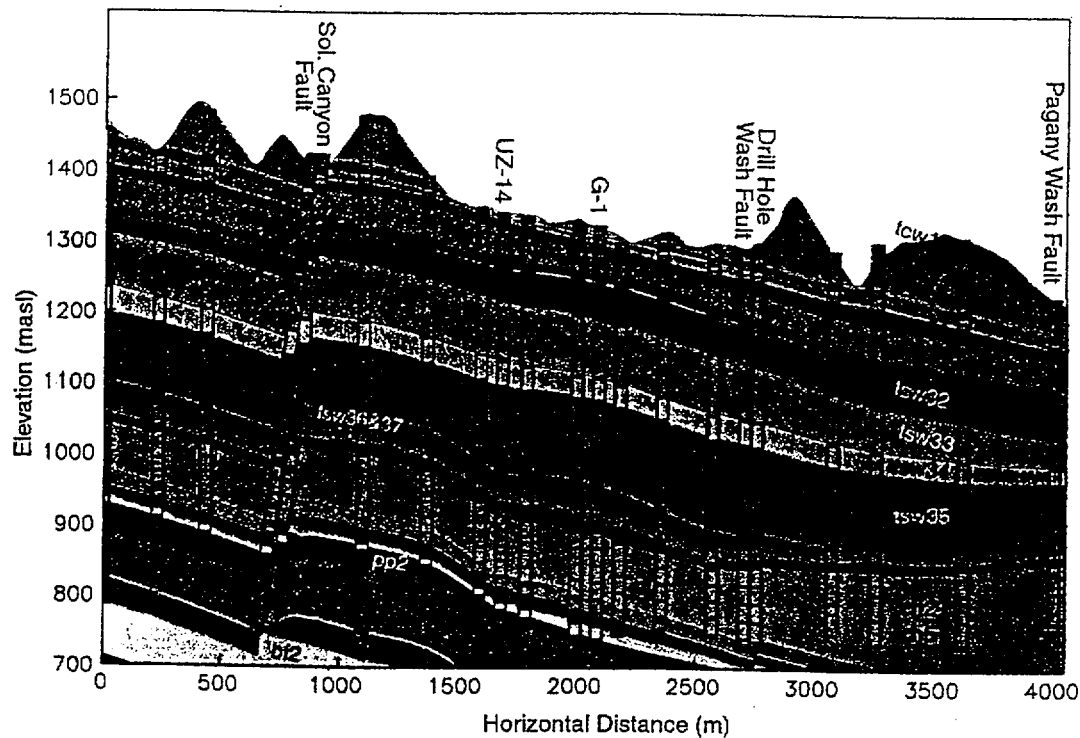


Figure V-6. East-West Cross-Section Comparison along A-A'. GFM3.1 stratigraphy (DTN: MO9901MWDGFM31.000) overlain with FY99 UZ Model calibration grid layering information (from DTN: LB990501233129.004).

Figure V-7 is an east-west cross section along transect B-B' that intersects the Solitario Canyon, Ghost Dance, Dune Wash, and Imbricate faults. Again, the overall layer thickness and elevation match is good between the UZ Model grid and GFM3.1. The greatest discrepancy in layer contact elevation occurs adjacent to fault zones. The software used for grid development, WinGridded V1.0, cannot represent intersecting faults. This is because fault columns are generated using vertical columns of gridblocks that do not pinch out or intersect at depth. Section 6.6.1 of this AMR discusses the general methodology for fault gridding using WinGridded. Vertical representation of the Solitario Canyon fault in the UZ Model calibration grid changes from nonvertical to vertical at an elevation of about 1050 masl in cross section B-B' because of the proximity of another fault—the western splay of Solitario Canyon fault (see Figure V-3). According to GFM3.1, these two faults intersect at an elevation of about 750 masl. Vertical representation of the Dune Wash fault also becomes vertical not only at depth but near the land surface on account of constraints set on column width.

Figure V-8 is a north-south cross section along transect C-C' that intersects the Pagany Wash, Drill Hole Wash, and Splay “S” faults. The overall layer thickness and elevation match is acceptable throughout the cross section, including grid columns adjacent to fault zones.

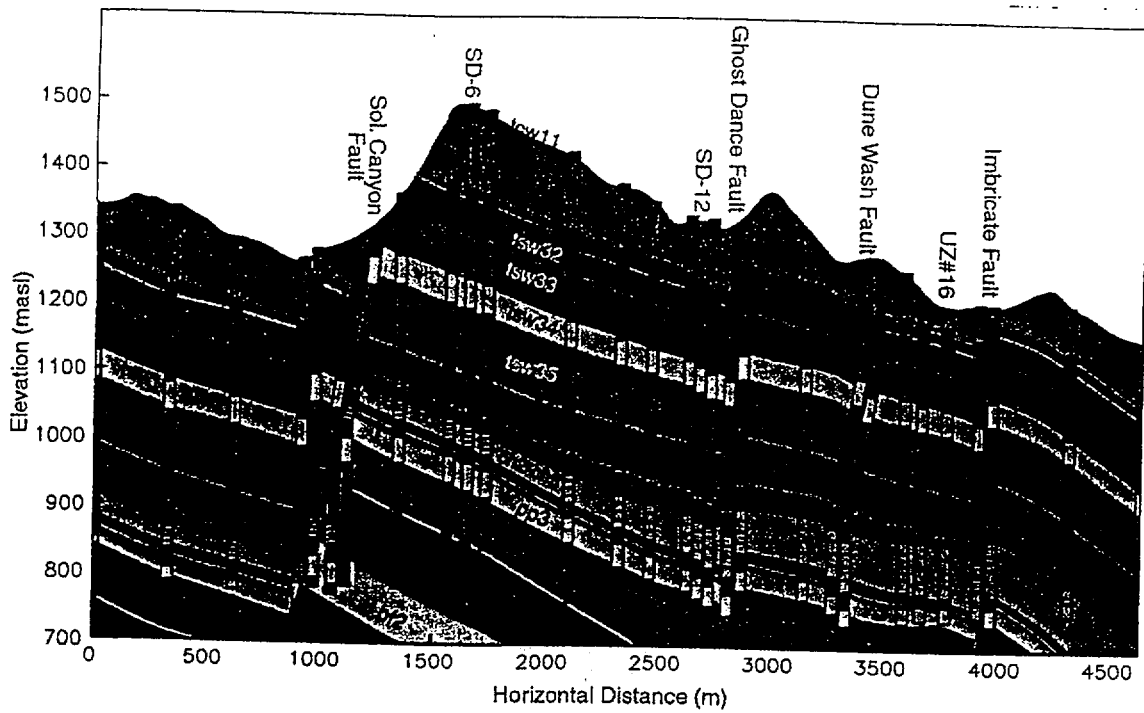


Figure V-7. East-West Cross-Section Comparison along B-B'. GFM3.1 stratigraphy (DTN: MO9901MWDGFM31.000) overlain with FY99 UZ Model calibration grid layering Information (from DTN: LB990501233129.004).

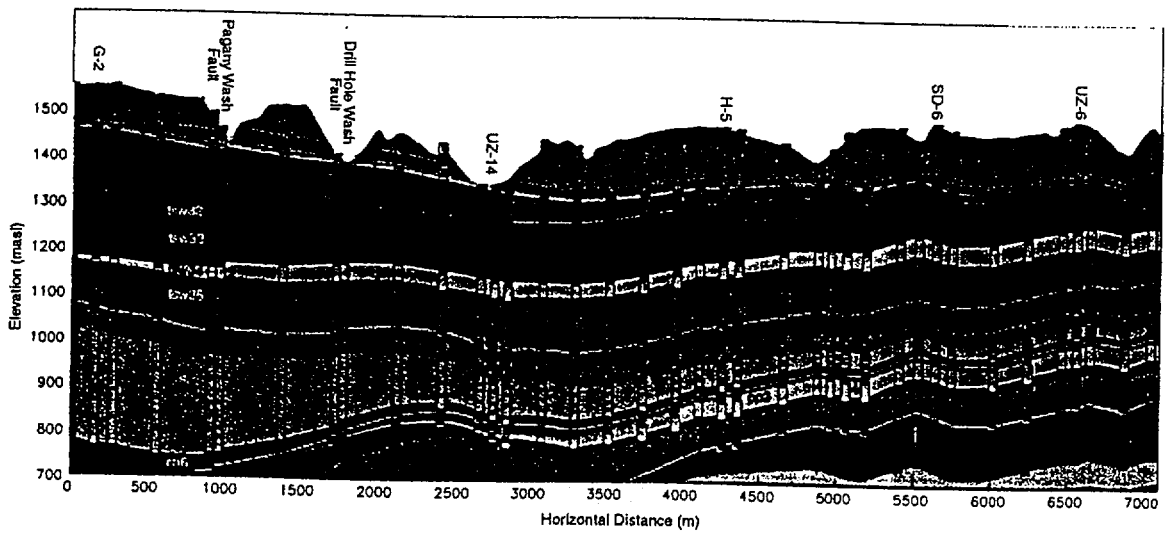


Figure V-8. North-South Cross-Section Comparison along C-C'. GFM3.1 stratigraphy (DTN: MO9901MWDGFM31.000) overlain with FY99 UZ Model calibration grid layering Information (from DTN: LB990501233129.004).

To summarize the results from the cross-section comparisons, UZ Model layer thicknesses are in close agreement with GFM3.1 layer thicknesses (as expected, since the UZ Model was

ATTACHMENT VI.

Development of a 3-D Numerical Grid for Calculation of Flow Fields for PA.

In general, the 3-D numerical grid generated for development of FY 99 UZ Model flow fields for PA is similar to the 3-D calibration grid. The major difference is that the 3-D grid for generating flow fields consists of a plan-view with repository refinement, but no discretization along the ESF or ECRB. In addition, the southwestern-most fault in the UZ Model domain, branching west off the main trace of the Solitario Canyon fault, is shortened in order to resolve problems with fault-slope representation along the large-displacement, nonvertical Solitario Canyon fault.

The primary 3-D grid is generated using formatted GFM3.1 fault data (as discussed in Section 6.3 of this AMR) and layer isochore and elevation data (as discussed in Sections 6.4.1 and 6.4.2). Vitric and zeolitic material names are assigned to gridblocks in UZ Model layers ch1, ch2, ch3, ch4, and ch5 based on the location of the vitric-zeolitic boundary (see Section 6.6.3, Figure 5). Dual-permeability meshes are generated from the primary mesh using fracture data presented in Table 5.

The mesh files identified by DTN: **LB990701233129.001** and created for use in generating 3-D flow fields for Performance Assessment include:

- The primary (ECM) mesh, “**primary.mesh**.”
- The dual-k mesh “**3d2kpa.mesh**,” which contains no perched-water adjustments.
- The dual-k mesh “**3d2kpa_pc1.mesh**” for perched-water conceptual model #1.
- The dual-k mesh “**3d2kpa_pc2.mesh**” for perched-water conceptual model #2.

The three dual-k meshes contain identical numerical values. The only difference between them is that certain material names have been modified (e.g., “tswM8” changed to “pcM38,” corresponding to the certain matrix gridblocks for UZ Model layer “tsw38”) so that special rock properties can be assigned in the TOUGH2 input card ROCKS in order to represent the different perched-water conceptual models (#1: flow-through, #2: reduced fracture permeability in zeolites). The mesh file “3d2kpa.mesh” contains no modified material names.

The detailed steps describing the generation of the mesh files are documented in Scientific Notebook YMP-LBNL-YSW-JH-2A (pp. 113-120).

Primary and dual-permeability grid statistics are summarized in Table VI-1.

Table VI-1. Statistics for the 3-D UZ Model Grids for Generating Flow Fields (from DTN: LB990701233129.001).

	Primary (ECM) Mesh	Dual-k Meshes
# of Columns	1,324	1,324
# of Gridblocks	50,312	97,976
# of Connections	174,553	396,770

Figures

The 2-D (plan-view) grid for generating 3-D UZ Model flow fields is shown in Figure VI-1. Selected cross sections from the 3-D grid (along transects A-A', B-B', and C-C' as indicated in Figure VI-1) are shown in Figures VI-2 through VI-4. Note the 5-m vertical resolution at the repository horizon and the 20-m maximum vertical resolution below the repository horizon in the cross-sectional figures.

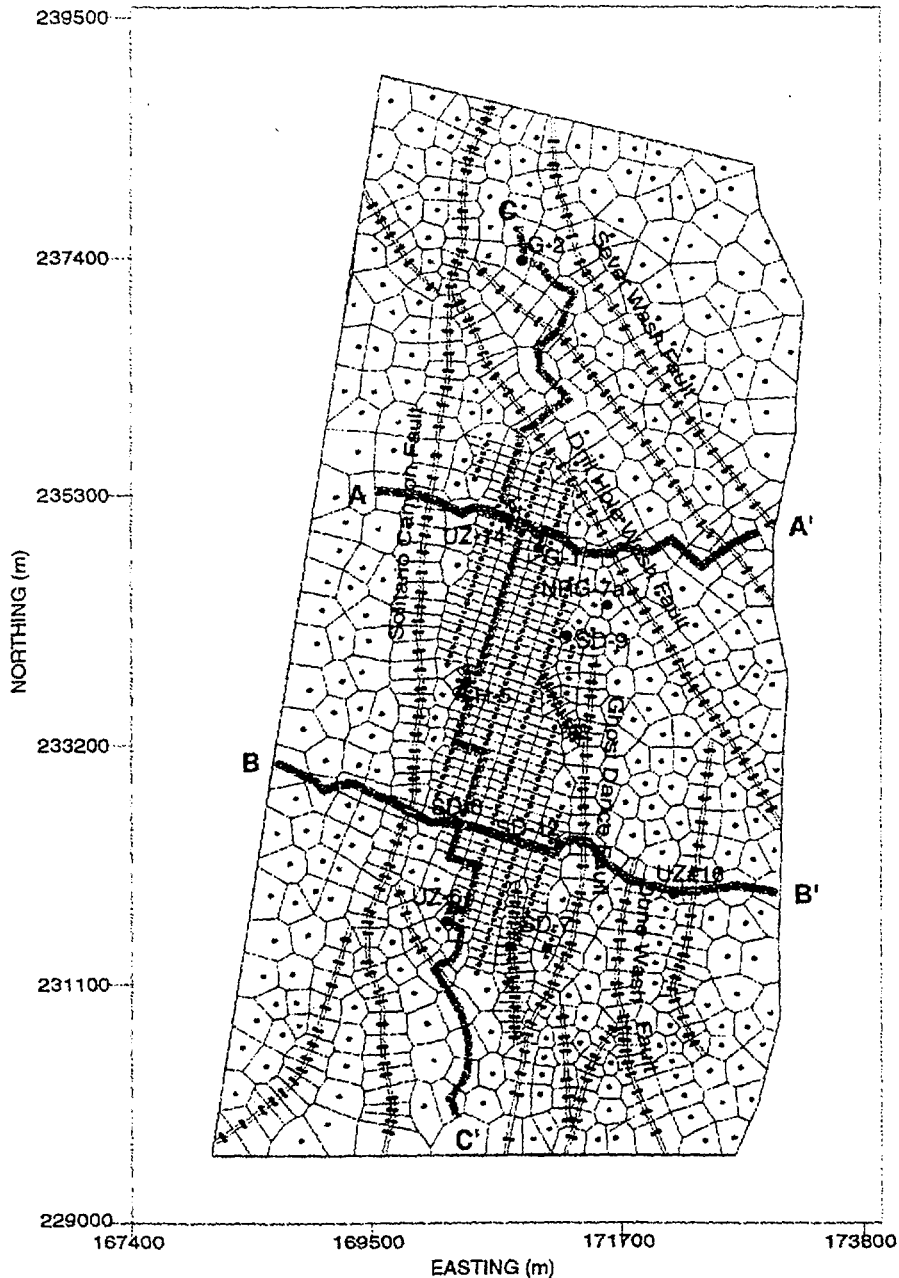


Figure VI-1. 2-D (Plan-View) Grid Design for FY99 UZ Model Flow-Field Calculations (from DTN: LB990701233129.001).

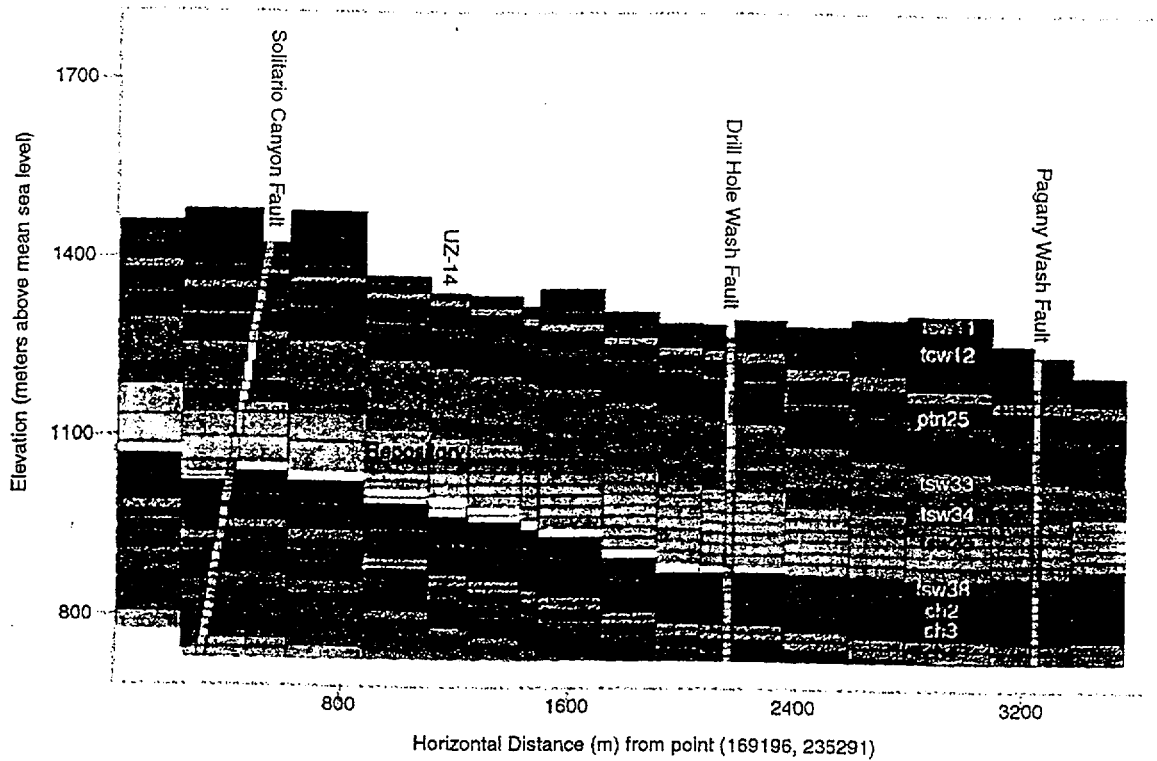


Figure VI-2. East-West Cross Section A-A' from the 3-D UZ Model Flow-Fields Grid (from DTN: LB990701233129.001).

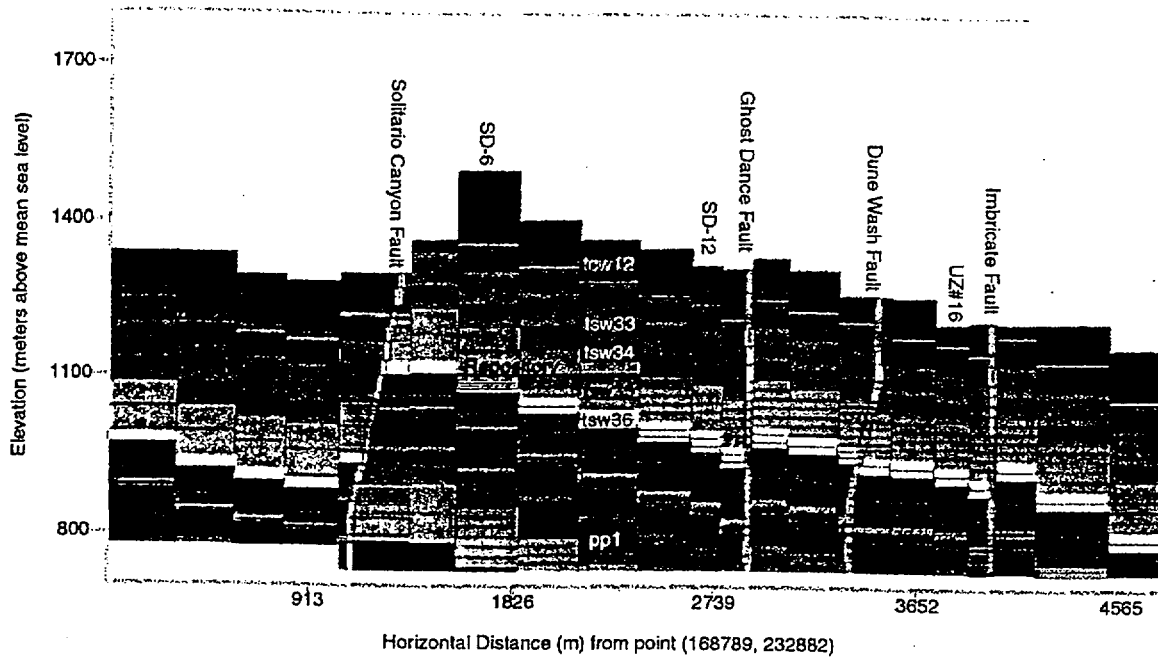


Figure VI-3. East-West Cross Section B-B' from the 3-D UZ Model Flow-Fields Grid (from DTN: LB990701233129.001).

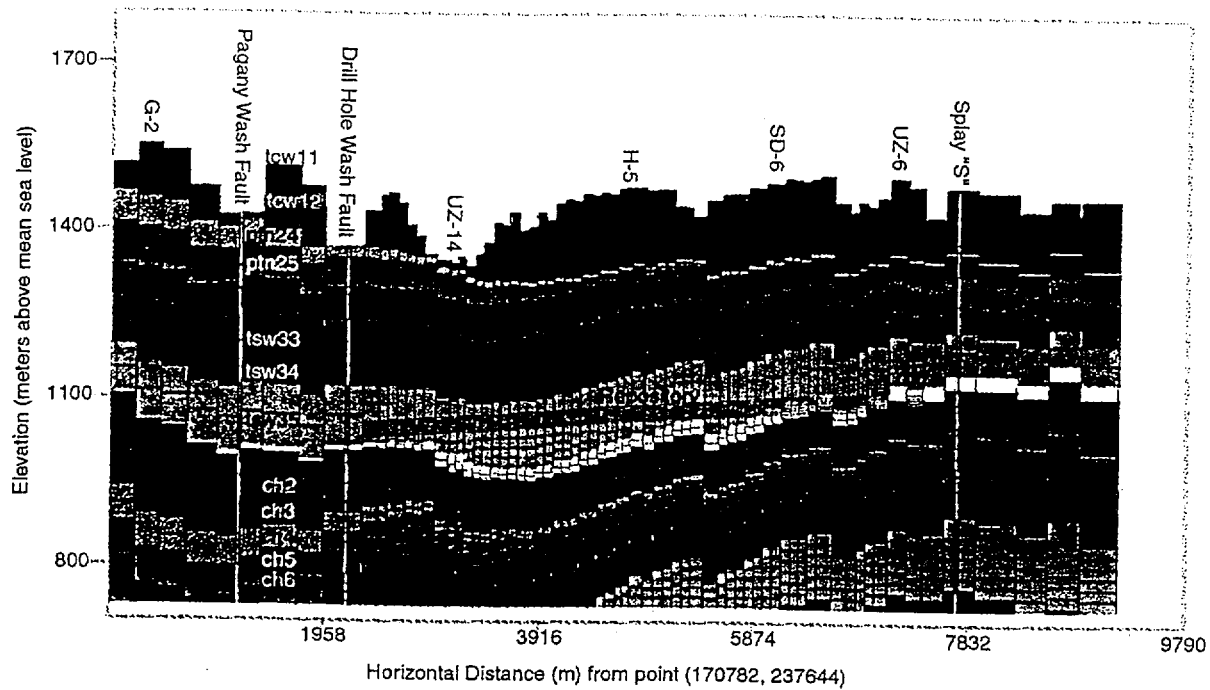


Figure VI-4. North-South Cross Section C-C' from the 3-D UZ Model Flow-Fields Grid (from DTN: LB990701233129.001).

Grid Verification

1. Gridblock Volume, Connection Length, and Interface Area Verification

Because the total number of gridblocks within the 3-D UZ Model flow-fields grids is so large, a subset of gridblocks from the model is evaluated to ensure the accuracy of the calculated gridblock volumes, connection lengths, and interface areas. Additional spot checks are performed that involve plotting simulated saturation contours along UZ Model cross sections in order to detect missing gridblock connections. These verification activities are described in Scientific Notebook YMP-LBNL-YSW-JH-2 (pp. 53-57).

2. Borehole Verification

Model layer contact elevations for eleven grid columns corresponding to borehole locations were compared against the observed stratigraphic contact elevations contained in the GFM3.1 file "pix99el.dat" (where contact elevations were absent from this file, values were back interpolated from GFM3.1 surface elevation grids). Given an estimated maximum error in layer contact elevations at column centers of about 5 m (see first paragraph of Section 6.6), a grid validation criterion of plus-or-minus 5 m for layer contact elevations in grid columns corresponding to borehole locations was established. Differences in layer contact elevations (values from the 3-D UZ Model grid subtracted from values from "pix99el.dat") are plotted in Figure VI-5 for the eleven boreholes. Line discontinuities indicate missing, or pinched out, layers for that particular borehole.

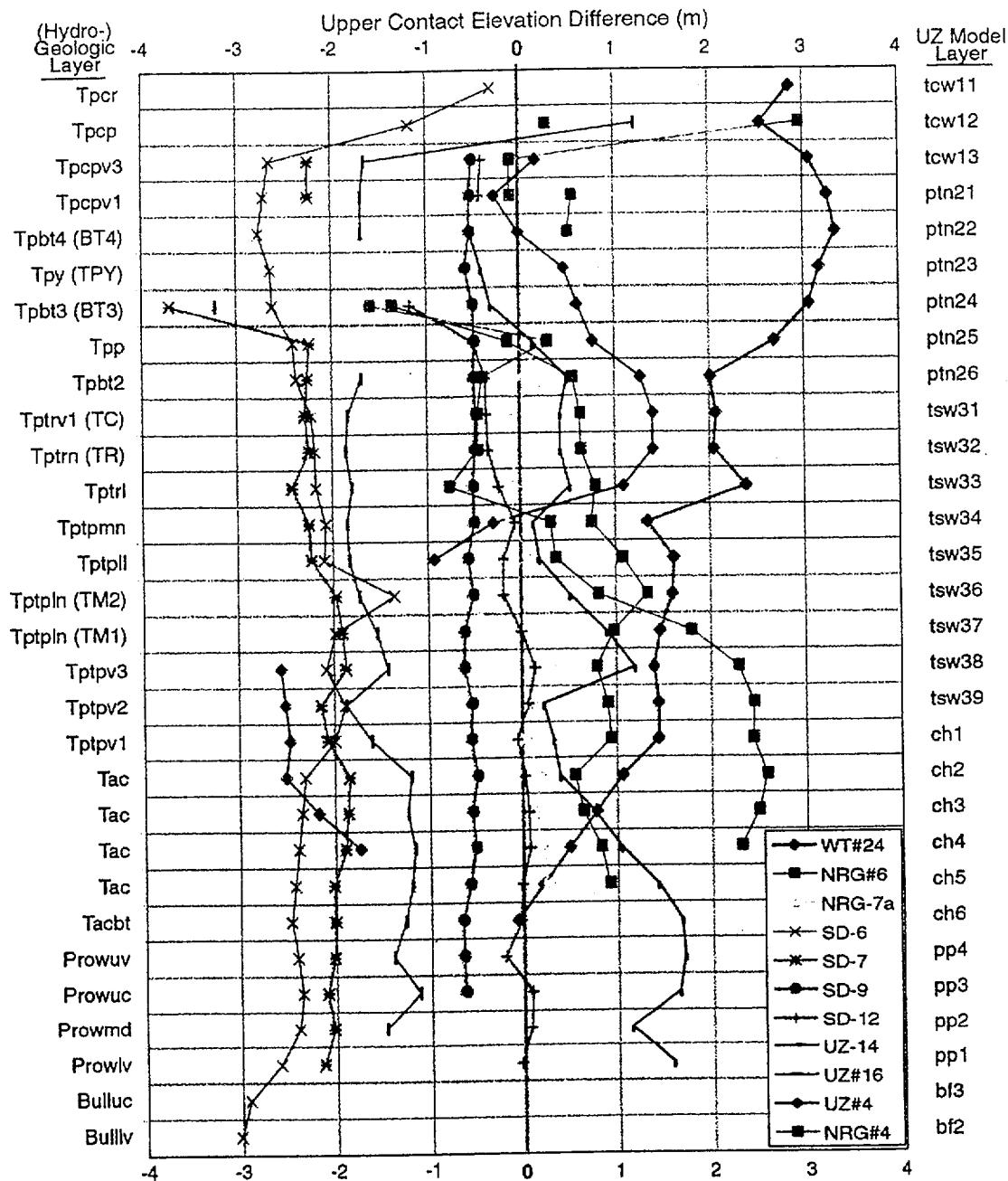


Figure VI-5. Upper Contact Elevation Differences: GFM3.1 "pix99el.dat" (DTN: MO9901MWDGFM31.000) Minus 3-D UZ Model (Flow-Fields) Grid (DTN: LB990701233129.001) at Selected Borehole Locations. [A negative value means the UZ Model layer contact elevation is higher than the stratigraphic pick.]

Figure VI-5 shows that the accuracy of the 3-D UZ Model grid is typically within about 3 m for these borehole locations. Differences in the bedrock surface elevations for boreholes NRG-7a, SD-7, SD-9, SD-12, and UZ#4, which correspond to the upper eroded surface of geologic layer Tpcp, are not shown in this figure because they range from about 7 to 19 m. These large differences at the bedrock surface arise due to fairly steep channel erosion that produces a

surface with highly varying slope. Though the nearest GFM3.1 data point may be only meters to a few tens of meters away, irregularities in the bedrock surface may cause an elevation change of tens of meters over that distance. Given that fracture flow is predominant in the welded Tiva Canyon Tuff (as suggested by pneumatic and geochemical signals) (Rousseau et al. 1999, p. 1), the overestimate of layer Tpcp elevation in the UZ Model grid is believed to have an insignificant impact on modeling results.

3. Cross Section Verification

This type of verification involves visual, cross-section comparisons between GFM3.1 and columns of gridblocks from the UZ Model in order to ensure that gridblock material names and elevations are correct. One of the goals of this activity is to evaluate the UZ Model representation of stratigraphy immediately adjacent to fault planes—an area in which gridding can become extremely complex.

Three GFM3.1 cross sections, corresponding to the traverses highlighted in the plan-view grid diagram (Figure VI-1), were extracted using EARTHVISION (EARTHVISION 4.0, STN: 30035 V4.0, Version 4.0). These data were used to develop the base map in each figure. In order to simplify the comparison, certain GFM3.1 layers are combined into single layers if they were grouped together in the UZ Model (e.g., Tptrl, Tptf, and Tptpul are combined into one layer equivalent to "tsw33"). Overlain on each base map are columns indicating the UZ Model representation of these layers along the same traverse. Of the three cross sections compared, only the one along B-B' is presented here (Figure VI-6). The other two cross-section comparisons, along A-A' and C-C' (see Scientific Notebook YMP-LBNL-JH-2A, pp. 137, 139), are nearly identical to the cross-section comparisons previously described for the 3-D UZ Model calibration grid (see Attachment V).

Data defining the top and bottom elevations of each hydrogeologic layer in the UZ Model were obtained as output directly from WinGridder (WinGridder V1.0, STN: 10024-1.0-00, Version 1.0) after grid generation. UZ Model gridblocks are color coded based on their material name in order to match the corresponding GFM3.1 layer (or combination of layers, in certain cases). Note that the column width shown is not to scale and that all grid layer interfaces in the UZ Model are horizontal, rather than tilted, as shown along faults.

Note in Figure VI-6 that the western Solitario Canyon fault splay is not represented in the UZ Model grid along this east-west cross section. This simplification in the grid is not expected to have any significant impact on model simulation results within the repository area because the splay lies west of the Solitario Canyon fault, which may serve as either a conduit for vertical flow or as a barrier to lateral flow. Overall, the layer thickness and elevation match is good between the UZ Model grid and GFM3.1.

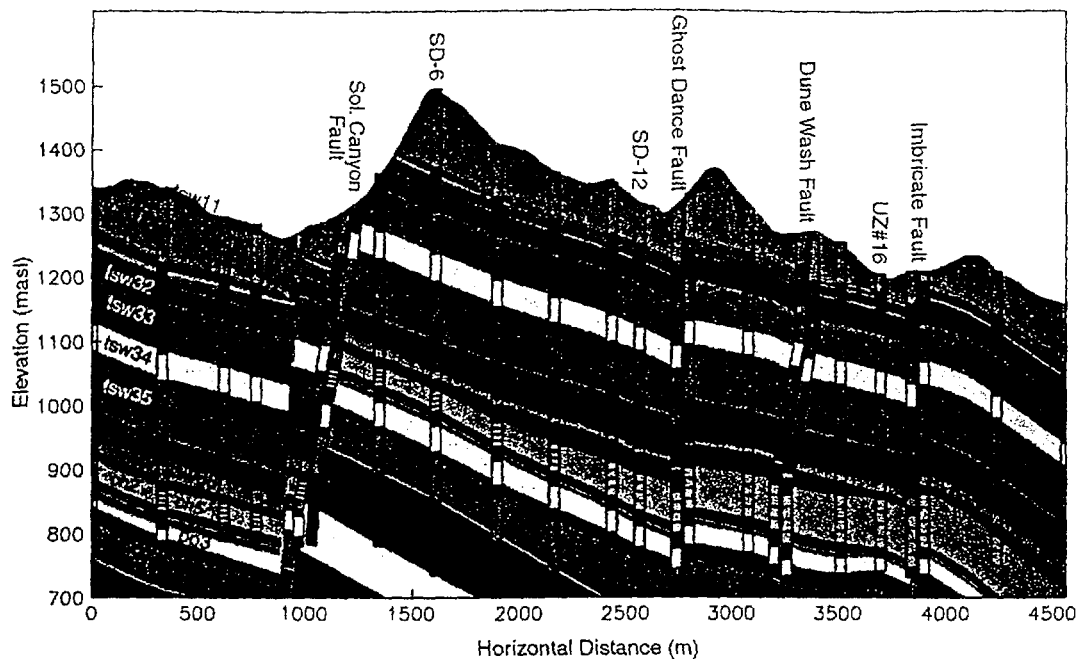


Figure VI-6. East-West Cross-Section Comparison along B-B'. GFM3.1 stratigraphy (DTN: MO9901MWDGFM31.000) overlain with FY99 UZ Model grid layering information (from DTN: LB990701233129.001).