OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET
Complete Only Applicable Items

1. QA: QA
Page: 1 of: ~~68~~ 70

2. [x] Analysis — Check all that apply

Type of Analysis:
- [ ] Engineering
- [ ] Performance Assessment
- [x] Scientific

Intended Use of Analysis:
- [ ] Input to Calculation
- [x] Input to another Analysis or Model
- [ ] Input to Technical Document
- [ ] Input to other Technical Products

Describe use:
To provide numerical grids to be used in UZ Flow and Transport Modeling activities

3. [x] Model — Check all that apply

Type of Model:
- [ ] Conceptual Model
- [ ] Abstraction Model
- [x] Mathematical Model
- [ ] System Model
- [ ] Process Model

Intended Use of Model:
- [ ] Input to Calculation
- [x] Input to another Model or Analysis
- [ ] Input to Technical Document
- [ ] Input to other Technical Products

Describe use:

4. Title:
Development of Numerical Grids for UZ Flow and Transport Modeling

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-NBS-HS-000015 REV 00 ICN 01

6. Total Attachments:
6

7. Attachment Numbers - No. of Pages in Each:
I-1, II-2, III-4, IV-3, V-9, VI-7

	Printed Name	Signature	Date
8. Originator	Jennifer Hinds Lehua Pan	Jennifer Hinds	12/18/01
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11. Responsible Manager	G. S. Bodvarsson	[signature]	12/18/01

12. Remarks:
REV 00:
Block 8: Jennifer Hinds prepared the entire document and performed analyses and modeling except for the analyses utilizing the software Wingridder, which were performed by Lehua Pan.
Block 9: The entire document was checked by Richard Stover and Peter Persoff.

REV 00 ICN 01:
Deficiency Report LVMO-00-D-039, Inaccurate Documentation And Validation of Software Routines And/or Macros, identified software issues that are addressed in MOL.20010816.0228 (Hinds 2001), additional software documentation. The information in the record will be integrated into the AMR as part of the next revision or ICN.

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

2. Analysis or Model Title:
U0000 Development of Numerical Grids for UZ Flow and Transport Modeling

3. Document Identifier (including Rev. No. and Change No., if applicable):

ANL-NBS-HS-000015 REV 00 ICN 01

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue
00 01	The following remaining TBVs have been resolved and removed: TBVs 3008, 3310, 3057, and 3060. These DTNs are either now qualified, have been superceded, have new qualified sources, or have been resolved through text changes to the AMR. Changes in ICN 01 of this AMR are marked with change bars in the document margins. Changes made affect the following Sections and pages: Section 1 (p. 11) Section 2 (p. 13) Section 3 (p. 15) Section 4 (pp. 17-20) Section 5 (pp. 25-28) Section 6 (pp. 29-30, 32, 40-41, 48-49) Section 7 (p. 61) Section 8 (pp. 63-66) Attachment I (p. I-1)

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FIGURES

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TABLES

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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
DIRS	Document Input Reference 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

ACRONYMS (CONTINUED)

STN	Software Tracking Number
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. Revision 00 of the work described herein follows the planning and work direction outlined in the *Development of Numerical Grids for UZ Flow and Transport Modeling* (CRWMS M&O 1999c). The technical scope, content, and management of ICN 01 of this AMR is currently controlled by the planning document, *Technical Work Plan for Unsaturated Zone (UZ) Flow and Transport Process Model Report* (BSC 2001a). The scope for the TBV resolution actions in this ICN is described in the *Technical Work Plan for: Integrated Management of Technical Product Input Department* (BSC 2001b, Addendum B, Section 4.1).

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

Applicable Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) Administrative Procedures (APs) and YMP-LBNL Quality Implementing Procedures (QIPs) for development of REV 00 of the AMR were identified in the "AMR Development Plan for U0000 Development of Numerical Grids for UZ Flow and Transport Modeling, Rev 00" (CRWMS M&O 1999c). The current version of applicable procedures identified in the *Technical Work Plan for Unsaturated Zone (UZ) Flow and Transport Process Model Report* (BSC 2001a) were utilized in the development of REV 00 ICN 01 of the AMR.

Revision 00 of 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). The activity evaluation for REV 00 ICN 01 is documented in *Technical Work Plan for Unsaturated Zone (UZ) Flow and Transport Process Model Report* (BSC 2001a).

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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 the Document Input Reference System (DIRS).

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	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, ESF4_XYZ V.03.XLS, and WinGridder V1.0 are qualified under *AP-SI.1Q, Software Management.*

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 directly or as corroborative information in numerical grid development are summarized in Table 2. The Q-status of each of these DTNs is provided in the DIRS.

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

Description	DTN or ACC	USE
Geologic Framework Model, GFM3.1	MO9901MWDGFM31.000	Direct
Hydrogeologic Unit Definitions	MOL.19980429.0512[1]	Corroborative (Assumption 4)
Integrated Site Model, ISM3.0	MO9901MWDISMRP.000	Corroborative (Assumption 5, 6)
Repository Layout Configuration	MOL.19990409.0100[2]	Corroborative (Assumption 8)
Water Table Elevations	MO9609RIB00038.000[3] MO0106RIB00038.001	Corroborative (Assumption 1)
Perched Water Elevations	GS990908312312.005	Corroborative (Assumption 3)
Fracture Data for Hydrogeologic Units	LB990501233129.001	Direct

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

[2] Data retrieved from CRWMS M&O 1999d.

[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. Note that the TDMS now shows DTN: M09901MWDGFM31.000 (Q) to be superseded by DTN: MO0012MWDGFM02.002, however, the new DTN does not include the data used for development of this analysis. The comment section on the Technical Data Information Form for the more recent DTN also contains the statement, "GFM2000 does not invalidate GFM3.1. Changes to rock layer elevations in the repository area are very small in magnitude; rarely as large as 25 feet." Because a variance of 25 feet is less than the uncertainty in the depths for stratigraphic layers in GFM2000 (BSC 2001c, Section 7), this ICN maintains the use of the original DTN.

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 have also been considered as discussed in Section 5.2 (Assumption 4). 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. As discussed in Section 5.2 (Assumption 5), the data considered in the numerical grid development for defining low-permeability, zeolitic volumes of rock are obtained from the ISM3.0 Rock Properties Model (DTN: MO9901MWDISMRP.000). The specific ISM3.0 files used in UZ Model grid development are listed in Attachment II.

As discussed in Section 5.2 (Assumption 8), an assumed repository layout configuration based on the Enhanced Design Alternative (EDA) II (CRWMS M&O 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.

As discussed in Section 5.1 (Assumption 1), the lower UZ Model boundary is based on water table elevations given in DTN: MO9609RIB00038.000 (specifically, Table 1, column labeled 1993). This DTN was qualified (TBV) when REV 00 of this AMR was issued, but the status of the data was later changed to unqualified. The data have been superseded by DTN: MO0106RIB00038.001 which is qualified. Table 1 of this new DTN includes a summary of mean water levels from selected wells in the Yucca Mountain area, and has been updated to include water level data from 1999. Table 4 of this ICN includes a comparison of the water level data from the two DTNs. The data used to develop REV 00 of this AMR (DTN: MO9609RIB00038.000) are not significantly different from the new qualifed data (DTN: MO0106RIB00038.001), and there is, therefore, no impact to the output of this document. Not included in Table 4 are perched water elevations for boreholes USW G-2 and USW WT-24 (DTN: GS990908312312.005), to be discussed in Section 5.1.

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

Table 4. Water Levels in Selected Boreholes

Borehole ID[1]	Water Table Elevation (masl) DTN: MO9609RIB00038.000	Water Table Elevation (masl) DTN: MO0106RIB00038.001
USW G-3 [2]	730.54	730.5
USW H-1 [2]	730.96	730.8
USW H-3 [2]	731.20	731.5
USW H-4 [2]	730.46	730.4
USW H-5 [2]	775.55	775.5
USW H-6 [2]	776.03	776.0
USW WT-1 [2]	729.96	730.4
USW WT-2 [2]	730.70	730.6
UE-25 WT#3	729.68	729.6
UE-25 WT#4 [2]	730.37	730.8
UE-25 WT#6 [2]	1034.14	1034.6
USW WT-7 [2]	775.86	775.8
USW WT-10	776.08	776.0

From Table 1 of DTN: MO9609RIB00038.000 and DTN: MO0106RIB00038.001

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) DTN: MO9609RIB00038.000	Water Table Elevation (masl) DTN: MO0106RIB00038.001
USW WT-11	730.65	730.7
UE-25 WT# 12	729.24	729.5
UE-25 WT#13	729.06	729.1
UE-25 WT#14	729.57	729.7
UE-25 WT#15	729.02	729.2
UE-25 WT#16	738.22	738.3
UE-25 WT#17	729.45	729.7
UE-25 WT#18 [2]	730.72	730.8
UE-25 J#13	728.46	728.4
UE-25 b#1 [2]	730.68	730.6
UE-25 c#2	729.98	730.2
UE-25 c#3	730.21	730.2

From Table 1 of DTN: MO9609RIB00038.000 and DTN: MO0106RIB00038.001

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
ch1Vl	6.9E-04	3.0E-04	1.0E-01	3.0E-01
ch2Vl	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch3Vl	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch4Vl	8.9E-04	2.6E-04	1.4E-01	4.3E-01
ch5Vl	8.9E-04	2.6E-04	1.4E-01	4.3E-01
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

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:

where is the fracture porosity for the 1-D calibration, is the fracture porosity as listed in the second column of Table 5, is the permeability of model layer "tsw34" (equal to 3.4E-13 m^2), and is the alternative permeability of model layer "tsw34" (equal to 1.6E-13 m^2) (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)
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:

where is the fracture porosity for the 1-D calibration, is the fracture porosity as listed in the second column of Table 5, is the permeability of model layer "tsw34" (equal to 3.4E-13 m^2), and is the alternative permeability of model layer "tsw34" (equal to 1.6E-13 m^2) (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. None of the assumptions listed below require verification.

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. The lower boundary for the UZ Model was established assuming 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). These data are given in DTN: MO9609RIB00038.000 (which has been superceded by DTN: MO0106RIB00038.001; see Section 4.1), and the 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 (at 1034, 1020, and 986 masl, respectively) can be interpreted to be 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 (Table 4). In boreholes USW G-2 and USW WT-24, not included in Table 4, water levels are approximately 1,020 masl and 840 masl, respectively (DTN: GS990908312312.005). 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 geologic data provided in GFM 3.1 cannot, by themselves, 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.

4. It is assumed that the 30 hydrogeologic units (HGUs) identified by the USGS (Flint 1998, pp. 1, 3-4) based on similarities in rock hydrogeologic properties are adequate to define the layering scheme used for the UZ Model grids (Section 6.3).

Since the hydrogeologic property sets to be utilized in UZ flow and transport modeling 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 grids.

The distribution of low-permeability zeolites within the Calico Hills nonwelded (CHn) hydrogeologic unit impacts flowpaths and groundwater travel times from the repository horizon to the water table and is, therefore, an important feature to capture in the UZ Model grids. The data considered in numerical grid development for defining low-permeability, zeolitic volumes of rock come from the ISM3.0 Rock Properties Model (DTN: MO9901MWDISMRP.000] [see Assumptions 5 and 6]). Note that DTN: MO9901MWDISMRP.000 was superseded by DTN: MO9910MWDISMRP.002 subsequent to the issuance of REV 00 of this document. An impact review of the newer data has been completed, and the changes were found to have no significant impact on the results of this document in the potential repository area (CRWMS M&O 2000).

The following two assumptions pertain to the definition of low-permeability, zeolitic regions within UZ Model layers corrosponding to portions of the CHn. Within UZ Model layers ch1, ch2, ch3, ch4, and ch5, the tuff has been altered from vitric to zeolitic in some areas and remains unaltered in other 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 within these UZ Model layers is assigned to either the vitric or zeolitic material.

5. It is assumed that saturated hydraulic conductivity (Ksat) data from the ISM3.0 Rock Properties Model (DTN: MO9901MWDISMRP.000) can be used as a surrogate for assigning gridblocks either vitric or zeolitic material names (and thus, seperate hydrogeologic properties) within certain layers of the Calico Hills nonwelded (CHn) hydrogeologic unit (Section 6.6.3).

There are two main reasons why Ksat data are used as a surrogate to assign gridblocks either vitric or zeolitic material names. First, existing data show that the Ksat 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 Ksat values than on mineralogic alteration (i.e., % zeolite).

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

Results from analyses by Flint (1998, p. 44) indicate that vitric Ksat values are on the order of 10^{-7} m/s, while zeolitic Ksat values are on the order of 10^{-10} to 10^{-11} m/s. No definitive Ksat cutoff value exists by which to distinguish vitric material from zeolitic material, as this transition occurs over about three orders of magnitude. The Ksat-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 next assumption pertains to the representation of faults within the UZ Model grids.

7. 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.

The configuration of the repository layout constitutes the final assumption.

8. It is assumed that the repository layout configuration that was proposed for the Enhanced Design Alternative (EDA) II (CRWMS M&O 1999d) is appropriate to define those areas within the numerical grid that require enhanced numerical resolution. (Section 6.3).

The Enhanced Design Alternative (EDA) II (CRWMS M&O 1999d) was the most recent representation of the repository layout at the time this document was prepared, and was considered to be the best source for this information. It is recognized that the repository design is still undergoing change, and that future adjustments to the grid resolution may be necessary depending on final design decisions.

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) and Assumption 4. 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 (Assumption 5, 6). 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. *See Attachment III for additional details.*
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 (Assumption 5, 6). Uses fracture hydrogeologic data in Table 5 to generate the dual-permeability meshes. *See Attachment IV for additional details.*
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 gridblocks 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. ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Assumption 5 and 6 uses fracture hydrogeologic data in Table 5 to generate the dual-permeability meshes. *See Attachment V 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) modications.

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. ISM3.0 data used to define vitric-zeolitic boundary (DTN: MO9901MWDISMRP.000). Assumption 5 and 6 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) modications.

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 km^2 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 (Assumption 1). 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: GS990908312312.005; 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.

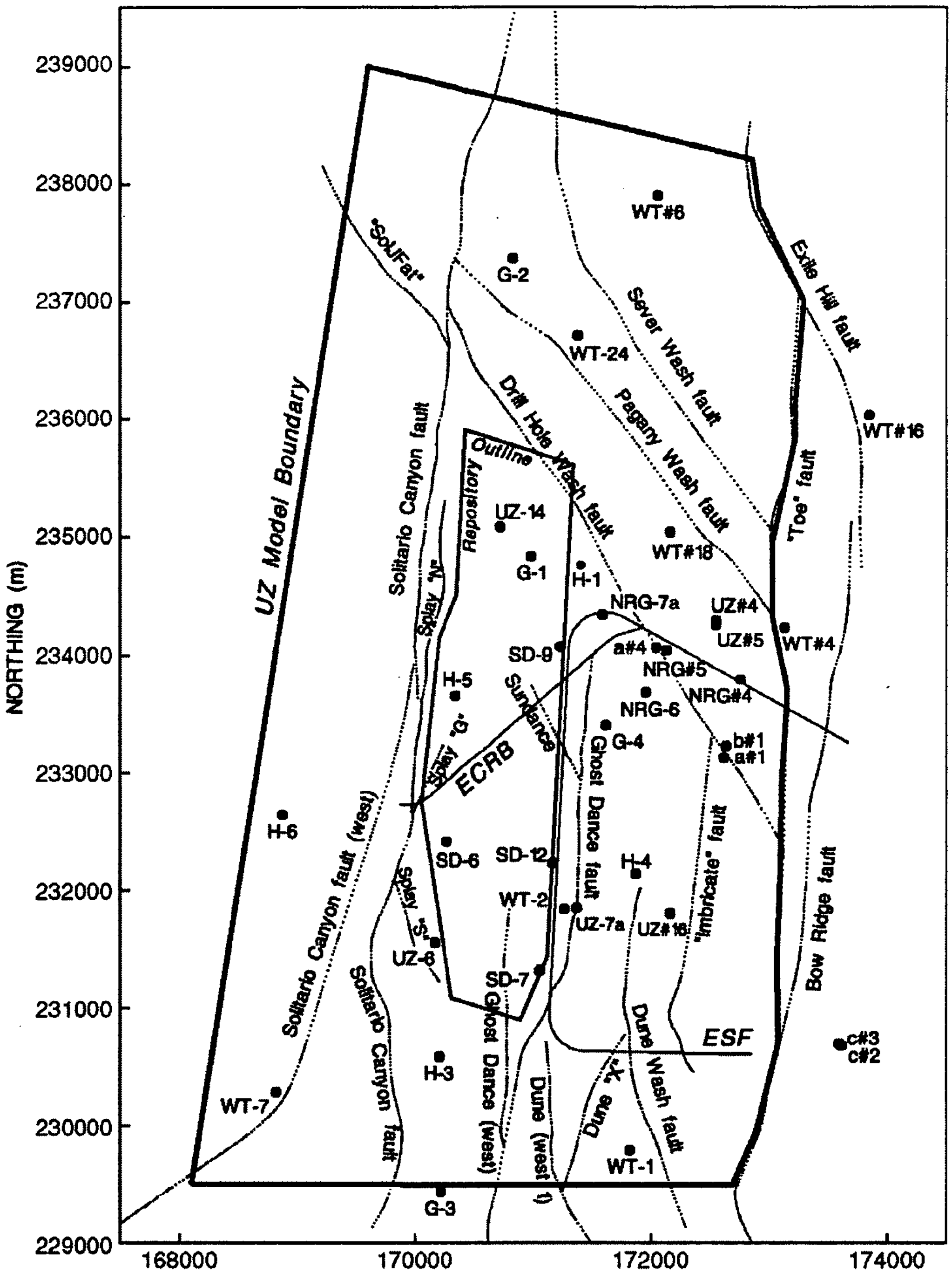


Figure 1. Plan-View Schematic Showing the UZ Model Boundary, the Repository Outline, Major Fault Locations Derived from GFM3.1, Selected Boreholes, the ESF, and the ECRB

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 BT1*a* (altered)
	Tpbt1		
	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)	pp1	PP1 (zeolitic)
	Tcpbt (Prowbt)		
	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 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)
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 1.0 – 2.6 (1.7) south	63.4 45.0	81.5 69.0	74.5 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 7, 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 (Assumption 4). 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
- ia31tacbtRWC.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 + ia31trnRWC.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 + ia31trnRWC.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 Tptrvl 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 Tpbt4 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 that 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.

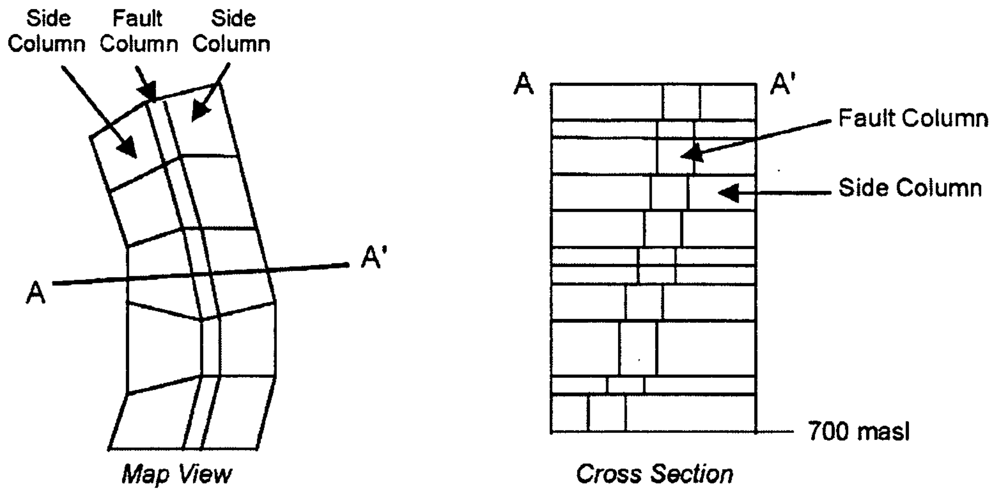


Figure 2. Schematic Illustration of Fault-Related Gridblocks in Map View and in Cross Section

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 (Assumption 8). 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 (Assumption 5, 6) 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.

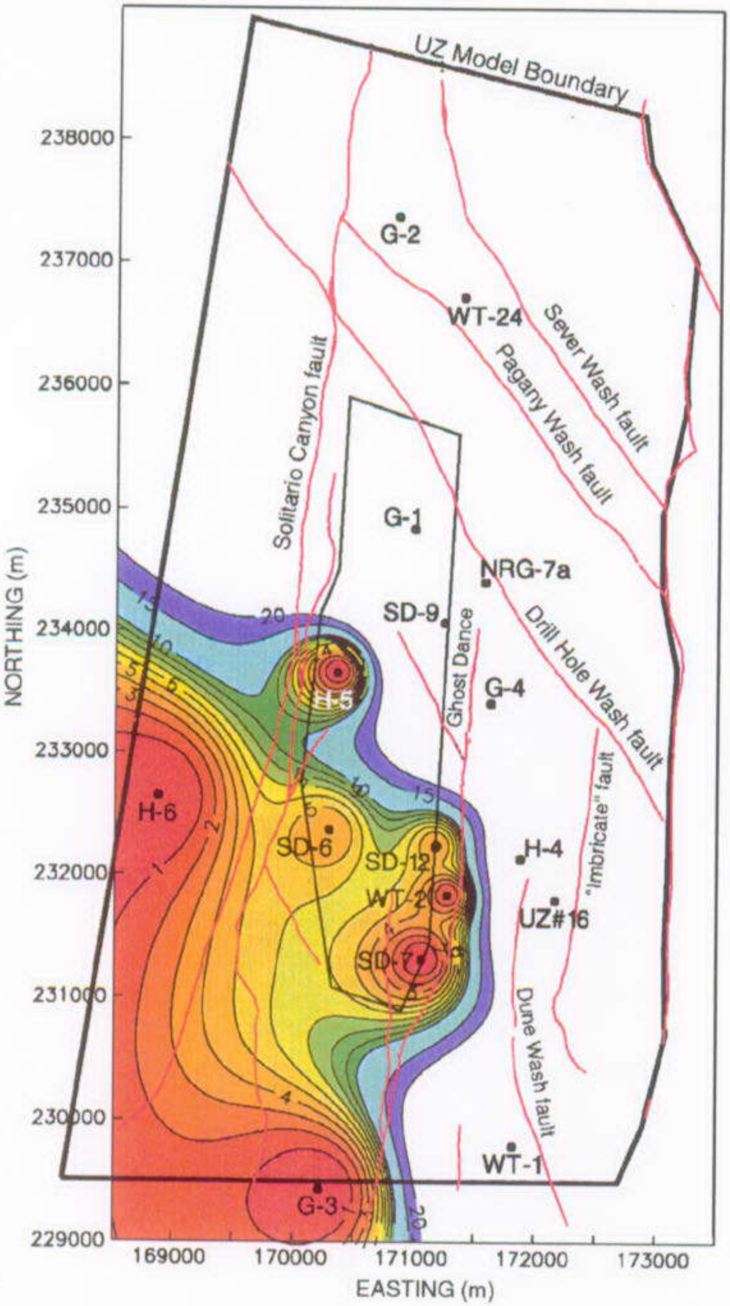
At high matrix saturations, groundwater flow within the CHn is believed to divert around zeolitic volumes of rock and preferentially flow through the less-altered, higher-permeability matrix. Consequently, only a low percentage of the total percolation flux is expected to travel through significantly 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 Tptpv1 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.

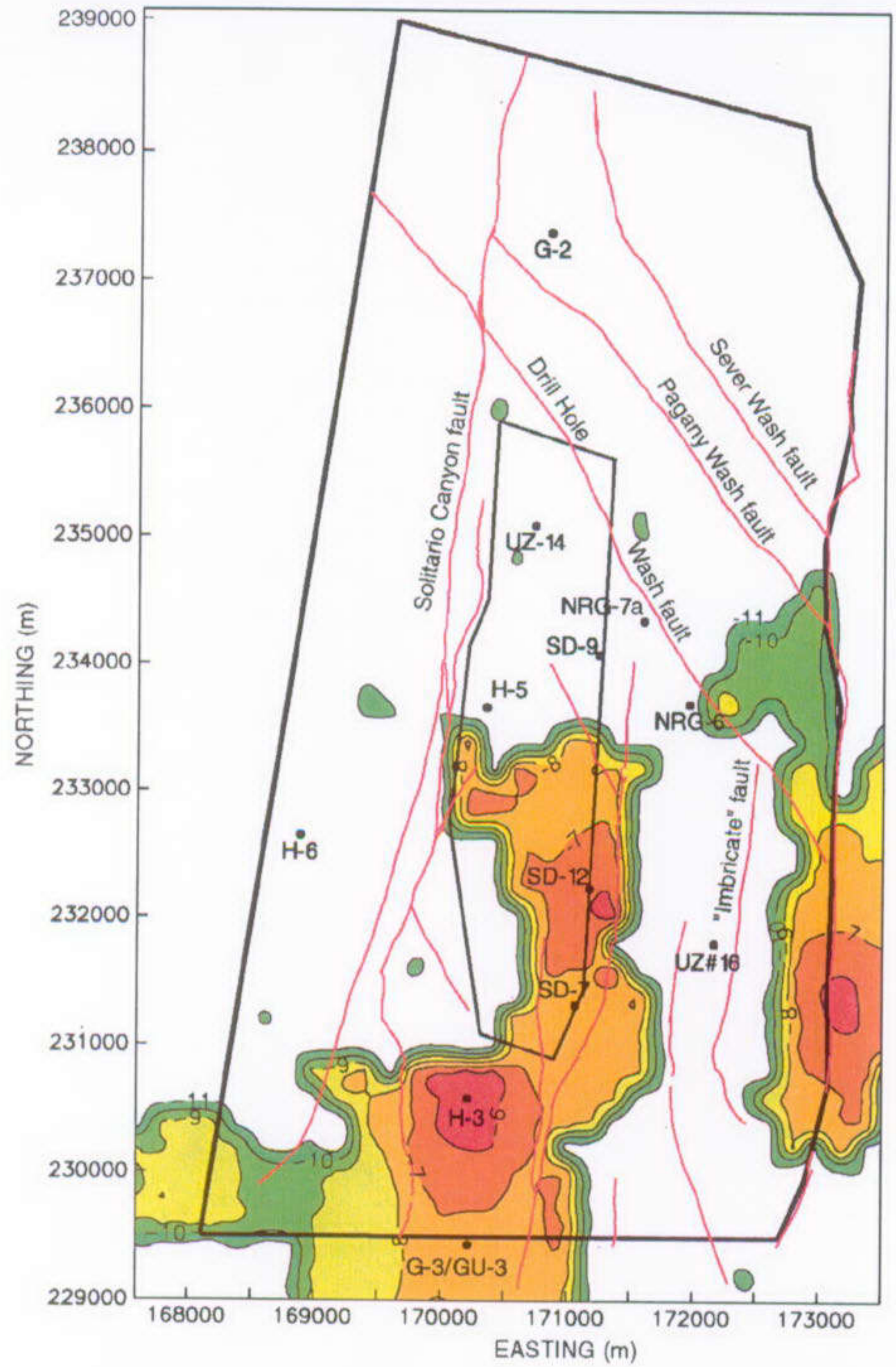
Results from the Rock Properties Model of ISM3.0 are also examined. The Rock Properties Model uses porosity (data that are relatively abundant at Yucca Mountain) as a surrogate to predict Ksat values. The limitations of this correlation are discussed in Rautman and McKenna (1997, pp. 13-14). Ksat distributions 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 6, 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 "$\log_{10}$" (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.

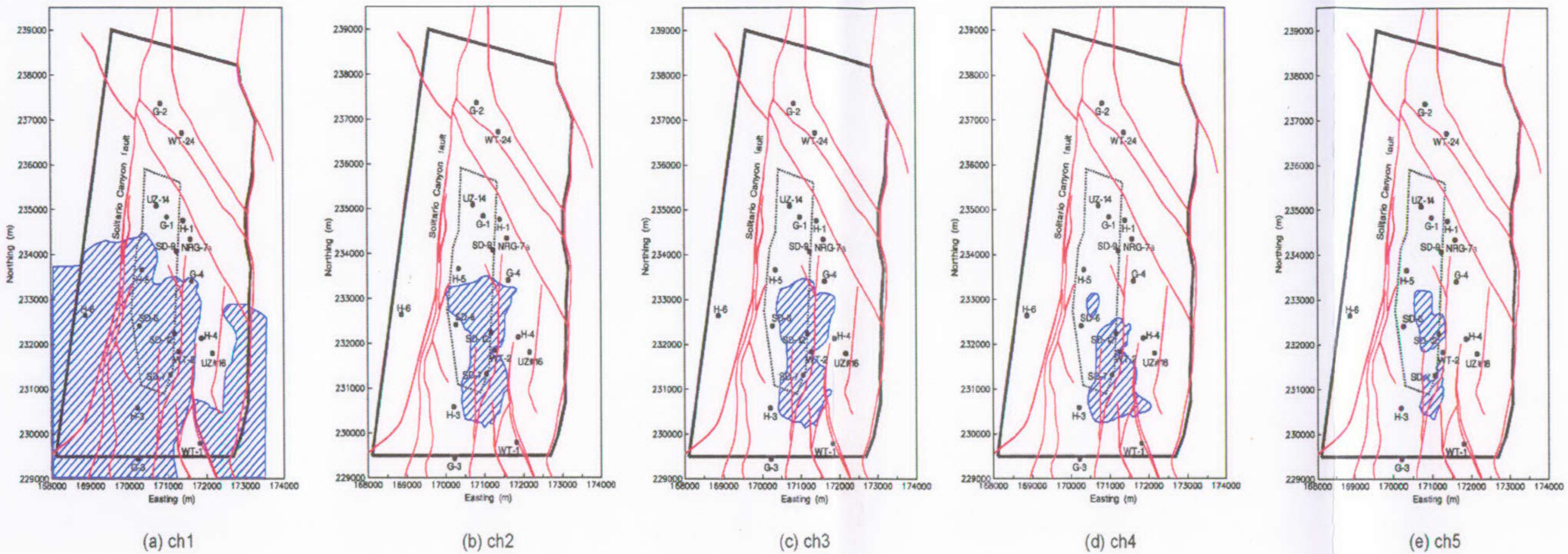
Volumes of fracture and matrix elements are computed with DKMgenerator V1.0 using the following formulas:

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

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. is the porosity or fractional volume of fractures within the bulk rock.



NOTE: White areas indicate "zeolitic" materal.

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

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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:

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

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

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

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

and

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

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:

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

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: LB990512331 29.001.

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 "ELEME" 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 (Ksat) 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 Ksat). 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 TECHNICAL PRODUCT OUTPUT

The technical product output for this AMR have been submitted to the TDMS and are included in the following DTNs:

LB990051233129.001

LB990501233129.002

LB990501233129.003

LB990501233129.004

LB990701233129.001.

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

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

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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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