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

1. QA: QA

2. ☒ Analysis — Check all that apply	3. ☒ Model — Check all that apply
Type of Analysis: ☐ Engineering ☐ Performance Assessment ☒ Scientific	Type of Model: ☒ Conceptual Model ☐ Abstraction Model ☐ Mathematical Model ☐ System Model ☒ Process Model
Intended Use of Analysis: ☐ Input to Calculation ☐ Input to another Analysis or Model ☒ Input to Technical Document	Intended Use of Model: ☐ Input to Calculation ☒ Input to another Model or Analysis ☒ Input to Technical Document
Describe use: The analysis is used to develop inputs for the calibrated properties model and supports the UZ PMR	Describe use: The developed calibrated properties are used as inputs to other models and analyses and the model supports the UZ PMR

4. Title:
Calibrated Properties Model

5. Document Identifier (including Rev. No. and Change No., if applicable):
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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

2. Analysis or Model Title:

Calibrated Properties Model

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

MDL-NBS-HS-00003 REV00

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue

DISCLAIMER

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Although this document has undergone technical reviews at the contractor organization, it has not undergone a DOE policy review. Therefore, the views and opinions of authors expressed may not state or reflect those of the DOE. However, in the interest of the rapid transfer of information, we are providing this document for your information per your request.

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ACRONYMS

1-D	one-dimensional
2-D	two-dimensional
3-D	three-dimensional
ACC	Accession Number
AMR	Analysis/Model Report
AP	Administrative Procedure (DOE)
CFu	Crater Flat undifferentiated hydrogeologic unit
CHn	Calico Hills non-welded hydrogeologic unit
CRWMS	Civilian Radioactive Waste Management System
DOE	Department of Energy
DTN	Data Tracking Number
ECM	Effective Continuum Method
ECRB	Enhanced Characterization of Repository Block
ESF	Exploratory Studies Facility
FY	Fiscal Year
GFM	Geologic Framework Model
HGU	Hydrogeologic Unit
ISM	Integrated Site Model
ITN	Input Tracking Number
LBNL	Lawrence Berkeley National Laboratory
M&O	Management and Operating Contractor
non-Q	non-Qualified
NSP	Nevada State Planar
OCRWM	Office of Civilian Radioactive Waste Management
PA	Performance Assessment
PMR	Process Model Report
PTn	Paintbrush non-welded hydrogeologic unit
Q	Qualified
QAP	Quality Assurance Procedure (M&O)
QARD	Quality Assurance Requirements and Description
QIP	Quality Implementing Procedure

ACRONYMS (Continued)

RIB	Reference Information Base
RIS	Records Information System
TBV	To Be Verified
TCw	Tiva Canyon welded hydrogeologic unit
TDMS	Technical Data Management System
TSw	Topopah Spring welded hydrogeologic unit
USGS	United States Geological Survey
UZ	Unsaturated Zone
UZ Model	Unsaturated Zone Flow and Transport Model
YMP	Yucca Mountain Site Characterization Project

1. PURPOSE

The purpose of this Analysis/Model Report (AMR) is to document the Calibrated Properties Model that provides calibrated parameter sets for unsaturated zone (UZ) flow and transport process models for the Yucca Mountain Site Characterization Project (YMP). This work was performed in accordance with the *AMR Development Plan for U0035 Calibrated Properties Model REV00* (CRWMS M&O 1999c). These calibrated property sets include matrix and fracture parameters for the UZ Flow and Transport Model (UZ Model), drift seepage models, drift-scale and mountain-scale coupled-processes models, and Total System Performance Assessment (TSPA) models as well as Performance Assessment (PA) and other participating national laboratories and government agencies. These process models provide the necessary framework to test conceptual hypotheses of flow and transport at different scales and predict flow and transport behavior under a variety of climatic and thermal-loading conditions.

This AMR documents the following calibrated property sets, which were previously submitted to the Technical Data Management System (TDMS):

- Mountain-scale, calibrated parameter sets based on one-dimensional inversions (DTN: LB997141233129.001 for base-case infiltration, LB997141233129.002 for upper bound infiltration, and LB997141233129.003 for lower bound infiltration)

- Drift-scale, calibrated parameter sets based on one-dimensional inversions (DTN: LB990861233129.001 for base-case infiltration, LB990861233129.002 for upper bound infiltration and LB990861233129.003 for lower bound infiltration)

- Calibrated, fault parameters (one set for all three infiltration scenarios) based on two-dimensional inversions (DTN: LB991091233129.004)

The objective of the calibration process is to provide calibrated parameters sets that can be used in process models to simulate flow and transport in the UZ at Yucca Mountain. The calibration process includes inversions utilizing the code ITOUGH2 (ITOUGH2 V 3.2, STN: 10054-3.2-00, Version 3.2). Property sets are generated corresponding to maps of the best estimate of present day net infiltration as well as maps representing the expected upper and lower bounds of net infiltration. The caveats and limitations of each of these property sets are documented in Section 6.0 and included as part of the data submittal package to the Technical Data Management System (TDMS).

This AMR supports the AMRs that document the UZ Flow Submodels and Models, the Mountain-Scale Coupled Thermo-Hydrologic (TH) Processes Models, the Drift-Scale Test (DST) Thermo-Hydrologic-Chemical (THC) Model, the THC Seepage Model, and the Seepage Model for PA. It supports the UZ Flow and Transport Process Model Report (PMR) and provides a direct feed of parameters to PA. This AMR also provides the documentation for the Milestone Deliverable SP3540M4, UZ Flow Model Parameters.

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2. QUALITY ASSURANCE

The activities documented in this AMR were evaluated with other related activities in accordance with QAP-2-0, Conduct of Activities, and were determined to be subject to the requirements of the U.S. DOE Office of Civilian Radioactive Waste Management (OCRWM) Quality Assurance Requirements and Description (QARD) (DOE 1999). This evaluation is documented in CRWMS 1999a, b; and Wemheuer 1999 (Activity Evaluation for Work Package WP 1401213UMI). This AMR has been prepared in accordance with procedure AP-3.10Q, Analyses and Models.

Other applicable Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) Administrative Procedures (APs) and YMP-LBNL Quality Implementing Procedures (QIPs) are identified in the "AMR Development Plan for U0035 Calibrated Properties Model" (CRWMS M&O 1999c).

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3. COMPUTER SOFTWARE AND MODEL USAGE

The software and routines used in this study are listed in Table 1. These are appropriate for the intended application and were used only within the range of validation. The software ITOUGH2 V3.2 and TOUGH2 V1.4 and infil2grid V1.6 were obtained from Configuration Management in accordance with AP-S1.1Q, Software Management. The use of this software prior to obtaining it from Configuration Management is being reviewed per the AP-3.17Q, Impact Reviews, but no impact on the technical products documented in this AMR is expected. The qualification status of this software is given in Attachment I.

Table 1. Computer Software and Routines

Software Name	Version	Software Tracking Number (STN)	Computer Platform
ITOUGH2	3.2	10054-3.2-00	SUN and DEC w/Unix OS
TOUGH2	1.4	10007-1.4-01	SUN and DEC w/Unix OS
infil2grid	1.6	10077-1.6-00	SUN and DEC w/Unix OS
Routines:		**Accession Number (ACC) or Software Tracking Number (STN):**	
aversp_1	1.0	MOL.19991011.0222	SUN and DEC w/Unix OS
factorOBJ	1.0	MOL.19991011.0223	SUN and DEC w/Unix OS
TBgas3D	1.0	MOL.19991012.0222	SUN and DEC w/Unix OS
e9-3in	1.0	10126-1.0-00	SUN and DEC w/Unix OS
inf	1.0	MOL.19991021.0465	SUN and DEC w/Unix OS

The code ITOUGH2 (ITOUGH2 V 3.2, STN: 10054-3.2-00, Version 3.2) in Table 1 was reverified as part of the implementation of AP-SI.1Q. The other codes TOUGH2 (TOUGH2 V 1.4, STN: 10007-1.4-01, Version 1.4) and infil2grid (infil2grid V 1.6, STN: 10077-1.6-00, Version 1.6) are being directly qualified under AP-SI.1Q. The routines aversp_1, TBgas3D, inf, and factorOBJ, were qualified per Section 5.1 of AP-SI.1Q, Rev. 1, ICN 0. This documentation is also included as Attachment IV. The routine e9-3in was qualified per Section 5.1 of AP-SI.1Q, Rev. 2, ICN 0.

Standard spreadsheet and visual display graphics programs (Excel 97 SR-1 and Tecplot V7.0) were also used but are not subject to software quality assurance requirements.

This AMR documents the Calibrated Properties Model. The input and output files for the model runs presented in this AMR are listed in Attachment III.

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4. INPUTS

4.1 DATA AND PARAMETERS

Source information on the data and parameter inputs are summarized in Table 2 and are further documented below.

4.1.1 Developed Data

Developed data that are used include the spatially varying infiltration maps from the Infiltration Model and several numerical grids, which are documented in separate AMRs. These data sets are too large to reproduce here but are listed by DTN in Table 2. Uncalibrated matrix and fracture properties and property estimate uncertainty data (e.g. standard deviation and number of samples) that are used as input to the calibration are listed in Tables 3 and 4. Matrix porosity, residual saturation, and satiated saturation are not calibrated. All other properties and uncertainty data are used as initial estimates and/or to constrain the calibration.

4.1.2 Acquired Data

Acquired data that are used include saturation, water potential, and pneumatic pressure. In all cases, the data sets are too large to reproduce here but are listed by DTN in Table 2. These data are developed prior to use in the inversions as documented in Sections 6.1.2 and 6.3.2. Data that are not used are also discussed.

4.1.2.1 Saturation Data

Saturation data measured on core from boreholes USW SD-6, USW SD-7, USW SD-9, USW SD-12, USW UZ-14, UE-25 UZ#16, and USW WT-24 are used for the one-dimensional (1-D) inversions. The location of these boreholes is shown in Figure 1. These boreholes do not intersect known large faults, and thus the saturation data from these boreholes are representative of the rock mass of Yucca Mountain. Saturation data measured on core from borehole USW UZ-7a (location shown in Figure 1) are used for the two-dimensional (2-D) inversions. This borehole intersects the Ghost Dance fault, and thus the saturation data from this borehole are representative of the faulted rock of Yucca Mountain.

Saturation data measured on core from several boreholes and tunnels at Yucca Mountain are not included in any of the inversions. Saturation data measured on core from boreholes USW NRG-6 and USW NRG-7a are not used because mishandling of the core caused excessive drying (Rousseau et al. 1999, p. 125). Saturation data measured on core from the neutron boreholes, designated either USW UZ-N** or UE-25 UZN #** (where the ** is a number), are not used because these boreholes do not penetrate significant portions of the unsaturated zone and thus would be of limited usefulness. Similarly, saturation data measured on core from the Exploratory Studies Facility (ESF), Enhanced Characterization of Repository Block (ECRB) Cross-Drift, alcoves, and niches are not used because they represent only one layer at any one column.

Geophysical measurements of saturation are not used because of larger uncertainties associated with these data and because the combination of data collected using different measurement techniques are likely to give inconsistent information about the natural system.

4.1.2.2 Water Potential Data

Water potential data measured *in situ* in boreholes USW NRG-6, USW NRG-7a, UE-25 UZ#4, and USW SD-12 are used in the 1-D inversions. These boreholes do not intersect known large faults, and thus the water potential data are representative of the rock mass of Yucca Mountain. Some water potential data measured *in situ* in the ECRB are also used in the 1-D inversions. Water potential data measured *in situ* in borehole USW UZ-7a are used for the 2-D inversions. This borehole intersects the Ghost Dance fault, and thus the water potential data are representative of the faulted rock of Yucca Mountain.

Water potential data measured *in situ* in borehole UE-25 UZ#5 are not used because it is less than 40 m from borehole UE-25 UZ#4 and thus falls within the same numerical model column.

Water potential data measured on core are not used because drying during drilling and/or handling may have substantially changed the water potential. In contrast with saturation data, for which the amount of change may be estimated (see Section 6.1.2), there is no way to reliably estimate the change in the water potential. Such an estimate would depend on both the amount of saturation change and the relationship between saturation and water potential, and would have unacceptably high uncertainty.

4.1.2.3 Pneumatic Pressure Data

Pneumatic pressure data measured *in situ* in boreholes UE-25 NRG#5, USW NRG-6, USW NRG-7a, USW SD-7, and USW SD-12 are used in the 1-D inversion. These boreholes do not intersect known large faults, and thus the pneumatic pressure data from these boreholes are representative of the rock mass of Yucca Mountain. Pneumatic pressure data measured *in situ* in borehole USW UZ-7a are used in the 2-D inversion. This borehole intersects the Ghost Dance fault, and thus the pneumatic pressure data from this borehole are representative of the faulted rock of Yucca Mountain.

Pneumatic pressure data from boreholes UE-25 UZ#4 and UE-25 UZ#5 are not used for the 1-D inversion because they are close to a small, unnamed fault, which, while it does not affect the *in situ* water potential data, could affect the pneumatic data. While data from these boreholes and from USW NRG-6 do show the influence of the ESF, which is being transmitted via faults, they are not used for calibration of fault parameters because 3-D models would be required and only a single paramenter, TSW horizontal fracture permeability, could be calibrated. Pneumatic pressure data from borehole USW SD-9 are not used because apparent errors in the files made the data unusable in a timely fashion.

Table 2. Input Data Sources and Data Tracking Numbers

DTN or Accession Number (ACC)	Data Description
GS000399991221.004	Saturation data from cores for boreholes USW SD-7, USW SD-9, USW SD-12, USW UZ-14, UE-25 UZ#16 & USW UZ-7a
GS000399991221.001	*In situ* water potential data for ECRB
GS980808312242.014	Saturation data from cores for boreholes USW SD-6
GS980708312242.010	Saturation data from cores for boreholes USW WT-24
GS950208312232.003 GS951108312232.008 GS960308312232.001 GS960808312232.004 GS970108312232.002 GS970808312232.005 GS971108312232.007 GS980408312232.001	*In situ* water potential data for boreholes USW NRG-6, USW NRG-7a, USW SD-12, UE-25 UZ#4, & USW UZ-7a
GS960208312261.001	*In situ* pneumatic pressure data for borehole UE-25 NRG#5
GS950208312232.003 GS951108312232.008 GS960308312232.001 GS960808312232.004	*In situ* pneumatic pressure data for borehole USW NRG-6 & USW NRG-7a
GS960908312261.004	*In situ* pneumatic pressure data for borehole USW SD-7
GS960308312232.001	*In situ* pneumatic pressure data for borehole USW SD-12 & USW UZ-7a
GS000399991221.002	Infiltration map – base-case
GS000399991221.002	Infiltration map – lower bound
GS000399991221.002	Infiltration map – upper bound
LB990501233129.002	1-D Grid
LB990501233129.003	2-D Grid
LB990501233129.001	fracture and matrix hydrologic properties and uncertainty data

Table 3. Uncalibrated Matrix Properties and Uncertainty Data. k is permeability. σ is standard deviation. N is number of samples. φ is porosity. α and m are fitting parameters for the van Genuchten water potential relationship. SE is standard error. S_r and S_s are residual and satiated liquid saturation.

UZ Model Layer	Permeability (m^2)					Porosity (-)	van Genuchten Parameters					
	k	log(k)	$\sigma_{log(k)}$	N	N non-detect	φ	α (Pa^{-1})	log(α)	m (-)	SE_m	S_r (-)	S_s (-)
tcw11	4.7E-15	-14.326	0.471	3	0	0.253	3.77E-5	-4.424	0.485	0.068	0.07	1.0
-	1.3E-15	-14.894	-	1	0	0.164	3.76E-5	-4.425	0.649	0.116	0.23	1.0
tcw12	2.6E-19	-18.579	1.459	39	25	0.082	8.80E-6	-5.056	0.253	0.028	0.19	1.0
tcw13	1.8E-16	-15.737	2.380	6	1	0.203	3.72E-6	-5.430	0.418	0.094	0.31	1.0
ptn21	4.0E-14	-13.397	2.047	10	0	0.387	1.91E-4	-3.720	0.202	0.043	0.23	1.0
ptn22	1.9E-12	-11.728	2.379	4	0	0.439	2.52E-5	-4.599	0.299	0.041	0.16	1.0
ptn23	1.5E-13	-12.833	1.582	3	0	0.254	5.46E-6	-5.263	0.405	0.076	0.08	1.0
ptn24	1.1E-13	-12.950	1.041	18	1	0.411	8.72E-5	-4.059	0.197	0.029	0.14	1.0
ptn25	1.1E-13	-12.964	0.389	11	0	0.499	3.93E-5	-4.406	0.293	0.085	0.06	1.0
ptn26	6.7E-13	-12.174	1.116	21	0	0.492	4.01E-4	-3.397	0.216	0.037	0.05	1.0
tsw31	2.9E-17	-16.535	3.377	10	5	0.053	2.41E-5	-4.618	0.278	0.036	0.22	1.0
tsw32	3.2E-16	-15.495	0.925	47	0	0.157	6.35E-5	-4.197	0.269	0.032	0.07	1.0
tsw33	2.3E-17	-16.637	1.511	51	14	0.154	1.81E-5	-4.743	0.280	0.022	0.12	1.0
tsw34	7.5E-19	-18.124	1.965	39	28	0.110	3.69E-6	-5.433	0.325	0.036	0.19	1.0
tsw35	3.1E-17	-16.510	1.573	65	21	0.131	6.41E-6	-5.193	0.242	0.034	0.12	1.0
tsw36	3.9E-19	-18.406	3.564	48	32	0.112	2.23E-6	-5.652	0.416	0.027	0.18	1.0
tsw37	2.8E-19	-18.558	1.285	23	13	0.094	1.01E-6	-5.995	0.460	0.052	0.25	1.0
tsw38	3.8E-18	-17.419	1.707	16	2	0.037	4.90E-7	-6.310	0.319	0.045	0.44	1.0
tsw39	4.4E-17	-16.355	1.499	9	0	0.173	1.60E-5	-4.797	0.360	0.106	0.29	1.0
ch1Ze	1.7E-19	-18.778	0.841	8	1	0.288	4.06E-7	-6.391	0.339	0.071	0.33	1.0
ch1VI	2.6E-14	-13.584	1.076	16	0	0.273	2.91E-5	-4.535	0.337	0.035	0.03	1.0
ch[2345]VI	8.9E-14	-13.050	1.639	24	0	0.345	7.20E-5	-4.143	0.220	0.057	0.07	1.0
ch[2345]Ze	5.4E-18	-17.269	0.890	125	17	0.331	8.12E-6	-5.090	0.248	0.026	0.28	1.0
ch6	1.0E-18	-17.995	1.608	14	8	0.266	3.36E-7	-6.473	0.505	0.036	0.37	1.0
pp4	4.4E-17	-16.356	2.275	10	2	0.325	1.80E-7	-6.744	0.684	0.042	0.28	1.0
pp3	6.6E-15	-14.179	0.940	55	0	0.303	7.89E-5	-4.103	0.337	0.038	0.10	1.0
pp2	5.2E-17	-16.286	0.920	25	0	0.263	3.39E-6	-5.470	0.376	0.032	0.18	1.0
pp1	4.2E-17	-16.376	1.454	40	4	0.280	3.22E-6	-5.493	0.401	0.059	0.30	1.0
bf3	3.9E-15	-14.414	1.815	5	1	0.115	1.69E-6	-5.771	0.416	0.082	0.11	1.0
bf2	3.9E-17	-16.410	2.669	5	3	0.259	2.49E-7	-6.603	0.585	0.040	0.18	1.0
tcwf	2.7E-19	-18.562	-	-	-	0.086	8.35E-6	-5.078	0.260	-	0.20	1.0
ptnf	1.2E-13	-12.906	-	-	-	0.446	3.68E-5	-4.434	0.255	-	0.10	1.0
tswf	1.8E-18	-17.755	-	-	-	0.127	3.18E-6	-5.497	0.296	-	0.16	1.0
chnf	4.0E-18	-17.398	-	-	-	0.259	9.79E-7	-6.009	0.386	-	0.23	1.0

DTN: LB990501233129.001 and DTN: LB991091233129.005

Table 4. Fracture Properties Prior Information. k is permeability (geometric mean). σ is standard deviation. N is number of samples. f is fracture frequency. α and m are fitting parameters for the van Genuchten water potential relationship.

FY '99 UZ Model Layer	permeability (m^2)				frequency (m^{-1})			van Genuchten		
	k	log(k)	$\sigma_{log(k)}$	N	f	σ_f	N	α (Pa^{-1})	log(α)	m (-)
tcw11	3.0E-11	-10.521	-	2	0.92	0.94	76	5.1E-3	-2.294	0.633
tcw12	5.3E-12	-11.279	0.778	80	1.91	2.09	1241	2.2E-3	-2.652	0.633
tcw13	4.5E-12	-11.344	1.147	3	2.79	1.43	60	1.9E-3	-2.728	0.633
ptn21	3.2E-12	-11.491	0.885	12	0.67	0.92	76	2.7E-3	-2.571	0.633
ptn22	3.0E-13	-12.524	0.202	4	0.46	-	-	1.4E-3	-2.861	0.633
ptn23	3.0E-13	-12.524	0.202	4	0.57	-	63	1.3E-3	-2.892	0.633
ptn24	3.0E-12	-11.527	-	1	0.46	0.45	18	3.0E-3	-2.529	0.633
ptn25	1.6E-13	-12.784	0.101	7	0.52	0.6	72	1.1E-3	-2.965	0.633
ptn26	2.2E-13	-12.661	-	1	0.97	0.84	114	9.7E-4	-3.015	0.633
tsw31	6.4E-13	-12.195	-	-	2.17	2.37	140	1.1E-3	-2.976	0.633
tsw32	7.1E-13	-12.146	0.658	31	1.12	1.09	842	1.4E-3	-2.864	0.633
tsw33	7.7E-13	-12.112	0.612	27	0.81	1.03	1329	1.6E-3	-2.806	0.633
tsw34	3.4E-13	-12.474	0.546	180	4.32	3.42	10646	6.8E-4	-3.169	0.633
tsw35	9.0E-13	-12.044	0.544	31	3.16	-	595	1.0E-3	-2.980	0.633
tsw3[67]	1.4E-12	-11.868	0.285	19	4.02	-	526	1.1E-3	-2.956	0.633
tsw38	6.4E-13	-12.195	-	-	4.36	-	37	8.4E-4	-3.077	0.633
tsw39	6.4E-13	-12.195	-	-	0.96	-	46	1.4E-3	-2.858	0.633
ch1Ze	2.5E-14	-13.606	-	-	0.04	-	3	1.4E-3	-2.852	0.633
ch1VI	2.2E-13	-12.661	-	-	0.10	-	11	2.1E-3	-2.680	0.633
ch[2345]VI	2.2E-13	-12.661	-	-	0.14	-	25	1.8E-3	-2.736	0.633
ch[2345]Ze	2.5E-14	-13.606	-	1	0.14	-	25	8.9E-4	-3.051	0.633
ch6	2.5E-14	-13.606	-	-	0.04	-	-	1.4E-3	-2.852	0.633
pp4	2.5E-14	-13.606	-	-	0.14	-	-	8.9E-4	-3.051	0.633
pp3	2.2E-13	-12.661	-	-	0.20	-	-	1.6E-3	-2.786	0.633
pp2	2.2E-13	-12.661	-	-	0.20	-	-	1.6E-3	-2.786	0.633
pp1	2.5E-14	-13.606	-	-	0.14	-	-	8.9E-4	-3.051	0.633
bf3	2.2E-13	-12.661	-	-	0.20	-	-	1.6E-3	-2.786	0.633
bf2	2.5E-14	-13.606	-	-	0.14	-	-	8.9E-4	-3.051	0.633
tr3	2.2E-13	-12.661	-	-	0.20	-	-	1.6E-3	-2.786	0.633
tr2	2.5E-14	-13.606	-	-	0.14	-	-	8.9E-4	-3.051	0.633
tcwf	2.7E-11	-10.571	-	-	1.90	-	-	3.8E-3	-2.418	0.633
ptnf	3.0E-12	-11.527	-	-	0.54	-	-	2.8E-3	-2.553	0.633
tswf	1.5E-11	-10.836	-	-	1.70	-	-	3.2E-3	-2.490	0.633
chnf	3.6E-13	-12.444	-	-	0.13	-	-	2.3E-3	-2.638	0.633

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4.2 CRITERIA

At this time, no specific criteria (e.g., System Description Documents) have been identified as applying to this analysis 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 (Subpart E, Section 114(1)).

The DOE interim guidance (Dyer 1999), requiring the use of the same subparts of the proposed NRC high-level waste rule, 10 CFR Part 63 (64 FR 8640) specified above, was released after completion of the work documented in this AMR; it has no impact on this work activity.

4.3 CODES AND STANDARDS

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

5. ASSUMPTIONS

The assumptions documented below are necessary to develop the Calibrated Properties Model. This section presents the rationale for the assumptions, and references the section of this AMR in which an assumption is used. Other assumptions basic to the Unsaturated Zone Flow and Transport Model (UZ Model) of Yucca Mountain are elements of the conceptual model, which is summarized at the beginning of Section 6 and will be fully documented in a future AMR supporting the Unsaturated Zone Flow and Transport PMR, so they will not be documented in this section.

The following assumptions are used to develop the Calibrated Properties Model.

1. It is assumed that one-dimensional (1-D) vertical flow adequately describes the flow patterns around the boreholes used for rock mass (nonfault) property calibration (Sections 6.1 and 6.2).

Inverse modeling involves many forward simulations, and therefore is computationally intensive. 1-D, columnar models are used because the time that is required for each forward simulation is short (a minute or less). Therefore many simulations, thousands in this case, can be accomplished in a reasonable (i.e., less than a day) time period. The effect of using 1-D columnar models is that all flow is forced to be vertical; there is no lateral flow. From the surface to the repository, lateral flow is not expected to be significant because perched water has not been found here. Below the repository, in the Calico Hills nonwelded unit (CHn: see Table 5) and the Crater Flat undifferentiated unit (CFu), areas of perched water exist where lateral flow may be significant. Properties needed to produce perched water and varying degrees of lateral flow are not addressed in this AMR but will be addressed in a future AMR supporting the Unsaturated Zone Flow and Transport PMR. This future AMR will also address the suitability of other CHn and CFu properties with respect to flow changes as a result of perched water and lateral flow.

2. It is assumed that 2-D flow (vertical and east-west) adequately describes the flow patterns around borehole USW UZ-7a used for fault property calibration (Section 6.3).

As above, inverse modeling is computationally intensive. For this reason, it is necessary to use the simplest model that will adequately simulate the system being modeled. For flow in and around a fault zone, a 2-D model is necessary to capture the interaction of the hanging wall, fault zone, and foot wall. An east-west, vertical cross section through USW UZ-7a and the Ghost Dance fault should capture this interaction. The cross section is aligned approximately parallel to the dip of the beds and parallel to the dip of the fault (perpendicular to the strike). Any lateral flow in or around the fault zone should follow the dip of the beds and the fault.

3. It is assumed that layers bf3 and bf2 are analogs for tr3 and tr2, respectively.

No data except geologic contacts exist for layers tr3 or tr2 (the Tram Tuff). Because the Tram Tuff has a structure similar to the Bullfrog Tuff and the two Tuffs are divided into model layers similarly (see Table 5), the hydrologic properties should also be similar. Further, model layers tr3 and tr2 constitute only a small portion of the unsaturated zone in the northern part of the model

area and along the foot wall of the Solitario Canyon fault, so the properties are not likely to have a large impact on future simulations of flow and transport.

4. It is assumed that calibrated fault properties based on inversion of data from the Ghost Dance fault apply to all faults in the UZ Model (Section 6.3).

The data from borehole USW UZ-7a represent the most complete data set from within a fault zone. Saturation, water potential, and pneumatic data are available from the surface down into the TSw. Other data sets that are influenced by faults from boreholes USW NRG-6, UE-25 UZ#4, and UE-25 UZ#5 include only pneumatic pressure data and are only relevant to the TSw. Because of the limited amount of data, it is best to characterize one fault as completely as possible and apply these properties to all other faults.

5. It is assumed that 30 days is a sufficient simulation time to establish fully dynamic, pneumatic initial conditions (Section 6.1.1).

Initial conditions for pneumatic simulations are either pneumatically static conditions or dynamic conditions from a previous simulation. When the barometric signal is applied to the upper boundary of the model, the pressure variations within the model quickly equilibrate to the boundary condition because propagation of the pressure fronts from the upper boundary is all that is necessary. The mean pressure, however, takes a little longer to equilibrate, because flow from the upper boundary must reach the entire model. Simulation output after the mean pressure has equilibrated is used for comparison to the data. Previous work has shown that 30 days is sufficient for the mean pressure to equilibrate (Ahlers et al 1998, p. 224).

6. It is assumed that common values of the active fracture parameter, γ, may be estimated for common rock types (Section 6.1).

The fracturing characteristics of the rocks of Yucca Mountain are assumed to be primarily dependent on the degree of welding and alteration. Data show that this is true of fracture frequency (as shown in Table 4). The welded rocks have higher fracture frequencies than the non-welded. Because of the general division between the fracture characteristics of welded and non-welded rocks and because there are no data on an appropriate active fracture parameter to use for these rocks, model layers are grouped together based on welding to estimate common values of the active fracture parameter. Alteration is believed to possibly influence the active fracture parameter, so it is also used as a criterion for grouping layers.

7. It is assumed that reported saturation values greater than 1.0 are equal to 1.0 (Section 6.1.2).

Measurement error causes calculated saturation values (based on measurements of initial, saturated, and dry weight) to be greater than 1.0, but this is not physical, if possible saturation is physically constrained to a maximum of 1.0.

8. Because of data limitations and the way data were interpreted, estimates of uncertainty cannot be directly calculated for some of the data. In these cases, an appropriate

uncertainty is selected (assumed) based on the uncertainties of similar data. The specific values and the rationale for each value are documented in Section 6.1.2.

All assumptions are confirmed based on the rationales stated for each and do not need further confirmation.

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6. MODELING

The UZ Model is used to represent past, present, and future thermo-hydrologic and chemical conditions within the unsaturated zone of Yucca Mountain. The UZ Model consists of hydrologic (flow and transport) and thermal properties and a numerical grid which together form input for the TOUGH family of simulators. This AMR documents the development of some of the hydrologic properties for the UZ Model. The development and features of the 1-D and 2-D submodel grids used for the modeling in this AMR are documented in the AMR entitled, "Development of Numerical Grids for UZ Flow and Transport Modeling" (CRWMS M&O 1999d, Attachments III and IV).

The conceptual model used to develop the numerical representation of the UZ Model will be documented in a future AMR supporting the Unsaturated Zone Flow and Transport PMR. The salient points of this conceptual model for the modeling documented herein are as follows:

1. Heterogeneity of hydrologic properties is predominantly a function of geologic layering, shown in Table 5, and thus any one geologic layer has homogeneous properties (referred to as layer average properties), except where faulting or variable alteration (e.g. zeolitization) are present. In these cases, a single, consistent change is made to the properties (e.g., two sets of properties are used for layers with variable alteration, one for the portion of the layer that is altered beyond some threshold and one for the remaining portion; AMR "Development of Numerical Grids for UZ Flow and Transport Modeling" CRWMS M&O 1999d documents this process).

2. Heterogeneity in faults is a function of major hydrogeologic units (HGU), shown in Table 5, with the CHn and CFu combined (i.e., only four sets of hyrologic properties are used for the faults).

3. Flow of liquid and gas through fractures and rock matrix is described using a dual-continuum model.

4. Flow of liquid and gas in the fractures and matrix is Darcian.

5. Unsaturated liquid flow in the fractures and matrix is described using van Genuchten's (1980, p. 893) relationships for water potential, relative permeability, and saturation.

6. Richard's equation is used to describe unsaturated liquid flow.

7. The active fracture model (Liu et al. 1998) is used with the continuum model to represent the effects of fingering flow in fractures. Finsterle (1998, p. 16) documents the full set of modifications to ITOUGH2 V 3.2 for the active fracture model.

8. Liquid flow under ambient conditions is steady-state.

9. Gas relative permeability, k_{rg}, is described by a modified Brooks-Corey relationship, where the unmodified relationship is (Brooks and Corey 1966, p . 71).

$$k_{rg} = (1 - S_e)^2 \left(1 - S_e^{\frac{2+\lambda}{\lambda}} \right) \qquad \text{(Eq. 1)}$$

where effective saturation S_e, is

$$S_e = \frac{S - S_r}{S_s - S_r} \qquad \text{(Eq. 2)}$$

S is liquid saturation, S_r is residual liquid saturation, S_s is satiated liquid saturation, and λ is related to the van Genuchten parameters n and m by (van Genuchten 1980, p. 895)

$$\lambda = n - 1 = \frac{m}{1 - m}. \qquad \text{(Eq. 3)}$$

Substituting Equation 3 into Equation 1 gives

$$k_{rg} = (1 - S_e)^2 \left(1 - S_e^{\frac{2-m}{m}} \right) \qquad \text{(Eq. 4)}$$

10. Liquid flow in the PTn (see Table 5) and vitric portions of the CHn is dominantly in the matrix, while in all other layers it is predominantly in the fractures. In order to accomplish the transition from dominant matrix flow to dominant fracture flow in the numerical model, downstream weighting is used for downward matrix-to-matrix flow from the PTn to the TSw and from the vitric CHn to the zeolitic CHn. At these interfaces, downstream weighting means that the lower permeability of the TSw or zeolitic rock is used for downward matrix to matrix flow. This should cause preferential matrix to fracture flow via a higher permeability path.

Table 5. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation (CRWMS M&O 1999d, Table 10)

Major Unit	GFM3.1* Lithostratigraphic Nomenclature	FY 99 UZ Model Layer	Hydrogeologic Unit
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		
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

NOTE: * GFM3.1 refers to the Geologic Framework Model Version 3.1.

Table 5. GFM3.1 Lithostratigraphy, UZ Model Layer, and Hydrogeologic Unit Correlation (CRWMS M&O 1999d, Table 10) (Cont.)

Major Unit	GFM3.1* Lithostratigraphic Nomenclature	FY 99 UZ Model Layer	Hydrogeologic Unit
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)		
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: * GFM3.1 refers to the Geologic Framework Model Version 3.1.

11. Calibrated properties are necessary on two scales, mountain-scale and drift-scale. Calibration of the mountain-scale properties considers pneumatic pressure data which reflects the mountain-scale process of barometric pumping. Mountain-scale properties are intended for use in models of processes at the mountain-scale. Calibration of the drift-scale properties in the repository horizon does not consider the pneumatic pressure data. Drift-scale properties are intended for use in models of processes at the drift-scale and in the repository horizon.

Alternative conceptual models and the rationale for not selecting them will be documented in a future AMR supporting the UZ Flow and Transport PMR. Briefly, these alternative conceptual models include an equivalent-continuum model, a weeps model, and a discrete fracture model.

Calibration of the UZ Model is a key step in its development. Calibration is necessary in order to refine the property estimates derived from laboratory and field data so that they are suitable for use in the UZ Model and so that the UZ Model accurately depicts hydrologic conditions in the mountain. The UZ Model considers hydrologic processes on a mountain scale, so where properties are scale-dependent, upscaling will inherently be part of the calibration process. The calibration process also reduces property-estimate uncertainty and bias. Property estimates from laboratory and field data, like any other estimate, will have uncertainty associated with them because of data limitations (e.g., sampling and measurement biases, few samples, etc.).

Data inversion is used to calibrate some of the numerical model parameters. Inversion is an iterative process where predictions from a numerical model are compared to data and the numerical model parameters are adjusted (calibrated) in order to improve the match between the model prediction and the data. The data that are inverted to provide the calibrated properties documented in this AMR include saturation in the rock matrix, water potential in the rock matrix, and pneumatic pressure in the fractures. Hydrologic-property estimates from laboratory and field measurements, which provide initial estimates for model parameters, also are included as data in the inversion. These data, which are referred to as prior information in this report, are just as important to the inversion as the data about the state of the system (e.g., saturation). The combination of the two types of information allows the inversion to match the data as well as possible while simultaneously estimating model parameters that are reasonable according to the prior information.

Model parameters to be estimated are fracture and matrix (identified with a subscript F or M, respectively) permeability, k, van Genuchten parameters α and m (van Genuchten 1980, pp. 892–893), where $m = 1\text{-}1/n$ for the fractures and matrix, and a fracture activity parameter, γ (Liu et al. 1998). These parameters are estimated for 31 model layers (as shown in Table 5), though in some cases a common parameter value is estimated for groups of layers, and for three of the four layers in the faults. The details of which layers are grouped for parameter estimation are given in Section 6.1. A total of 199 rock parameters are to be estimated. This set of parameters is chosen for calibration because they represent the smallest set that will uniquely represent ambient conditions in the UZ.

Other hydrologic parameters that are not calibrated are fracture and matrix porosity, residual saturation, and satiated saturation. The liquid flow simulations, because they are steady-state, are insensitive to porosity variations, so porosity could not be calibrated by inversion of saturation and water potential data. For the pneumatic simulations, diffusivity, which is proportional to the ratio of permeability to porosity, is the sensitive parameter. Permeability is chosen to be calibrated because it is already needed for the liquid flow portion of the calibration. Further, matrix porosity is a well constrained property because the techniques used to measure porosity are simple and the measurement error is low. Fracture porosity, though not well constrained, would not, alone, provide sufficient range to calibrate the pneumatic simulations to the data.

Residual and satiated saturation are parameters that do not influence the calibration to ambient data as strongly as the van Genuchten parameters α and m. This is because the ambient saturation and water potential data are generally not at the extremes of the relationships where these bounding values play a stronger role. Like matrix porosity, matrix residual saturation is another

property that is simple to measure with low error, so it makes more sense to calibrate the parameters that are not well constrained.

Parameter calibration is performed using the base-case, upper bound, and lower bound infiltration scenarios. The infiltration scenarios are a key input to the UZ Model because flow and transport are dependent on the amount of water infiltrating into the mountain. The base-case infiltration scenario gives the expected, spatially varying infiltration rates over Yucca Mountain, and parameters calibrated using this scenario are the base-case parameter set. The upper and lower bound infiltration scenarios give bounds to the uncertainty of the base-case infiltration scenario. Parameters calibrated using the bounding scenarios are also provided. This gives the parameter sets which consider underestimation and overestimation of the present-day infiltration by the base-case scenario.

Calibration of the UZ Model is carried out in a series of steps. One-dimensional vertical-column submodels are used for the calibration of the rock mass (nonfault) parameters for the mountain-scale and drift-scale conceptual models. The one-dimensional submodels correspond to 11 surface-based boreholes from which saturation, water potential and pneumatic pressure have been measured. Table 6 shows the types of data used from each borehole, and Figure 1 shows the locations of the boreholes with respect to other boreholes and features at Yucca Mountain. Water flow (and gas flow in the pneumatic simulations) is simulated simultaneously in all columns. Layer-averaged effective parameters are estimated, i.e., the same set of parameter values is used for each geologic layer in all eleven columns.

Table 6. Data used for 1-D and 2-D Calibration from Each of Twelve Boreholes

Borehole (1-D or 2-D calibration)	**Matrix Liquid Saturation (core)**	**Matrix Liquid Water Potential (*in situ*)**	**Fracture Pneumatic Pressure (*in situ*)**
UE-25 NRG#5 (1-D)			✔
USW NRG-6 (1-D)		✔	✔
USW NRG-7a (1-D)		✔	✔
USW SD-6 (1-D)	✔		
USW SD-7 (1-D)	✔		✔
USW SD-9 (1-D)	✔		
USW SD-12 (1-D)	✔	✔	✔
UE-25 UZ#4 (1-D)		✔	
USW UZ-7a (2-D)	✔	✔	✔
USW UZ-14 (1-D)	✔		
UE-25 UZ#16 (1-D)	✔		
USW WT-24 (1-D)	✔		

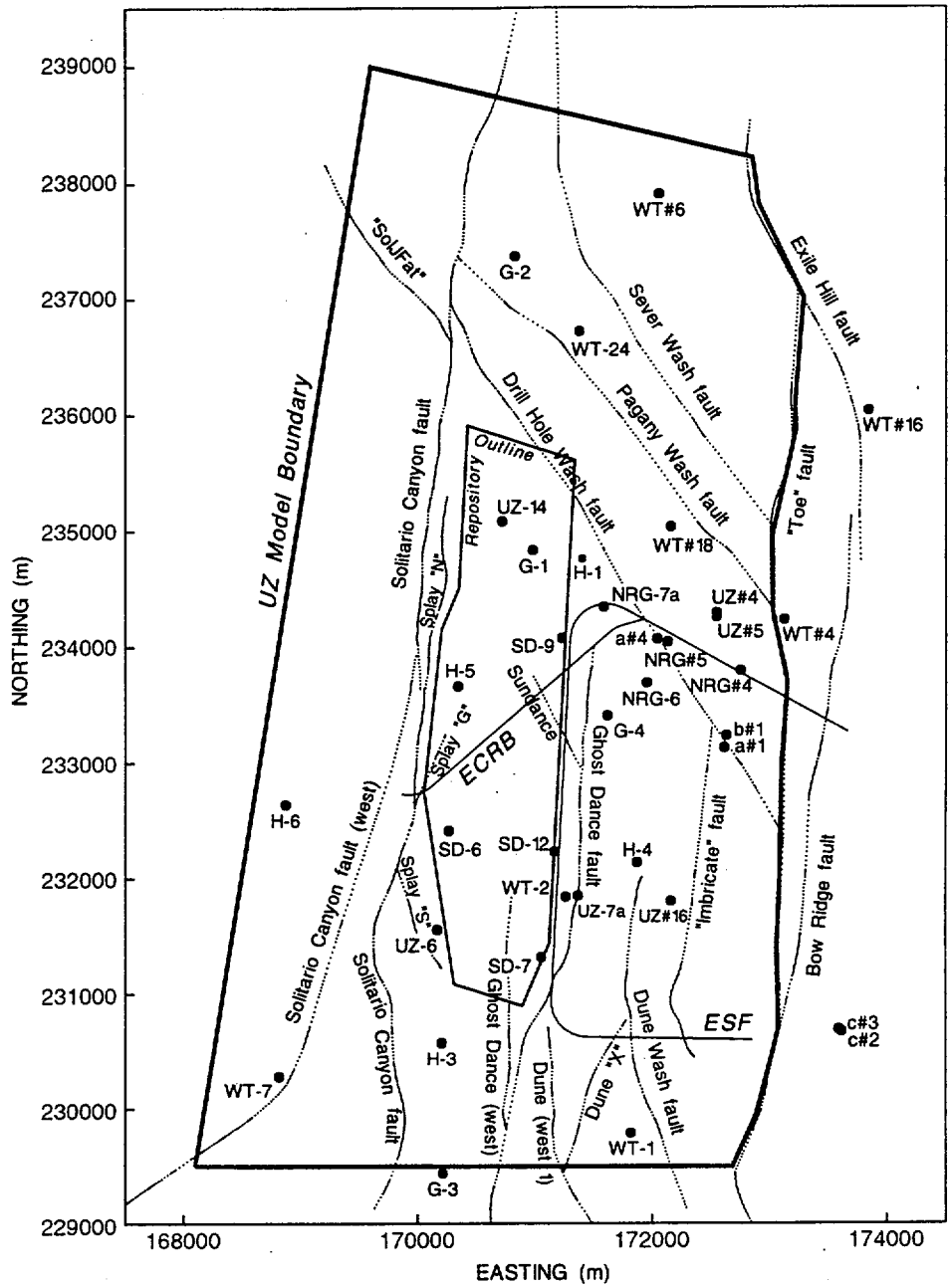

Figure 1. Borehole Locations (CRWMS M&O 1999d, Figure 1)

A two-dimensional model is used to calibrate parameters for the faults. The two-dimensional model is an east-west vertical cross section through borehole USW UZ-7a. Data from USW UZ-7a are the most comprehensive with respect to faults. Saturation, water potential, and pneumatic pressure data are available within the Ghost Dance fault zone from the surface to the upper layers of the TSw. Pneumatic-only data (that show fault influence) are available from three other boreholes but are not used in this analysis (rationale documented in Section 4.1.2.3). Because the

data on faults are so limited (one borehole that only partially penetrates the UZ compared to 11 boreholes, some of which fully penetrate the UZ in the rock mass), they are separated into four layers to reduce the number of parameters used to characterize the fault zones. The layers are the TCw, PTn, TSw, and CHn/CFu. Data for inversion are available for only the first three layers, so only the parameters of these layers are calibrated.

The software, ITOUGH2 V 3.2 (Finsterle 1999), is used to carry out the automatic portion of the inversion process. This software not only allows the consideration of both data and prior information, but also allows them to be weighted. The data and prior information are weighted according to the uncertainty of the estimated value. The software attempts to minimize the sum of the squared, weighted residuals (called the objective function). It does this by iteratively adjusting (calibrating) selected model parameters. When the objective function reaches a minimum, the resulting parameter set is considered to be the best estimate. The objective function is judged to have reached a minimum when it is either near an apparent asymptotic value or ITOUGH2 V 3.2 cannot reduce the objective function. Finsterle (1998; 1999) describes further details of ITOUGH2 V 3.2.

Important aspects of the conceptual model and some data cannot be easily integrated into the format of ITOUGH2 V 3.2. This information is considered for the calibrated property sets by manually adjusting parameters. Two main considerations are not integrated into the ITOUGH2 V 3.2 objective function. The first is conceptual model item 10 above. Flow proportions through each column are checked against this criteria. The second is that attenuation of the pneumatic signal through the TSw must be consistent with the data. The method for considering this is given below in Section 6.1.3 under the heading "TSw k_F Calibration."

When all three criteria, minimization of the objective function, flow proportions consistent with conceptual model item 10, and pneumatic attenuation through TSw consistent with data, are met, then a parameter set is considered acceptable.

Because of its superior numerical solver, TOUGH2 V 1.4 is used to calculate initial conditions prior to each step when ITOUGH2 V 3.2 cannot. To further ease the calculation of initial conditions prior to the pneumatic inversion steps, routine e9-3in is used to convert between the ITOUGH2 V 3.2/TOUGH2 V 1.4 EOS9 module initial condition format and the ITOUGH2 V 3.2/TOUGH2 V 1.4 EOS3 module initial condition format.

The key scientific notebooks (with relevant page numbers) used for the modeling activities described in this AMR are listed in Table 7.

Table 7. Scientific Notebooks

LBNL Scientific Notebook ID	M&O Scientific Notebook ID	Pages	Accession Number (ACC)
YMP-LBNL-GSB-1.1.2	SN-LBNL-SCI-003-V1	76-79, 86-112, 127-145	MOL.19990720.0203
YMP-LBNL-GSB-LHH-2	SN-LBNL-SCI-098-V1	38-51, 52-56	MOL.19990902.0134

6.1 ONE-DIMENSIONAL MOUNTAIN-SCALE CALIBRATION

Saturation, water potential, and/or pneumatic pressure data from eleven boreholes at Yucca Mountain, listed in Table 6, are used to calibrate the parameters for the 31 model layers. In addition, the prior information on k_F, k_M, α_F, α_M, m_F, and m_M is included in the inversion. Common parameters are estimated for some groups of layers.

1. Because there are no data for model layers tr3 and tr2, they are assumed to be analogous to model layers bf3 and bf2, respectively (Assumption 3, in Section 5). This assumption is made based on the common depositional profile of the Tram and Bullfrog Tuffs. Because the Bullfrog Tuff represents a very small portion of the UZ within the UZ Model boundaries (it is present above the water table only immediately next to the Solitario Canyon fault and in the extreme northern portion of the UZ Model), the impact of this assumption is not significant.

2. Common values of k_F, k_M, α_F, α_M, m_F, and m_M are estimated for the vitric Tac (material types ch2v, ch3v, ch4v, and ch5v) and for the zeolitic Tac (material types ch2z, ch3z, ch4z, and ch5z). As reflected in Table 5, these layers do not represent actual geologic or hydrogeologic divisions but are employed in order to better characterize which portions of the Tac are vitric or zeolitic as documented in the AMR entitled, "Development of Numerical Grids for UZ Flow and Transport Modeling" (CRWMS M&O 1999d, pp. 48-52).

3. The lower nonlithophysal layer of the TSw (Tptpln) is subdivided into two layers based on matrix property development consistent with Flint (1998). This division does not exist for the fracture properties (see Table 4), so common values of k_F, α_F, and m_F are estimated for material types tsw36 and tsw37.

4. Common values of γ are estimated for the TCw, PTn, most of the TSw, vitric portions of the CHn, zeolitic portions of the CHn and CFu, and devitrified/welded portions of the CHn and CFu. Table 8 gives the material types included in each of these groups. Values of γ are estimated individually for tsw31 because matrix-to-fracture flow is expected to be high in this layer, as a result of the transition from matrix-dominated flow in the PTn to fracture-dominated flow in the TSw.

The one-dimensional mountain-scale property calibration is documented in scientific notebook YMP-LBNL-GSB-1.1.2, pp. 76-79 and 89-112 and in scientific notebook YMP-LBNL-GSB-LHH-2, pp. 38-51.

6.1.1 Model Development

The one-dimensional, vertical-column, numerical grids for the eleven boreholes are available under DTN: LB990501233129.002.

Prior information for k_F, k_M, α_F, α_M, m_F, and m_M, also used as initial parameter guesses, is available under DTN: LB990501233129.001 and is shown in Tables 3 and 4.

No prior information exists for the active fracture parameter, γ. initial estimates for γ for this inversion are shown in Table 8.

Table 8. Initial Estimates of the Active Fracture Parameter, γ, for Saturation and Water Potential Data Inversion for Base-case Infiltration

Material Type (group)	γ
tcw11, tcw12, tcw13 (TCw)	0.3
ptn21, ptn22, ptn23, ptn24, ptn25, ptn26 (PTn)	0.1
tsw31	0.1
tsw32, tsw33, tsw34, tsw35, tsw36, tsw37, tsw38, tsw39 (TSw)	0.4
ch1v, ch2v, ch3v, ch4v, ch5v (CHn vitric)	0.1
ch1z, ch2z, ch3z, ch4z, ch5z, ch6, pp4, pp1, bf2 (CHn & CFu zeolitic)	0.1
pp3, pp2, bf3 (CHn & CFu welded/devitrified)	0.3

Three calibrated parameter sets are produced, one for each present day infiltration case. The base-case, present day infiltration map and the lower and upper bound, present day infiltration maps, are used to calculate infiltration rates corresponding to the calibration boreholes. For each infiltration map, the infiltration rate at each calibration borehole, shown in Table 9, is determined, using routine inf, as an averaged infiltration rate value over a circular area of 200 m radius with the center at the borehole location. A relatively large value of the radius is used due to the consideration of capillary dispersion (lateral redistribution of moisture due to a capillary gradient from wet areas under high infiltration zones to dry areas under low infiltration zones) within the PTn unit. A value of 0.05 mm/yr is assigned to boreholes with calculated values smaller than 0.05 mm/yr also due to the consideration of capillary dispersion.

Table 9. Infiltration Rates (mm/yr) Used in the 1-D Data Inversions

Borehole	lower bound	base-case	upper bound
UE-25 NRG#5	0.05	1.81	5.80
USW NRG-6	0.05	0.52	2.68
USW NRG-7a	0.05	0.22	3.16
USW SD-6	0.98	6.51	15.38
USW SD-7	0.05	1.06	2.59
USW SD-9	0.08	1.05	3.65
USW SD-12	0.80	3.25	7.65
UE-25 UZ#4	0.05	0.29	3.21
USW UZ-14	0.20	2.28	8.70
UE-25 UZ#16	0.05	0.22	2.91
USW WT-24	1.82	5.93	13.28

The time-varying pneumatic pressure boundary condition used to simulate barometric pumping is a combination of records from the surface at boreholes USW NRG-6 and USW NRG-7a. The record from USW NRG-7a is used as the basis for the surface signal. Where there are gaps in the data from USW NRG-7a, data from USW NRG-6 are used to fill them. Four, discontinuous, 60 day periods are combined end to end into a 240 day record of barometric pressure. The four 60

day periods cover the four 30 day periods selected for data inversion (see Table 10 below) and the 30 days immediately preceding each. The 30 days preceding the data sets are included in the simulations to develop a dynamic pressure history in the simulation (Assumption 5, in Section 5). Because pressures are constantly changing in the real system, pneumatic pressure is never in equilibrium (i.e., pneumatically static conditions are never achieved). Initial pressure conditions are pneumatically static. Previous work with the Yucca Mountain models have shown that after thirty days, the effects of the initial conditions are insignificant (i.e., dynamic pneumatic conditions corresponding to the current dynamic boundary conditions are developed) (Ahlers et al 1998, p.224). This is also true when the initial conditions are the dynamic conditions at the end of a 60-day period (i.e., when switching from one 60 day boundary condition period to the next). The mean pressure at the collar (surface) of each borehole is different because each borehole is at a different elevation. The mean pressure of the pneumatic boundary condition for each boundary node is calculated based on pneumatically static conditions.

6.1.2 Data

Saturation, water potential, and gas pressure data, which are inverted to obtain the calibrated parameter sets, are developed so that they can be compared to the numerical model predictions. The core saturation data are available on intervals of as small as 0.3 m. In order to compare these data to the saturation profiles predicted by the numerical model on intervals of as large as 60 m (maximum model layer thickness), the data are averaged. The *in situ* water-potential and gas-pressure data are measured on depth intervals equal to or greater than the numerical grid spacing, so these data do not need to be averaged. The *in situ* water-potential data do need to be analyzed, as discussed below, to determine when the sensor is in equilibrium with the surrounding rock.

Saturation Data from Core—The number, arithmetic mean, and standard deviation of the core measurements (see Section 4.1.2.1 for description of data) that correspond to the intervals covered by each numerical grid element are calculated using routine aversp_1. Values greater than 1.0 are assumed to be 1.0 (Assumption 7, in Section 5).

ITOUGH2 allows the data to be weighted. The weight of each saturation data point is estimated from the number of measurements, the standard deviation of the measurements, and estimates of handling and measurement error. The total error, *TE*, which is equal to the inverse of the weight is

$$TE=SE+ME+HE \qquad \text{(Eq. 5)}$$

where *SE* is the standard error, *ME* is the measurement error, and *HE* is the handling error. Standard error, *SE*, is defined here as

$$SE = \frac{\sigma}{\sqrt{N}} \qquad \text{(Eq. 6)}$$

where σ is the unbiased estimate of the standard deviation and N is the number of measurements. If there is no estimate of the standard deviation because of only one sample, σ and thus *SE* is assumed to be 0.05 (Assumption 8, in Section 5).

Flint (1998, p. 17) reports that the measurement error for bulk properties is less than 0.5%. The measurement error for saturation is thus taken to be 0.005.

Drying of core during handling is a potential source of error for saturation data (Flint 1998, pp. 18-19; Rousseau et al. 1999, pp. 129-131). This quantity is not easily quantifiable because of the variable nature of the forces driving the drying. Drying during handling at the surface is related to saturation, water potential (and variation of water potential with saturation), and temperature of the core as well as temperature, pressure, relative humidity, and speed of the air around the core. Drying of the core during drilling is related to similar factors. Rather than correct the measured saturation data by an uncertain estimate of drying, a contribution to the total uncertainty of the saturation data is made by an estimate of drying losses. This contribution is included as the handling error, *HE*, in Equation 1 above.

A simplified model of core drying during handling is used to estimate the rate of evaporation from the core. Drying during drilling is not considered. A fully saturated core is approximated as a spherical rock with a surface that is always completely wet and that has the same area as the core. A solution for evaporation from a spherical drop of water in an air stream is given by Bird et al. (1960, pp. 648) as

$$W = \eta \, \pi \delta^2 \frac{x_0 - x_\infty}{1 - x_\infty} \qquad \text{(Eq. 7)}$$

where W is the evaporation rate, η is the mass transfer coefficient of water vapor in air, δ is the diameter of the spherical equivalent of the core (calculated assuming that they have the same surface area), x_0 is the water mole fraction in the air at the surface of the core, and x_∞ is the water mole fraction in air far away from the core. The mass transfer coefficient of water vapor in air, η, is given by Bird et al. (1960, pp. 649) as

$$\eta = \frac{cD}{\delta}\left[2 + 0.6\left(\frac{v\delta\rho}{\mu}\right)^{1/2}\left(\frac{\mu}{D\rho}\right)^{1/3}\right] \qquad \text{(Eq. 8)}$$

where c is the total molar concentration of the air-water mixture, D is the effective binary diffusivity of water vapor in air, v is air speed, ρ is density of air, and μ is viscosity of air. Effective binary diffusivity, D [cm^2/s], for an air and water-vapor (components A and B) mixture is given by Bird et al. (1960, pp. 505) as

$$D = \frac{3.64\times10^{-4}}{p}\left(\frac{T}{\sqrt{T_{cA}T_{cB}}}\right)^{2.334}(p_{cA}p_{cB})^{1/3}(T_{cA}T_{cB})^{5/12}\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2} \qquad \text{(Eq. 9)}$$

where p is pressure [atm], T is temperature [K], and p_c, T_c, and M are the critical pressure [atm], critical temperature [K], and molecular weight [g/g-mole], respectively, of components A and B.

It is assumed that the temperature of the core is 25°C and that the temperature, pressure, relative humidity, and speed of the air far from the core are 30°C, 1 atm, 25%, and 3 kph, respectively. These are all reasonable assumptions given the field conditions at Yucca Mountain. Assuming that the effect of the water vapor in the air is negligibly small, the physical properties of air at 27.5°C (the average temperature) are $c = 4.05\times10^{-5}$ g-mole/cm^3, $\rho = 0.00118$ g/cm^3, and $\mu = 1.84 \times 10^{-4}$ g/cm s (Roberson and Crowe 1990, p. A-22). The molecular weight, critical temperature and critical pressure of air are 28.97 g/g-mole, 132 K, and 36.4 atm, respectively (Bird et al. 1960, p. 744). The molecular weight and critical temperature and pressure of water are 18.02 g/g-mole, 647.25 K, and 218.3 atm, respectively (Weast 1987, pp. B-94, F-66). The mole fraction of water vapor in air at the surface of the core, x_0, is 0.0313 (Weast 1987, p. D-190). Given a relative humidity of 25%, the mole fraction of water vapor in air far from the core, x_∞, is 0.0126 (Weast 1987, p. D-190). The core is 7 cm in diameter and 10 cm in length (Flint 1998, p. 11). Using these values, an evaporation rate of 2.69×10^{-4} g-mole/s is calculated.

At this evaporation rate, the saturation of a fully saturated core of average porosity, 22.3%, will be reduced by 2.2% after 5 minutes, which is the handling time given by Flint (1998, p.11). A fully dry core will have no reduction in saturation. Using these two points, a linear dependence of saturation change on saturation yields the relation

$$\Delta S = 0.022S \qquad \text{(Eq. 10)}$$

where S is the uncorrected saturation value and ΔS is saturation change resulting from handling. Average porosity for the entire mountain is calculated as a layer thickness weighted average of individual layer porosities.

Non-Q, corrected saturation data from boreholes SD-7, SD-9, USW SD-12, and UZ-14 corroborate the relationship given in Equation 3. Non-Q corrected saturation data are calculated based on several factors including porosity and drilling rate (Flint 1998, pp. 18-19; Rousseau et al. 1999, pp. 129-131). A linear correlation of uncorrected saturation to the difference between corrected and uncorrected saturation gives a correlation factor of 0.022. Values greater than 1.0 in the uncorrected and corrected saturation data were changed to 1.0 (Assumption 7, in Section 5).

***In Situ* Water Potential Data**—Measuring water potential *in situ* requires the rock near the borehole and the fill of the borehole to come into equilibrium with the surrounding rock. Prior to installation of the *in situ* sensors, these boreholes were open, and rock immediately around the borehole may have dried out (Rousseau et al. 1999, pp. 143-151). Thus the *in situ* data (see Section 4.1.2.2 for description of data) need to be evaluated in order to determine the equilibrium value of the data.

Data are available from boreholes USW NRG-6 and USW NRG-7a from 11/94 through 3/98, from borehole UE-25 UZ#4 from 6/95 through 3/98, and from borehole USW SD-12 from 11/95 through 3/98 in the DTNs listed above in Section 4. Each DTN covers from three to six months of data. The arithmetic average and trend (i.e., slope) of the data points for the time period covered by each DTN for each borehole, depth, and instrument station (there are two instrument stations per depth) were calculated. Values for each instrument station were then compared between DTNs

(providing an approximate time history of water potentials) to find the value that best represented the equilibrium value. The change in the average value is used as the primary indicator to judge whether the measurement represented the equilibrium value. The trend is used as a secondary indicator to flag instrument stations that may be drifting or out of calibration.

Rousseau et al. (1999, p. 144) gives ± 0.2 MPa as the 95% confidence interval (two standard deviations) for the *in situ* water potential measurements. One standard deviation, 0.1 MPa, is used as an estimate for the uncertainty. Because water potential is lognormally distributed, the standard error of log(water potential), $SE_{\log(\Psi)}$, is estimated as

$$SE_{\log(\Psi)} = \log(\Psi + 0.1) - \log(\Psi) \qquad \text{(Eq. 11)}$$

where Ψ is the value of the water potential data point in MPa.

Because saturation data points outnumber water potential data points approximately 8 to 1, saturation data are likely to dominate the inversion. Saturation data are available for all layers while water potential data are available for about half the layers but in fewer locations thus accounting for the discrepancy in numbers of data points. For layers where water potential data are available, such data must be included equally in the inversion. To accomplish this, the water potential data weighting, the inverse of standard error, is increased so that it represents half as much information (because there is water potential data for about half as many layers) as the saturation data. A new standard error is calculated by

$$\frac{1}{SE_{\log(\Psi)}'} = \frac{1}{SE_{\log(\Psi)}} \frac{1}{2} \frac{N_s}{N_{wp}} \qquad \text{(Eq. 12)}$$

where $SE_{\log(\Psi)}'$ is the modified standard error, N_s is the number of saturation data points, and N_{wp} is the number of water potential data points.

In situ water potential data for model layers tsw36 and tsw37 are not available from the surface based boreholes listed above. Data from the ECRB in the vicinity of borehole USW SD-6 are available and better constrain the calibrated properties for these and neighboring layers. These data are assigned to tsw36 and tsw37 in USW SD-6 for inversion. Weighting is calculated as described above for the other *in situ* water potential data.

Pneumatic Pressure Data—Thirty days of data from each borehole (see Section 4.1.2.3 for description of data) are used for the inversions. Several criteria are used to select data for the inversion. The data must include both diurnal pressure changes and longer-period, weather-associated, pressure changes, and the data must have been obtained prior to any influence from construction of the ESF. Table 10 shows the starting and ending dates for the data that were used in the inversion. Data from the instrument station or port nearest the bottom of the TCw are included because they show the lack of attenuation and lag of the barometric signal through the TCw. Data from stations between the lowermost in the TCw and the surface are not included because they would not add information to the inversion and would weight the TCw data more than other data. Data from all instrument stations or ports in the PTn are included because there is

substantial attenuation and lag of the barometric pumping signal through the PTn. Individual layers in the PTn are expected to have widely variable permeability, so it is important to include data that show the amount of attenuation and lag of the barometric signal in different layers of the PTn. Data from the uppermost and lowermost instrument stations or ports in the TSw are included because they show the lack of significant attenuation and lag of the barometric pumping signal characteristic through the TSw. Data from the stations in between the uppermost and lowermost stations are not included for the same reason cited above for the TCw data. Table 10 also shows the elevations of the sensors from which data were extracted for use in the inversion and the subunit in which the sensors are placed. Data from the two lowest instrument stations in borehole USW SD-12 are not included because these data are affected by the presence of perched water, which is not adequately reproduced in the 1-D simulations. Data from the third-lowest instrument station in USW SD-12 are not included because it was not properly isolated from the surface (Rousseau et al. 1997, p. 31).

Table 10. Pneumatic Pressure Data Used for Inversion

Borehole	Elevation [m]	Subunit	Dates
UE-25 NRG#5	1211.3	Tpcp	7/17 – 8/16/95
	1194.8	Tpy	7/17 – 8/16/95
	1177.1	Tpp	7/17 – 8/16/95
	1161.0	Tpbt2	7/17 – 8/16/95
	1143.9	Tptrn	7/17 – 8/16/95
	1008.3	Tptpmn	7/17 – 8/16/95
USW NRG-6	1207.6	Tpcp	3/31 18:00 – 4/26/95
	1192.4	Tpp	3/27 – 4/26/95
	1161.9	Tptrn	3/27 – 4/26/95
	1027.8	Tptpmn	3/27 – 4/26/95
USW NRG-7a	1276.8	Tpcp	3/27 – 4/26/95
	1235.7	Tpy	3/27 – 4/26/95
	1164.0	Tptrn	3/27 – 4/26/95
	1078.7	Tptpul	3/27 – 4/26/95
USW SD-7	1271.6	Tpcp	4/5 – 5/5/96
	1256.4	Tpp	4/5 – 5/5/96
	1241.4	Tptrn	4/5 – 5/5/96
	1119.2	Tptpmn	4/5 – 5/5/96
USW SD-12	1258.5	Tpcp	12/1 – 12/31/95
	1232.0	Tpbt2	12/1 – 12/31/95
	1217.1	Tptrn	12/1 – 12/31/95
	1001.3	Tptpll	12/1 – 12/31/95

(DTNs given in Table 2)

Prior Information—Uncertainties for weighting the prior information are shown in Table 11. For matrix permeability, the weight is estimated as the inverse of the standard error given in Equation 2. Because permeability is lognormally distributed, σ and thus SE are estimated for the

log transformed permeabilities, i.e. log(k). The number of samples used for calculation of the standard error does not include non detect samples (i.e., N in Equation 2 is the total number of samples minus the number of non detect samples as shown in Table 3). Fracture permeabilities are calibrated in one of three ways depending on the layer, and different uncertainties are used for each technique. Fracture permeabilities for layers tcw11 through ptn26 are calibrated by ITOUGH2 V 3.2 by inversion of pneumatic data (see Section 6.1.3.2). Because the pneumatic data represent mountain-scale data, significant upscaling of the borehole-scale, fracture permeability measurements is expected and their uncertainty should be large. Further, it is questionable whether the measurements made on layers in the PTn truly represent a fracture-only permeability because the matrix in the PTn is also very permeable. For these layers, an uncertainty of two orders of magnitude is assigned (Assumption 8, in Section 5). For layers tsw31 through tsw37, fracture permeabilities are calibrated by a technique that does not require weighting, so no uncertainties are used (see Section 6.1.3.2). For layers tsw38 and below, the fracture permeabilies are calibrated by ITOUGH2 V 3.2 by inversion of saturation and water potential data. However, all of the prior information fracture permeabilities for these layers are based on analogs, and thus any standard deviation data that might have been used to calculate an uncertainty do not represent the true uncertainty of the prior information for these layers. These permeabilities are also not expected to change as much as those above because the match to the matrix moisture data is not very sensitive to fracture permeability. An uncertainty of one order of magnitude is used for these layers (Assumption 8, in Section 5).

Table 11. Uncertainties Used for Weighting Prior Information

	$\log(k_M)$	$\log(a_M)$	m_M	$\log(k_F)$	$\log(a_F)$	m_F
tcw11	0.272	0.65	0.068	2.0	1.001	0.25
tcw12	0.390	0.65	0.028	2.0	0.087	0.25
tcw13	1.064	0.65	0.094	2.0	0.663	0.25
ptn21	0.647	0.65	0.043	2.0	1.001	0.25
ptn22	1.190	0.65	0.041	2.0	1.118	0.25
ptn23	0.913	0.65	0.076	2.0	1.118	0.25
ptn24	0.252	0.65	0.029	2.0	1.002	0.25
ptn25	0.117	0.65	0.085	2.0	1.001	0.25
ptn26	0.244	0.65	0.037	2.0	1.000	0.25
tsw31	1.510	0.65	0.036	-	1.000	0.25
tsw32	0.135	0.65	0.032	0.118	0.119	0.25
tsw33	0.248	0.65	0.022	0.118	0.118	0.25
tsw34	0.592	0.65	0.036	0.041	0.041	0.25
tsw35	0.237	0.65	0.034	0.098	0.509	0.25
tsw36	0.891	0.65	0.027	0.065	0.504	0.25
tsw37	0.406	0.65	0.052	0.065	0.504	0.25
tsw38	0.456	0.65	0.045	1.000	1.118	0.25
tsw39	0.500	0.65	0.106	1.000	1.118	0.25
ch1z	0.318	0.65	0.071	1.000	1.118	0.25

These data have been developed as documented in this AMR and submitted under DTNs: LB991091233129.001, LB991091233129.002

Table 11. Uncertainties Used for Weighting Prior Information (Cont.)

	$\log(k_M)$	$\log(a_M)$	m_M	$\log(k_F)$	$\log(a_F)$	m_F
ch1v	0.269	0.65	0.035	1.000	1.118	0.25
ch[2345]v	0.335	0.65	0.057	1.000	1.118	0.25
ch[2345]z	0.086	0.65	0.026	1.000	1.118	0.25
ch6	0.656	0.65	0.036	1.000	1.118	0.25
pp4	0.804	0.65	0.042	1.000	1.118	0.25
pp3	0.127	0.65	0.038	1.000	1.118	0.25
pp2	0.184	0.65	0.032	1.000	1.118	0.25
pp1	0.242	0.65	0.059	1.000	1.118	0.25
bf3	0.908	0.65	0.082	1.000	1.118	0.25
bf2	1.887	0.65	0.040	1.000	1.118	0.25

These data have been developed as documented in this AMR and submitted under DTNs: LB991091233129.001, LB991091233129.002

For m_M, the uncertainty is equal to the fitting error, SE_m, given in Table 3. m_F is based on data from several layers, so the uncertainty of the estimate for any one layer will be large. An uncertainty of 0.25 is used for all layers (Assumption 8, in Section 5) which is judged to be reasonable as it is about two times the maximum uncertainty used for m_M.

The uncertainty of matrix α_M is estimated by the fitting error for the desaturation data from about 0.02 to 0.4 orders of magnitude. Uncertainty is given for $\log(\alpha)$ because α is lognormally distributed. Because the estimates of α_M from the desaturation data fitting are modified by data representing field moisture conditions, the uncertainty estimate based on the fitting error is judged to be too low. An uncertainty of 0.65 orders of magnitude, or about three times the average fitting error and more than 1.5 times the maximum fitting error, is given for all α_M prior information (Assumption 8, in Section 5). The value of α_F is estimated based on fracture permeability and fracture frequency data. Standard error for α_F, $SE_{\log(\alpha)}$, is calculated as a combination of the standard errors for fracture permeability, $SE_{\log(k)}$, and fracture frequency, $SE_{\log(f)}$,

$$SE_{\log(\alpha)}{}^2 = SE_{\log(k)}{}^2 + SE_{\log(f)}{}^2 \qquad \text{(Eq. 13)}$$

where the standard error of log transformed fracture frequency, $SE_{\log(f)}$, is approximated by

$$SE_{\log(f)} = \log\left(f + SE_f\right) - \log(f) \qquad \text{(Eq. 14)}$$

where f is fracture frequency and SE_f is standard error of fracture frequency estimated by Equation 2. Where fracture frequency data are not available from the ESF or ECRB, the standard error, $SE_{\log(f)}$, is assumed to be 0.5 (Assumption 8, in Section 5), which is about twice the maximum uncertainty of the data from the ESF or ECRB.

6.1.3 Data Inversion

One-dimensional data inversion is carried out in a series of steps. First, the parameters are calibrated by inversion of saturation and water potential data. Second, the calibrated parameters from the first step are used as initial estimates for further parameter calibration by pneumatic data inversion. Third, the calibrated parameter set from the second step is checked against the saturation and water potential data and further calibrated if needed. If further calibration is carried out in the third step, then the new parameter set is checked against the pneumatic data. For the three final parameter sets documented below, this fourth step is all that was necessary. More generally, though, this iterative approach would be continued until satisfactory matches to the saturation, water potential, and pneumatic data are achieved.

In the saturation and water potential inversions (the first and third steps above), fracture permeabilities for layers tcw11 down to tsw37 are not included as parameters to be calibrated. Trial runs showed that these fracture permeabilities are much better constrained during the pneumatic data inversion. The calibrated values tend to be higher than the prior information, so these permeabilities are set to 1.0E-10 m^2 for tcw11, tcw12, and tcw13, 5.0E-12 m^2 for ptn21 through ptn26, and 5.0E-11 m^2 for tsw31 through tsw37. In the pneumatic inversion (the second step), these permeabilities are the only parameters calibrated because they are the only parameters well constrained by the pneumatic data.

6.1.3.1 Saturation and Water Potential Inversion

The EOS9 module (Richard's equation) of ITOUGH2 V 3.2 is used for moisture flow calibration.

Calibration of the parameter set for the base-case infiltration scenario—For the base-case infiltration scenario, the initial estimates for all parameters except 7 remain the same as the prior information. The initial estimates of k_M for material types tsw34, tsw36, tsw37, and tsw38 are increased from their prior information values to 10^{-17} m^2. The initial estimate of k_M for material type ch1v is increased from its prior information value to 10^{-13} m^2. The initial estimates of α_M for material types tsw37 and tsw38 are increased from their prior information value to $10^{-5.6}$ Pa^{-1}. These k_M and α_M values were changed because matrix saturations near 1.0 are predicted in these layers when using the prior information parameter values while lower saturation and water potential values are observed. When the prior information values of these parameters are perturbed to evaluate the parameter selection criteria, the saturation and water potential changes are likely to be very small, and so these parameters are not likely to be selected even though the data do not match the model predictions. Parameter selection is a feature of ITOUGH2 V 3.2 that reduces the parameters being calibrated during any one iteration based on objective function sensitivity criteria (Finsterle 1999, pp. 52-53). By setting the initial estimates of these parameters higher, the perturbation will produce larger saturation and water potential changes, making it more likely that these parameters are selected, so that ITOUGH2 can properly match the observed data in these layers.

The objective function is reduced approximately 78% in 34 iterations. The matches between the data and the calibrated simulation predictions, and between the calibrated parameter set and the

prior information, are inspected to make sure that there are no unreasonable differences. An unreasonable difference would be one that is much larger than the average difference. This is a qualitative judgement, but one that helps minimize the number of moisture and pneumatic inversion iterations necessary to produce an acceptable parameter set.

Inversion of saturation and water potential data for upper and lower bound infiltration scenarios—For each infiltration map (see Table 2 for data tracking information), two inversion runs were performed. In the first run, reasonable matches were obtained between the simulated and observed matrix water saturation and potential profiles in the calibration boreholes. Then, the output parameters from the first run are modified as the new initial estimates for the second run. The objective of the modification is to be consistent with conceptual model item 10. The details of the modification are documented in the scientific notebook YMP-LBNL-GSB-LHH-2 on pp. 41–44.

The objective function values were reduced by 86% and 58% for the upper and lower bound infiltration scenarios, respectively. Again, the matches between the data and the calibrated simulation predictions, and between the calibrated parameter set and the prior information, were inspected to make sure that there were not unreasonable differences.

6.1.3.2 Pneumatic Inversion

The EOS3 module of ITOUGH2 V 3.2 is used for the pneumatic simulations. Both the gas phase and the liquid phase are considered in the flow calculations.

The pneumatic inversion is carried out in two steps. First, the fracture permeabilities for layers tcw11 through ptn26 are calibrated. Then, the permeabilies for layers tsw31 through 37 are calibrated as a group by multiplying the prior information for all seven layers by the same factor.

TCw and PTn k_F calibration—As described above, trial inversions showed that the calibrated fracture permeabilities resulting from inversion of pneumatic data are higher than the prior information. The initial estimates for the fracture permeabilities are 1.0E-10 m^2 for tcw11, tcw12, and tcw13, and 5.0E-12 m^2 for ptn21 through ptn26. The large differences between the initial estimates and the prior information of fracture permeability are necessary because approaching the calibrated values from higher values is more successful. Prior information for the fracture permeabilities remains unchanged.

The permeabilities of layers tsw31 through 37 are set to $10^{1.6}$ times the prior information based on trial runs (see "TSw k_F calibration," below, for the rationale of a constant factor applied to all TSw fracture permeabilities).

Inversions of pneumatic data for all three infiltration scenarios result in calibrated parameters that provide nearly identical matches to the data.

TSw k_F calibration—The lack of significant attenuation in the TSw unit is considered an important feature shown by the gas pressure data. The calibrated fracture permeabilities for the model layers in the TSw unit need to be consistent with this feature. Therefore, fracture

permeabilities in the TSw need to be determined in such a way that the simulated and observed gas pressure signals at the upper and lower sensor locations in the TSw have similar degrees of attenuation for borehole USW SD-12. Borehole USW SD-12 is chosen for this analysis because the distance between the two TSw sensors within this borehole is the largest among all the relevant boreholes. The degree of attenuation of the barometric signal through the TSw in USW SD-12, or the relative difference between the signals at the two sensor locations, was determined by the routine factorOBJ, which evaluates

$$F = \frac{1}{N}\left\{\sum_{i=1}^{N}\left[(P_u(t_i) - P_u(t_1)) - (P_b(t_i) - P_b(t_1))\right]^2\right\}^{1/2} \qquad \text{(Eq. 15)}$$

where N is the total number of calibration time points, P is the gas pressure, and subscript, u and b, refer to the sensors in the upper and lower (bottom) portions of the TSw within the borehole USW SD-12. Obviously, if the gas signals from the two sensors are identical, F should be equal to zero. For the given gas signal data, the F value is 2.01E-3 (kPa). In this study, fracture permeabilities need to be determined that will predict F values similar to the value calculated from the data, such that the simulated and observed gas pressure signals have similar degrees of attenuation.

Since the gas pressure data from the TSw are limited as a result of the almost insignificant amount of attenuation and lag between the upper-most and lower-most sensors, the fracture permeabilities for different model layers in this unit could not be independently estimated in a reliable manner. Therefore, the ratios of the permeabilities of layers tsw31 through tsw37 are held constant, and the prior information permeability values are multiplied by a single factor, d. For a given infiltration map, a number of values, log(d), between 1 and 2 with an interval of 0.1 are tested to determine the d resulting in an F value closest to the F value corresponding to the data. To calculate an F value for a d factor, the outputs from the TCw and PTn fracture permeability calibrations are used to run a forward simulation for generating gas pressures used in Equation 8. In a forward simulation, all the rock properties are the same as those determined from the corresponding TCw and PTn fracture permeability calibration, except the fracture permeabilities for model layers tsw31 to tsw37 are determined using the d factor and the prior information.

The determined log(d) values are shown in Table 12 for the three infiltration maps. The log(d) values range from 1.6-1.7, indicating that the fracture permeabilities for the relevant model layers are increased by almost two orders of magnitude compared with the prior information. This results from the scale effects and will be further discussed in Section 6.2.

Table 12. The Calculated log(d) Factors for the Three Infiltration Maps

Base-case	Upper Bound	Lower Bound
1.7	1.6	1.6

6.1.3.3 Saturation and Water Potential Check/Inversion

Parameter Set for Base-case Infiltration Scenario—Matches to the saturation and water potential data were checked and found to be satisfactory. The proportions of fracture and matrix

flow were also checked, as was done for the other two infiltration scenarios as described above. Parameter adjustments are made as documented in scientific notebook YMP-LBNL-GSB-1.1.2 on pp. 107-108, resulting in matrix-dominated flow in the PTn and in the vitric portion of the CHn.

With the calibrated parameter set and the modified parameters as initial estimates, the saturation and water potential data are inverted to try to improve the data match as much as possible. As in the previous saturation and water potential inversions, the fracture permeabilities for layers tcw11 through tsw37 are fixed. The objective function is improved by 13%.

Parameter Sets for Upper and Lower Bound Infiltration Scenarios—Further parameter adjustments to ensure that the conceptual model of matrix-dominated flow through the PTn and vitric portion of the CHn is met were done. Then the resultant parameters were used as initial estimates for new inversions with the saturation and water potential data to improve the match to the data. The objective function is improved 6% and 8% for the upper and lower bound infiltration scenarios, respectively.

6.1.3.4 Pneumatic Check

Because parameter sets have been changed, the match to the pneumatic data is reevaluated for all three infiltration scenarios. The matches are not significantly changed.

6.1.4 Summary of One-Dimensional, Mountain-Scale Calibration

Model Calibration Results for Basecase Infiltration Scenario—The one-dimensional calibrated parameter set for the base-case infiltration scenario is presented in Table 13. Matches to the data achieved with this parameter set for USW SD-12 are shown for saturation in Figure 2, for water potential in Figure 3, and for pneumatic pressure in Figure 4.

Table 13. Calibrated Parameters from One-Dimensional Inversion of Saturation, Water Potential, and Pneumatic Data for the Base-case Infiltration Scenario

Model Layer	k_M (m^2)	α_M (1/Pa)	m_M (-)	k_F (m^2)	α_F (1/Pa)	m_F (-)	γ (-)
tcw11	3.86E-15	4.00E-5	0.470	2.41E-12	3.15E-3	0.627	0.30
tcw12	2.74E-19	1.81E-5	0.241	1.00E-10	2.13E-3	0.613	0.30
tcw13	9.23E-17	3.44E-6	0.398	5.42E-12	1.26E-3	0.607	0.30
ptn21	9.90E-13	1.01E-5	0.176	1.86E-12	1.68E-3	0.580	0.09
ptn22	2.65E-12	1.60E-4	0.326	2.00E-11	7.68E-4	0.580	0.09
ptn23	1.23E-13	5.58E-6	0.397	2.60E-13	9.23E-4	0.610	0.09
ptn24	7.86E-14	1.53E-4	0.225	4.67E-13	3.37E-3	0.623	0.09
ptn25	7.00E-14	5.27E-5	0.323	7.03E-13	6.33E-4	0.644	0.09
ptn26	2.21E-13	2.49E-4	0.285	4.44E-13	2.79E-4	0.552	0.09
tsw31	6.32E-17	3.61E-5	0.303	3.21E-11	2.49E-4	0.566	0.06
tsw32	5.83E-16	3.61E-5	0.333	3.56E-11	1.27E-3	0.608	0.41
tsw33	3.08E-17	2.13E-5	0.298	3.86E-11	1.46E-3	0.608	0.41
tsw34	4.07E-18	3.86E-6	0.291	1.70E-11	5.16E-4	0.608	0.41
tsw35	3.04E-17	6.44E-6	0.236	4.51E-11	7.39E-4	0.611	0.41
tsw36	5.71E-18	3.55E-6	0.380	7.01E-11	7.84E-4	0.610	0.41
tsw37	4.49E-18	5.33E-6	0.425	7.01E-11	7.84E-4	0.610	0.41
tsw38	4.53E-18	6.94E-6	0.324	5.92E-13	4.87E-4	0.612	0.41
tsw39	5.46E-17	2.29E-5	0.380	4.57E-13	9.63E-4	0.634	0.41
ch1z	1.96E-19	2.68E-7	0.316	3.40E-13	1.43E-3	0.631	0.10
ch1v	9.90E-13	1.43E-5	0.350	1.84E-12	1.09E-3	0.624	0.13
ch2v	9.27E-14	5.13E-5	0.299	2.89E-13	5.18E-4	0.628	0.13
ch3v	9.27E-14	5.13E-5	0.299	2.89E-13	5.18E-4	0.628	0.13
ch4v	9.27E-14	5.13E-5	0.299	2.89E-13	5.18E-4	0.628	0.13
ch5v	9.27E-14	5.13E-5	0.299	2.89E-13	5.18E-4	0.628	0.13
ch2z	6.07E-18	3.47E-6	0.244	3.12E-14	4.88E-4	0.598	0.10
ch3z	6.07E-18	3.47E-6	0.244	3.12E-14	4.88E-4	0.598	0.10
ch4z	6.07E-18	3.47E-6	0.244	3.12E-14	4.88E-4	0.598	0.10
ch5z	6.07E-18	3.47E-6	0.244	3.12E-14	4.88E-4	0.598	0.10
ch6	4.23E-19	3.38E-7	0.510	1.67E-14	7.49E-4	0.604	0.10
pp4	4.28E-18	1.51E-7	0.676	3.84E-14	5.72E-4	0.627	0.10
pp3	2.56E-14	2.60E-5	0.363	7.60E-12	8.73E-4	0.655	0.46
pp2	1.57E-16	2.67E-6	0.369	1.38E-13	1.21E-3	0.606	0.46
pp1	6.40E-17	1.14E-6	0.409	1.12E-13	5.33E-4	0.622	0.10
bf3	2.34E-14	4.48E-6	0.481	4.08E-13	9.95E-4	0.624	0.46
bf2	2.51E-17	1.54E-7	0.569	1.30E-14	5.42E-4	0.608	0.10

These data have been developed as documented in this AMR and submitted under DTN: LB997141233129.001.

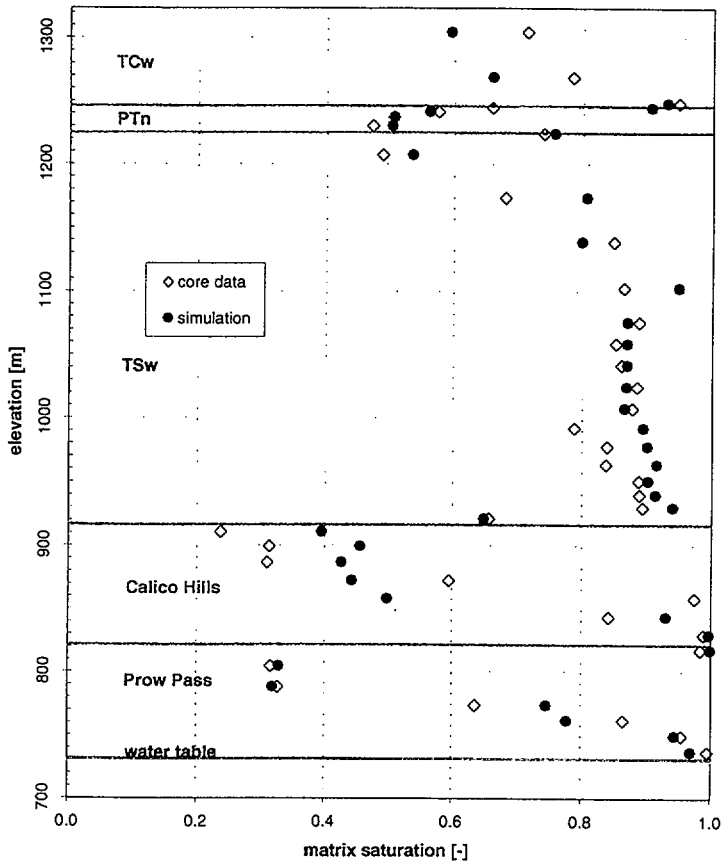

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Figure 2. Saturation Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Base-case Infiltration Scenario

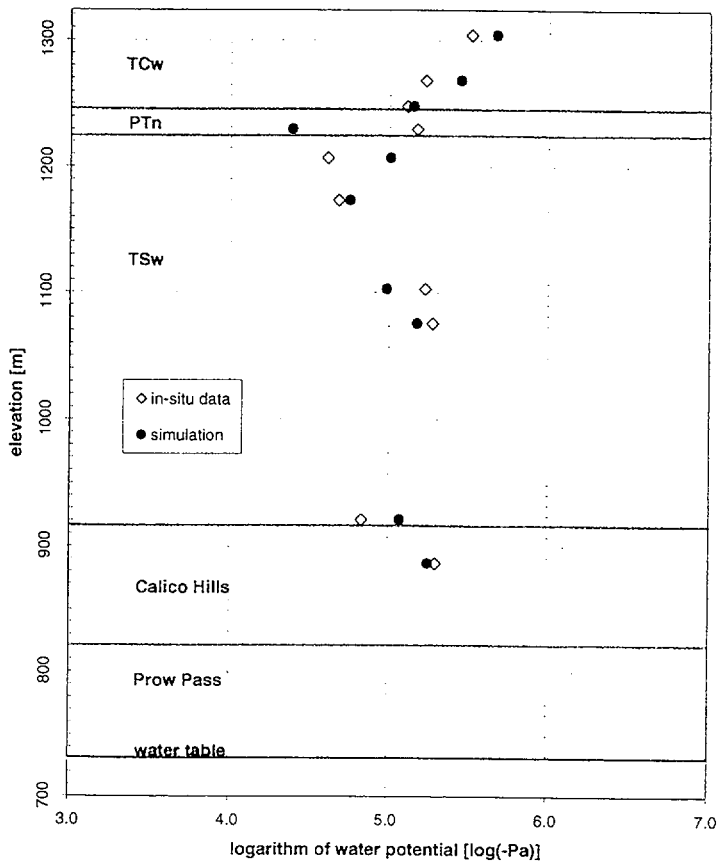

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Figure 3. Water Potential Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Base-case Infiltration Scenario

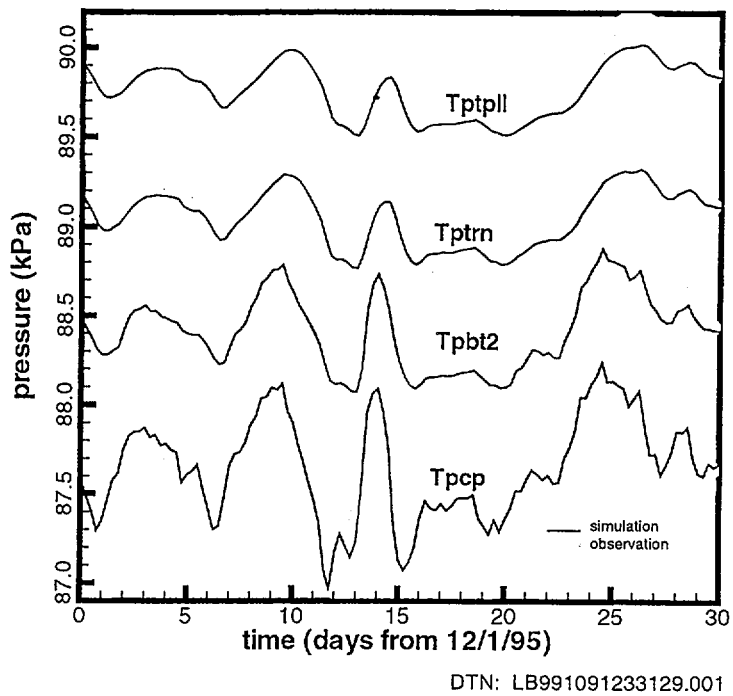


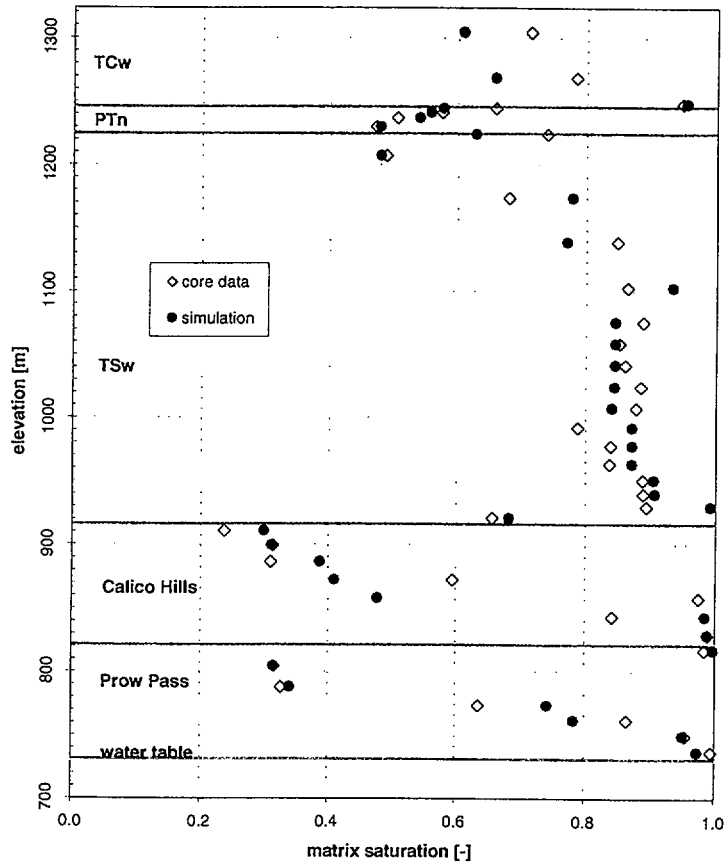
Figure 4. Pneumatic Pressure Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Base-case Infiltration Scenario

Model Calibration Results for Upper Bound Infiltration Scenario—The one-dimensional calibrated parameter set for the upper bound infiltration scenario is presented in Table 14. Matches to the data achieved with this parameter set for USW SD-12 are shown for saturation in Figure 5 and for water potential in Figure 6. The matches to the pneumatic data are virtually identical to those shown in Figure 4.

Table 14. Calibrated Parameters from One-Dimensional Inversion of Saturation, Water Potential, and Pneumatic Data for the Upper Bound Infiltration Scenario

Model Layer	k_M (m^2)	α_M (1/Pa)	m_M (-)	k_F (m^2)	α_F (1/Pa)	m_F (-)	γ (-)
tcw11	3.98E-15	4.27E-5	0.484	2.75E-12	4.67E-3	0.636	0.31
tcw12	3.26E-19	2.18E-5	0.229	1.00E-10	2.18E-3	0.633	0.31
tcw13	1.63E-16	2.17E-6	0.416	2.26E-12	1.71E-3	0.631	0.31
ptn21	1.26E-13	1.84E-4	0.199	1.00E-11	2.38E-3	0.611	0.08
ptn22	5.98E-12	2.42E-5	0.473	1.00E-11	1.26E-3	0.665	0.08
ptn23	3.43E-13	4.06E-6	0.407	1.96E-13	1.25E-3	0.627	0.08
ptn24	3.93E-13	5.27E-5	0.271	4.38E-13	2.25E-3	0.631	0.08
ptn25	1.85E-13	2.95E-5	0.378	6.14E-13	1.00E-3	0.637	0.08
ptn26	6.39E-13	3.54E-4	0.265	3.48E-13	3.98E-4	0.367	0.08
tsw31	9.25E-17	7.79E-5	0.299	2.55E-11	1.78E-4	0.577	0.09
tsw32	5.11E-16	4.90E-5	0.304	2.83E-11	1.32E-3	0.631	0.38
tsw33	1.24E-17	1.97E-5	0.272	3.07E-11	1.50E-3	0.631	0.38
tsw34	7.94E-19	3.32E-6	0.324	1.35E-11	4.05E-4	0.579	0.38
tsw35	1.42E-17	7.64E-6	0.209	3.58E-11	9.43E-4	0.627	0.38
tsw36	1.34E-18	3.37E-6	0.383	5.57E-11	8.21E-4	0.623	0.38
tsw37	7.04E-19	2.70E-6	0.447	5.57E-11	8.21E-4	0.623	0.38
tsw38	4.47E-18	5.56E-7	0.314	4.06E-13	7.69E-4	0.622	0.38
tsw39	3.12E-17	1.82E-5	0.377	5.89E-13	1.30E-3	0.633	0.38
ch1z	8.46E-20	4.23E-7	0.336	5.70E-13	1.29E-3	0.631	0.10
ch1v	4.36E-14	4.23E-5	0.363	7.90E-13	1.66E-3	0.656	0.10
ch2v	3.89E-13	4.86E-5	0.312	4.64E-13	1.45E-3	0.626	0.10
ch3v	3.89E-13	4.86E-5	0.312	4.64E-13	1.45E-3	0.626	0.10
ch4v	3.89E-13	4.86E-5	0.312	4.64E-13	1.45E-3	0.626	0.10
ch5v	3.89E-13	4.86E-5	0.312	4.64E-13	1.45E-3	0.626	0.10
ch2z	1.16E-17	1.13E-6	0.229	2.64E-14	8.45E-4	0.628	0.10
ch3z	1.16E-17	1.13E-6	0.229	2.64E-14	8.45E-4	0.628	0.10
ch4z	1.16E-17	1.13E-6	0.229	2.64E-14	8.45E-4	0.628	0.10
ch5z	1.16E-17	1.13E-6	0.229	2.64E-14	8.45E-4	0.628	0.10
ch6	3.32E-20	3.57E-7	0.502	2.21E-14	1.31E-3	0.631	0.10
pp4	2.00E-18	1.83E-7	0.683	1.07E-13	7.99E-4	0.633	0.10
pp3	1.47E-14	1.02E-5	0.395	7.10E-12	1.29E-3	0.749	0.56
pp2	1.05E-16	2.43E-6	0.367	2.53E-13	1.65E-3	0.629	0.56
pp1	5.49E-17	1.01E-6	0.393	6.25E-13	8.18E-4	0.630	0.10
bf3	2.98E-14	3.83E-6	0.490	1.43E-12	1.50E-3	0.636	0.56
bf2	3.86E-17	2.29E-7	0.582	2.26E-14	8.18E-4	0.631	0.10

These data have been developed as documented in this AMR and submitted under DTN: LB997141233129.002.



DTN: LB991091233129.001

Figure 5. Saturation Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Upper Bound Infiltration Scenario

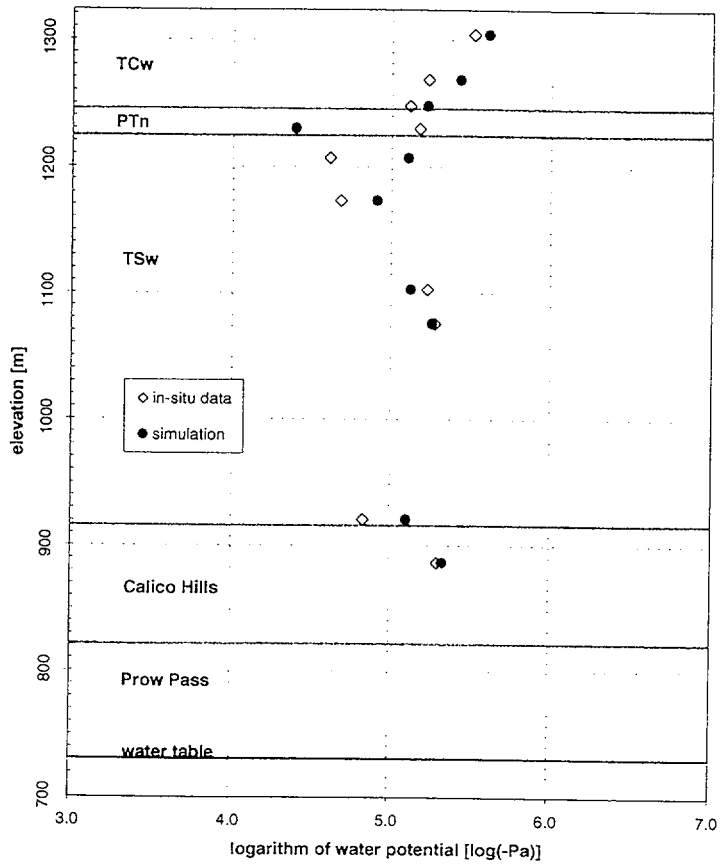


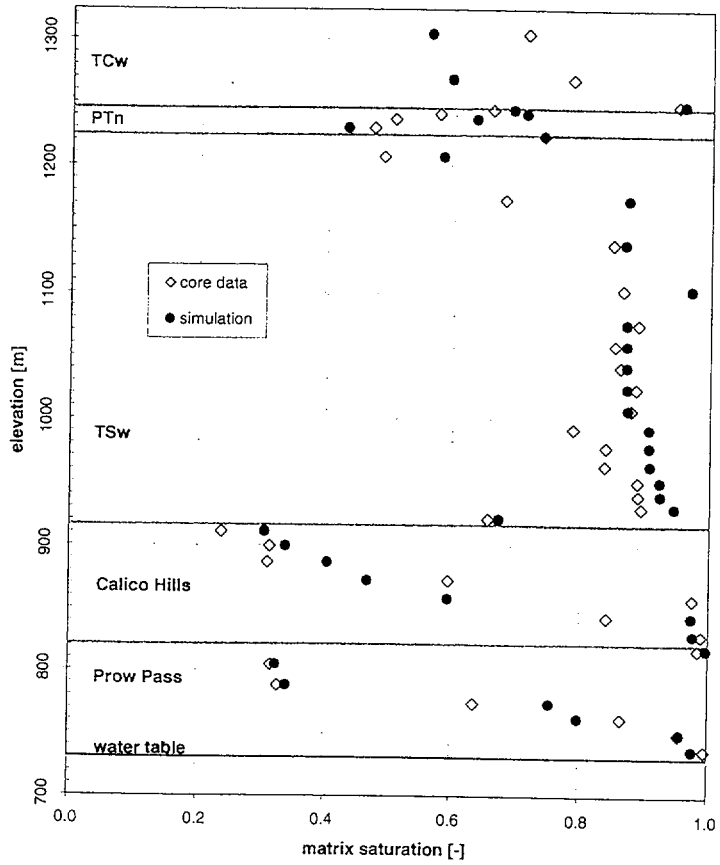
Figure 6. Water Potential Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Upper Bound Infiltration Scenario

Model Calibration Results for Lower Bound Infiltration Scenario—The one-dimensional calibrated parameter set for the lower bound infiltration scenario is presented in Table 15. Matches to the data achieved with this parameter set for USW SD-12 are shown for saturation in Figure 7 and for water potential in Figure 8. The matches to the pneumatic data are virtually identical to those shown in Figure 4.

Table 15. Calibrated Parameters from One-Dimensional Inversion of Saturation, Water Potential, and Pneumatic Data for the Lower Bound Infiltration Scenario

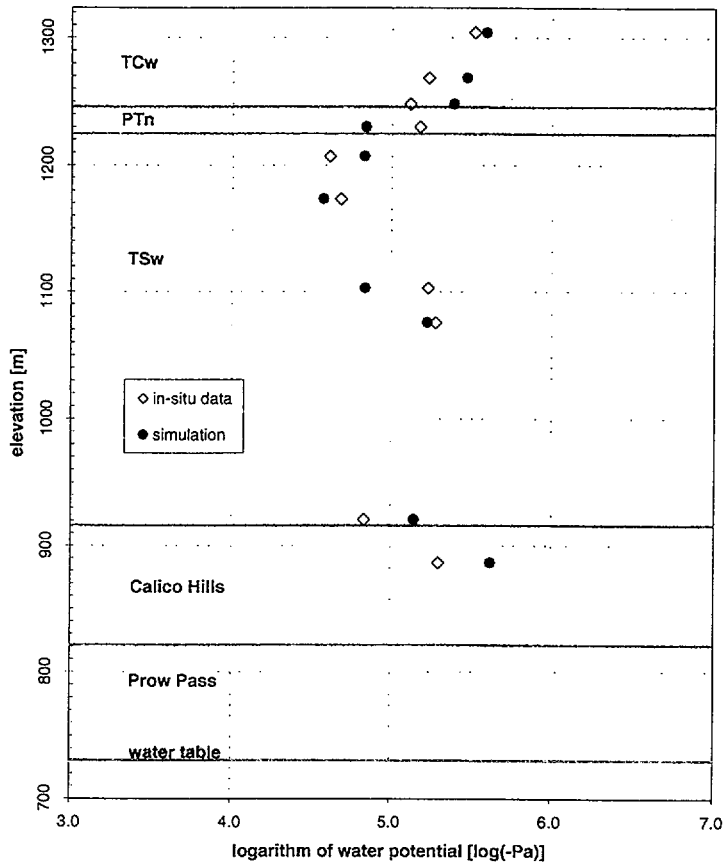
Model Layer	k_M (m^2)	α_M (1/Pa)	m_M (-)	k_F (m^2)	α_F (1/Pa)	m_F (-)	γ (-)
tcw11	4.63E-15	1.61E-5	0.460	2.70E-12	2.40E-3	0.598	0.25
tcw12	8.87E-20	2.89E-5	0.241	1.00E-10	2.05E-3	0.608	0.25
tcw13	6.61E-17	1.42E-6	0.368	1.79E-12	9.21E-4	0.600	0.25
ptn21	1.86E-13	6.13E-5	0.165	1.00E-11	1.66E-3	0.503	0.01
ptn22	3.27E-12	1.51E-5	0.390	1.00E-11	9.39E-4	0.651	0.01
ptn23	4.20E-13	2.04E-6	0.387	1.84E-13	1.28E-3	0.518	0.01
ptn24	3.94E-13	2.32E-5	0.210	4.31E-13	2.02E-3	0.594	0.01
ptn25	2.22E-13	2.04E-5	0.296	7.12E-13	7.42E-4	0.555	0.01
ptn26	5.43E-13	1.82E-4	0.264	3.08E-13	2.00E-4	0.401	0.01
tsw31	6.38E-17	2.81E-5	0.317	2.55E-11	4.42E-4	0.545	0.06
tsw32	6.28E-16	6.35E-5	0.279	2.83E-11	1.21E-3	0.603	0.23
tsw33	1.82E-17	2.44E-5	0.248	3.07E-11	1.36E-3	0.600	0.23
tsw34	3.50E-19	3.54E-6	0.309	1.35E-11	2.48E-4	0.515	0.23
tsw35	1.27E-17	7.57E-6	0.187	3.58E-11	6.26E-4	0.612	0.23
tsw36	1.19E-18	3.74E-6	0.328	5.57E-11	4.90E-4	0.540	0.23
tsw37	5.63E-19	3.28E-6	0.423	5.57E-11	4.90E-4	0.540	0.23
tsw38	1.44E-18	3.72E-6	0.291	5.65E-13	4.00E-4	0.603	0.23
tsw39	1.09E-17	2.37E-5	0.321	3.12E-13	6.43E-4	0.605	0.23
ch1z	2.75E-20	7.26E-7	0.304	1.87E-13	1.00E-3	0.611	0.12
ch1v	2.05E-14	9.86E-6	0.402	9.03E-13	1.43E-3	0.658	0.12
ch2v	3.17E-13	1.91E-5	0.326	1.94E-13	6.84E-4	0.544	0.12
ch3v	3.17E-13	1.91E-5	0.326	1.94E-13	6.84E-4	0.544	0.12
ch4v	3.17E-13	1.91E-5	0.326	1.94E-13	6.84E-4	0.544	0.12
ch5v	3.17E-13	1.91E-5	0.326	1.94E-13	6.84E-4	0.544	0.12
ch2z	6.28E-18	2.44E-6	0.135	4.10E-14	2.08E-4	0.613	0.12
ch3z	6.28E-18	2.44E-6	0.135	4.10E-14	2.08E-4	0.613	0.12
ch4z	6.28E-18	2.44E-6	0.135	4.10E-14	2.08E-4	0.613	0.12
ch5z	6.28E-18	2.44E-6	0.135	4.10E-14	2.08E-4	0.613	0.12
ch6	8.20E-20	5.06E-7	0.445	1.12E-14	6.10E-4	0.604	0.12
pp4	2.05E-18	1.83E-7	0.653	3.40E-14	4.86E-4	0.635	0.12
pp3	1.91E-14	1.53E-5	0.355	2.23E-12	5.93E-4	0.699	0.43
pp2	1.08E-16	2.08E-6	0.399	1.42E-13	7.62E-4	0.608	0.43
pp1	6.52E-17	9.40E-7	0.392	7.15E-14	3.90E-4	0.638	0.12
bf3	9.47E-15	3.75E-6	0.509	3.43E-13	7.60E-4	0.611	0.43
bf2	1.27E-17	1.38E-7	0.568	9.21E-15	4.18E-4	0.598	0.12

These data have been dveloped as documented in this AMR and submitted under DTN: LB997141233129.003.



DTN: LB991091233129.001

Figure 7. Saturation Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Lower Bound Infiltration Scenario



DTN: LB991091233129.001

Figure 8. Water Potential Matches at USW SD-12 for One-Dimensional, Mountain-Scale, Calibrated Parameter Set for the Lower Bound Infiltration Scenario

Discussion of result uncertainties—Quantifiable uncertainties are difficult if not impossible to establish for the estimated parameter sets. In the moisture data portion of the inversions, 163 parameters are calibrated to 233 data points. This is what is called a poorly constrained problem. Further complicating the calibration process, many of the parameters are cross-correlated; that is, variations in two or more parameters may have the same effect on the predicted system response. Because the problem is poorly constrained, there is no well-defined global minimum in the objective function. Rather, there are likely to be many, equivalent, local minima. With respect to the moisture data alone, any of these minima provide an equally good parameter set.

There are, however, two mitigating factors for the results of the inversion of the moisture data. First, consistency with conceptual model item 10 provides further evidence, not included in the objective function, that the parameter set is appropriate. Second, and more important, most of the parameters calibrated to the moisture data are changed very little with respect to the prior information. Table 16 summarizes the average change for each parameter type except γ, for which

prior information is not available. These changes are within the average uncertainites, *SE*, for each parameter type and in some cases are much smaller. The prior information standard deviation of matrix permeability, $\sigma_{\log(k)}$, is greater than the parameter change in all but one case. The standard deviation is a measure of the variability of the data that provides a good bound on the maximum amount of allowable change. The ch1 vitric permeability for the base-case infiltration scenario was the only calibrated matrix permeability value that changed more than the standard deviation. This change was made to increase matrix flow in the CHn vitric zone consistent with conceptual model item 10. Standard deviations are not available for any of the other parameters calibrated to the moisture data.

Table 16. Average Difference Between Calibrated Parameters and Prior Information for Parameters Calibrated to Moisture Data and Conceptual Model Item 10

	$\Delta\log(k_M)$	$\Delta\log(k_F)$[1]	$\Delta\log(\alpha_M)$	$\Delta\log(\alpha_F)$	Δm_M	Δm_F
base-case	.42	.38	.30	.21	.025	.024
upper bound	.37	.44	.20	.09	.030	.023
lower bound	.42	.35	.34	.28	.042	.053

NOTE: [1] Only fracture permeabilities for layers tsw38 and below are included. Fracture permeabilities for layers tsw37 and above are calibrated to pneumatic data.

Calibrated fracture permeability uncertainty estimated by inversion of pneumatic data is low. Unlike the moisture data inversion this is a well-constrained problem. A total of 2637 pneumatic data points are used to calibrate the fracture permeabilities of 9 layers (tcw11 through ptn26). Similarly, the single *d* parameter is calibrated by inversion of 480 data points. While it would appear that the combination of a well-constrained problem and the good matches between the simulation and the data should give very low uncertainty, this is not necessarily the case. Other elements of the model that are fixed by the conceptual model add uncertainty. The uncertainty of the other 163 parameters that are fixed during the pneumatic data inversion must also be considered when evaluating the uncertainty of the fracture permeabilities calibrated by pneumatic data inversion.

Perhaps a reliable estimate of uncertainty is the set of uncertainties used to weight the prior information. These uncertainties could be evaluated either by Monte Carlo simulation or by linear error analysis, both of which are capabilities of ITOUGH2 V 3.2. Because of the large number of parameters, and thus degrees of freedom for the objective function, linear error analysis is not a very reliable method to use. Unfortunately, the large number of parameters also make uncertainty analysis by Monte Carlo simulation prohibitively time consuming. Uncertainties of the calibrated property set will be addressed further in an AMR supporting the UZ Flow and Transport PMR, which will document sensitivity studies for the UZ Model.

6.2 ONE-DIMENSIONAL DRIFT-SCALE CALIBRATION

As a result of the pneumatic inversion, the site-scale fracture permeabilities in most of the TSw model layers are increased by almost two orders of magnitude, compared with the prior information determined from the air-injection tests, mainly because the pneumatic pressure data

result from the mountain-scale gas-flow processes, while air-injection tests correspond to scales on an order of several meters or less. It is well documented in the literature that large-scale effective permeabilities are generally larger than smaller-scale ones (Neuman 1994). An intuitive explanation for this scale-dependent behavior is that a large observation scale, in an average sense, corresponds to a larger opportunity to encounter more permeable zones or paths when observations are made, which considerably increases values of the observed permeability. Because of the scale difference, mountain-scale fracture permeabilities, determined from the pneumatic data inversion, cannot be applied to drift-scale modeling. Therefore, development of drift-scale properties is needed.

Unlike the connected fracture networks and soils, studies on the scale-dependent behavior of matrix properties in unsaturated fractured rocks are very limited. However, it is reasonable to consider that the scale-dependent behavior of the matrix is different from fracture networks. For example, relatively large fractures can act as capillary barriers for flow between matrix blocks separated by these fractures, even when the matrix is essentially saturated (water potential is close to the air entry value). This might limit the matrix scale-dependent behavior to a relatively small scale associated with the spacing between relatively large fractures. Although it is expected that estimated large-scale matrix permeabilities should be larger than those measured on a core-scale, no evidence exists to indicate that the matrix properties should be very different on both the site and drift scales, which are much larger than the scale characterized by the fracture spacing. This point is also supported by the inversion results for the site-scale properties. For example, the differences between the estimated site-scale matrix permeabilities and the prior information are generally much smaller compared with those for the fracture permeabilities.

Based on the above discussions, only fracture permeabilities for the drift-scale property sets are recalibrated while other properties remain the same as those in the corresponding site-scale properties. Since the drifts are located within the TSw units, the calibration is further limited to model layers tsw32-37. Data used for the calibration are the same as those used for the site-scale property calibration, except that the pneumatic data are excluded. The initial estimates are the prior information for the fracture permeabilities given in Table 4. Unlike the mountain-scale property calibration, the permeabilities for each of the layers are estimated independently, except that a single value is estimated for layers tsw36 and tsw37. Uncertainties used for weighting are calculated using Equation 2 and data from Table 4.

The calibrated results are given in Table 17 for the base-case, upper bound and lower bound infiltration rates. As expected, the calibrated fracture permeabilities are much lower than those corresponding to the site scale and are closer to the prior information. Except in two cases (upper bound infiltration scenario permeabilities for layers tsw32 and tsw35), all the estimated permeabilities are within a factor of two of the prior information. Note that the fracture permeabilities for the upper-bound infiltration rates are generally higher than those for the base-case and lower-bound infiltration rates. This is because relatively large fracture fluxes occur for the upper bound infiltration map, and permeabilities of some layers may need to be adjusted upward to accommodate the increased liquid flow. For the base-case and lower-bound infiltration scenarios, fracture permeabilities are more than enough to carry the small amount of liquid flow,

so the objective function is not very sensitive to the estimated fracture permeabilities. They will be mainly determined by the prior information, to which they are close as noted above.

Table 17. Calibrated Drift-Scale Fracture Permeabilities (m^2) for the Model Layers in TSw

Model Layer	Basecase	Upper Bound	Lower Bound
Tsw32	1.26E-12	7.08E-12	8.91E-13
Tsw33	5.50E-13	1.50E-12	6.07E-13
Tsw34	2.76E-13	4.63E-13	4.99E-13
Tsw35	1.29E-12	5.09E-12	1.82E-12
Tsw36	9.91E-13	1.48E-12	1.43E-12
Tsw37	9.91E-13	1.48E-12	1.43E-12

These data have been developed as documented in this AMR and submitted under DTNs: LB990861233129.001, LB990861233129.002, and LB990861233129.003.

Finally, it is important to note that the property sets developed in this section are only for drift-scale studies within the TSw unit. Uncertainties are not easily determined as discussed above in Section 6.1.4. Sensitivity studies are planned to better characterize uncertainties and will be documented in a future AMR supporting the UZ Flow and Transport PMR.

The one-dimensional drift-scale property calibration is documented in scientific notebook YMP-LBNL-GSB-LHH-2, pp. 52-56.

6.3 TWO-DIMENSIONAL FAULT CALIBRATION

Saturation, water potential, and pneumatic pressure data from borehole USW UZ-7a are inverted to calibrate the fault parameters for three of the four fault layers. There are no data, other than the prior information, for the lower fault layer, CHn/CFu, so the fault parameters for this layer are not included as part of the calibration. The prior information values are recommended for use in the UZ Model.

Of the criteria for a successful calibration given in Section 6 and used for the 1-D, mountain-scale calibration, only one is used here. Minimization of the objective function is the only criterion used. The two pneumatic data sets from the TSw are measured at points that are too close together to draw any conclusions about the amount of attenuation across the TSw in the fault. The proportion of fracture flow to matrix flow specifically in the fault is not an element of the conceptual model.

The two-dimensional fault property calibration is documented in scientific notebook YMP-LBNL-GSB-1.1.2, pp. 127-145.

6.3.1 Model Development

The numerical grid for the two-dimensional, vertical, cross section is available under DTN: LB990501233129.003.

Prior information for k_F, k_M, α_F, α_M, m_F, and m_M for the faults, which are also used as initial parameter guesses, are available under DTN: LB990501233129.001.

As with the one-dimensional calibration, there is no prior information for the active fracture parameter, γ, for the faults. initial estimates for γ for this inversion are shown in Table 18. The initial estimate for tcwf is increased over the initial estimate and calibrated value from the 1-D inversion because enhanced fracturing in the faults near the surface will reduce the relative area for fracture-matrix interaction. The initial estimate for chnf is an average of the 1-D base-case calibrated values for the zeolitic and devitrified layers of the CHn and CFu (see Table 13).

Table 18. Initial Estimates of the Active Fracture Parameter, γ, for Faults

Material type	γ
tcwf	0.4
ptnf	0.1
tswf	0.4
chnf	0.3

The base-case, lower bound and upper bound present-day infiltration maps, are used as input to infil2grid V1.6 to calculate infiltration rates for the upper boundary of the grid.

Pneumatic boundary conditions are developed in a manner similar to that documented in Section 6.1.1 using routine TBgas3D as documented in scientific notebook YMP-LBNL-GSB-1.1.2, pp. 140-142.

6.3.2 Data

Saturation, water potential, and pneumatic pressure data, which are inverted to obtain the calibrated parameter sets, are developed so that they can be compared to the numerical grid in a way similar to that described in Section 6.1.2. However, because geologic layering data from USW UZ-7a are not included in the geologic model used to develop the numerical grid, there is no one-to-one correlation between the grid layer elevations and the geology of USW UZ-7a. This problem is overcome by interpolating the data onto the grid. The specifics of this interpolation are documented in scientific notebook YMP-LBNL-GSB-1.1.2 on pp. 130-137 and p. 140.

Saturation and Water Potential Data—The calculation for the average saturations from core and *in situ* water potentials and their weighting for the inversion is the same as described in Section 6.1.2 above, except for the necessity of interpolation (based on geology) to assign data to the appropriate model layers.

Pneumatic Pressure Data—The same criteria for selecting an appropriate time interval for the data as described in Section 6.1.2 are used to select data from USW UZ-7a. Table 19 shows the dates, subunits, and elevations for the data that were used in the inversion. As with the one-dimensional pneumatic inversion, data are taken from the lowest TCw instrument station, all instrument stations in the PTn and in the TSw within the fault zone. Three instrument stations in

the foot wall (below the fault zone) are not included in the inversion because they represent interactions at the edge of the fault on a subgrid block scale not captured by the UZ Model.

Table 19. Pneumatic Pressure Data Used for Inversion

Borehole	Elevation [m]	Subunit	Dates
USW UZ-7a	1243.0	Tpc	12/1 – 12/31/95
	1232.3	Tpcpv1	12/1 – 12/31/95
	1221.6	Tpbt2	12/1 – 12/31/95
	1213.4	Tptrv3/2	12/1 – 12/31/95
	1177.8	Tptrn	12/1 – 12/31/95

6.3.3 Data Inversion

The data inversion for calibration of the fault parameters is carried out in the same sequence of steps used for the one-dimensional mountain-scale inversion. First, the saturation and water potential data are inverted. Second, the pneumatic data are inverted. Third, the calibrated parameters are checked against the saturation and water potential data and further calibrated if needed. And fourth, a final check against the pneumatic data is performed.

The selection of parameters to be calibrated to each data set is also the same as the one-dimensional mountain-scale inversion. Fracture permeabilities are fixed during the saturation and water potential inversion and are the only parameters calibrated to the pneumatic data.

initial estimates for the parameters are modified based on improving the match to the saturation and water potential data by trial and error. At several points during the trial-and-error process, automated inversion of the saturation and water potential data was attempted, but was not successful at significantly improving the match to the data (the objective function). As with the one-dimensional mountain-scale calibration, the fracture permeabilities are fixed from the beginning at values higher than the prior information because trial runs showed that they would be significantly increased during the pneumatic inversion.

Using the parameter set from the initial calibration step, the fracture permeabilities are calibrated by inversion of the pneumatic data. Automated inversion successfully improves the objective function and provides an excellent match to the pneumatic data. The criterion of the objective function approaching an asymptotic value is met.

Using the parameter set from the pneumatic calibration step as the initial estimate, automated inversion of the saturation and water potential data is performed and results in a slight improvement to the match. The criterion of ITOUGH2 V 3.2 terminating the inversion because it cannot improve the objective function further is met. The match to the pneumatic data is checked for the final fault parameter set and is found not to have changed significantly.

6.3.4 Parameter Check for Upper and Lower Bound Infiltration Scenarios

Because the nonfault parameters are assumed to have a significant effect on the behavior in the fault zone, the fault parameters calibrated for the base-case infiltration scenario are checked to

determine whether they are satisfactory for the other two infiltration scenarios. Saturation and water potential matches are slightly affected, but not significantly enough to warrant separate fault parameter sets for each of the infiltration scenarios.

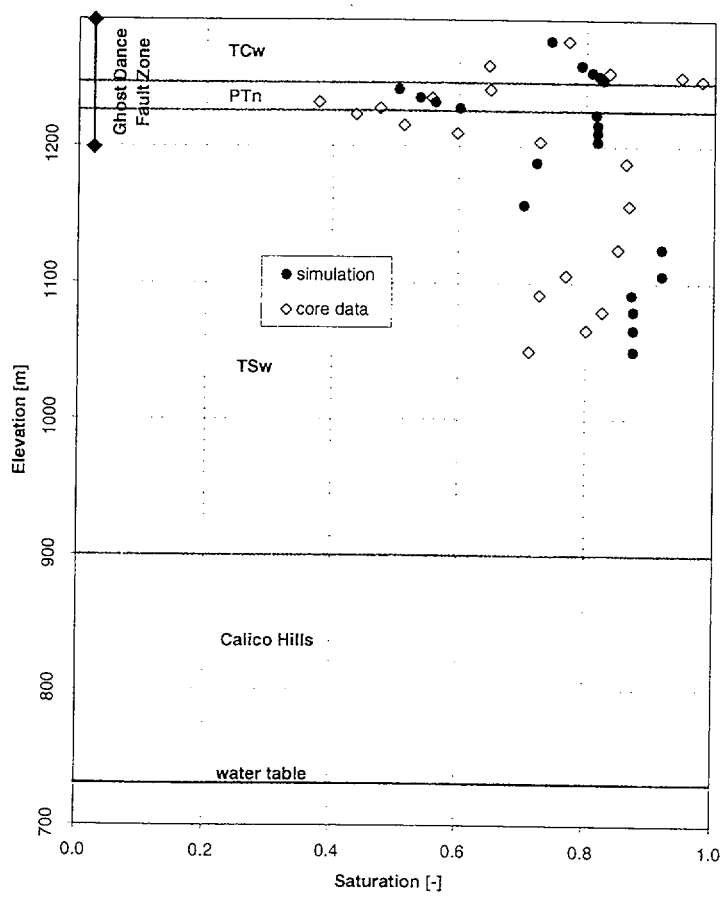
6.3.5 Summary of Two-Dimensional Fault Calibration

The calibrated fault parameter set is presented in Table 20. Matches to the data achieved with this parameter set for USW UZ-7a are shown for saturation in Figure 9, for water potential in Figure 10, and for pneumatic pressure in Figure 11.

Table 20. Calibrated Fault Parameters from Two-Dimensional Inversion of Saturation, Water Potential, and Pneumatic Data

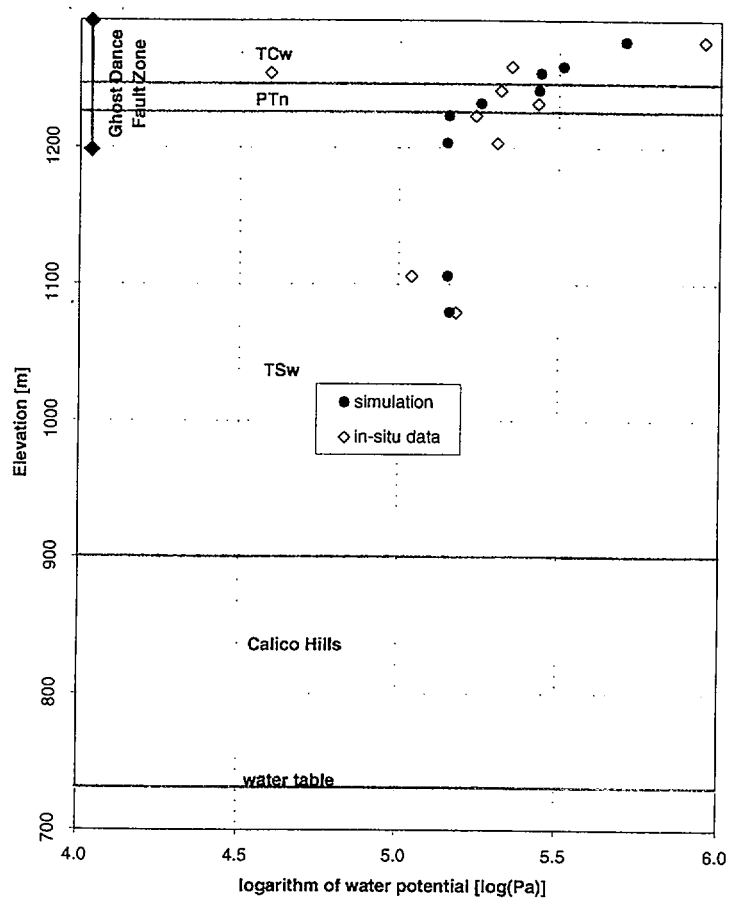
Model Layer	k_M (m^2)	α_M (1/Pa)	m_M (-)	k_F (m^2)	α_F (1/Pa)	m_F (-)	γ (-)
Tcwf	4.97E-19	9.92E-6	0.181	8.88E-11	3.80E-3	0.633	0.30
Ptnf	1.21E-13	3.71E-5	0.254	2.37E-11	2.80E-3	0.633	0.10
Tswf	1.11E-15	6.36E-6	0.401	6.38E-11	1.27E-3	0.633	0.50
Chnf[1]	4.0E-18	9.79E-7	0.386	3.6E-13	2.3E-3	0.633	0.30

NOTE: [1] Note that parameters for layer chnf are not calibrated but are taken directly from DTN: LB990501233129.001.
These data have been developed as documented in this AMR and submitted under DTN: LB991091233129.004.



DTN: LB991091233129.003

Figure 9. Saturation Matches at USW UZ-7a for Two-Dimensional Calibrated Fault Parameter Set for the Base-case Infiltration Scenario



DTN: LB991091233129.003

Figure 10. Water Potential Matches at USW UZ-7a for Two-Dimensional Calibrated Fault Parameter Set for the Base-case Infiltration Scenario

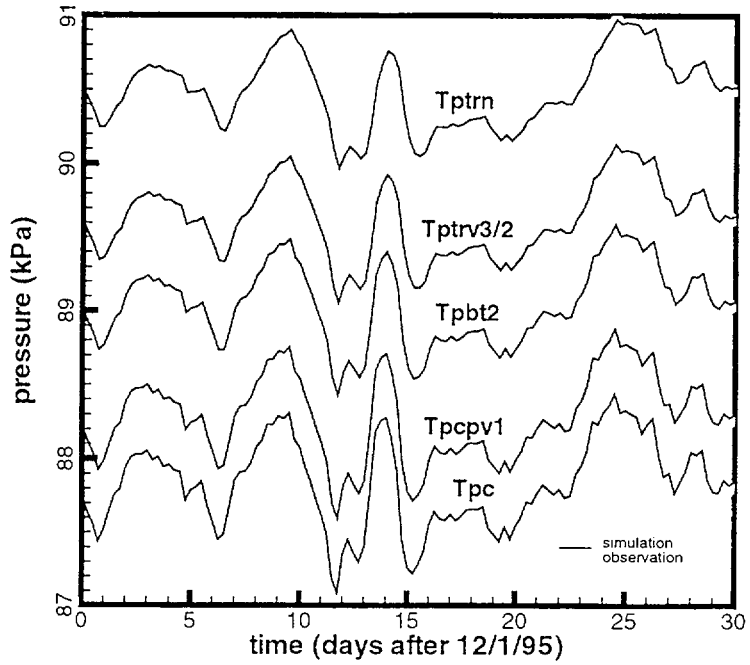


Figure 11. Pneumatic Pressure Matches at USW UZ-7a for Two-Dimensional Calibrated Fault Parameter Set for the Base-case Infiltration Scenario

Though not as extreme a case as the 1-D inversions, the 2-D inversions may still be characterized as overparameterized. Thus, the discussion of uncertainties that was given for the 1-D calibrated properties (see Section 6.1.4) also applies here.

6.4 VALIDATION

Validation activities for the Calibrated Properties Model are carried out within the limited scope of the intended use of the calibrated properties. The calibrated property sets are intended for specific uses as documented in item 11 on the list of conceptual model issues at the beginning of Section 6. The mountain-scale calibrated properties, documented in Sections 6.1 and 6.3, are intended for use in models that simulate or predict flow and transport coupled processes at the mountain scale (hundreds of meters vertically and kilometers horizontally) and across all layers within the UZ. The drift-scale calibrated properties, documented in Section 6.2, are intended to be used more narrowly. They are targeted specifically at simulations and predictions of flow and transport coupled processes at the drift-scale (tens of meters vertically and horizontally) within layers of the proposed repository and those immediately above and below (model layers tsw32, tsw33, tsw34, tsw35, tsw36, and tsw37).

The validity of the Calibrated Properties Model for its intended uses can be partially confirmed by evaluating several criteria:

1. Calibration within experimental data sets.

2. Comparison of predictions using the calibrated property sets and the UZ Flow and Transport Model to data not used in the calibration process.

3. Review of model calibration parameters for reasonableness, or consistency in explanation of all relevant data

4. Technical review through publication in the open literature.

The first criterion is partially met because the property sets documented in this AMR are developed using a calibration methodology. Formation and fault mountain-scale properties are calibrated to saturation data, *in situ* water potential data, pneumatic pressure data, and prior property information. Formation drift-scale properties are calibrated to saturation data, *in situ* water potential data, and prior property information. This criterion is considered only partially met because data are not available for all the ambient conditions (e.g., there are no saturation or water potential data available for fractures).

The second criterion is partially met by favorable comparison of simulation results from the three-dimensional UZ Flow and Transport Model to *in situ* water potential data and pneumatic pressure data that are not the same as those used in the calibration process as documented by CRWMS M&O (2000, U0050, Sections 6.8.2 and 6.8.4, respectively). Additional simulation results from the three-dimensional UZ Flow and Transport Model compare favorably to temperature data and ambient geochemistry data as documented by CRWMS M&O (2000, U0050, Sections 6.3 and 6.4, respectively). This criterion is considered only partially met because the additional *in situ* water potential and pneumatic pressure data do not represent all model layers and because comparisons to the temperature and ambient geochemistry data also involve calibration of other model elements.

The third criterion is partially met because most of the calibrated parameters are consistent with the prior information and for those that are not, the change can be reasonably explained in light of other data. As discussed in Section 6.1.4 and shown in Table 16, there is not a large difference between the prior information and most of the calibrated properties. Fracture permeabilities for the TCw and TSw are the mountain-scale calibrated parameters that have changed most significantly with respect to the prior information. But this change can reasonably be explained as reflecting upscaling from the borehole-scale air-permeability data to the mountain-scale pneumatic pressure data. Large changes in permeability and the van Genuchten α parameter near welded/non-welded interfaces can also be reasonably explained to have occurred because of conceptual model item 10, which requires matrix dominated liquid flow in the unaltered, non-welded layers and fracture dominated flow in the welded layers. Flow behavior at these interfaces is complex. The model geometry and spatial and parameter discretization simplifies these processes, but this requires that the calibrated properties at these interfaces be adjusted to compensate for the simplification. This is one of the important features of a calibrated model. Selected model parameters can be adjusted to compensate for simplifications in other model elements, and thus the model, as a whole, will reproduce the observed behavior. Again this criterion is considered only partially met because the relevant data does not cover all of the processes that are of interest.

The fourth criterion is partially met through the publication in open literature of previous UZ Flow Model calibration efforts (Bandurraga and Bodvarsson 1999; Ahlers et al. 1999) that are essential the same as the methodology used here. This criterion is not considered fully met only because these are from previous studies and not the one documented in this AMR.

The validity of the uncertainties proposed in Section 6.1.4 for the calibrated property sets has not been confirmed.

The evaluation of the four criteria above indicates that the Calibrated Properties Model is partially validated for each criterion. The combination of these confidence-building efforts provides sufficient evidence that these calibrated properties are appropriate for their intended purpose of modeling flow and transport under ambient conditions. Their intended uses, though, also include simulation and prediction of system response for possible future scenarios including changing climate and repository heating. These conditions are not, and could not be, included in the calibration process and thus the appropriateness of the model for these predictions can only be assumed from the performance of the model with respect to ambient conditions.

7. SUMMARY AND CONCLUSIONS

This report has documented the methodologies and the data used for developing rock property sets for three infiltration maps. Validation of these property sets will be documented in a future AMR supporting the Unsaturated Zone Flow and Transport PMR.

Model calibration is an important step in dealing with the upscaling issue. Although some hydrogeologic property data (prior information) are available, these data cannot be directly used to predict flow and transport processes because they were measured on scales smaller than those characterizing property distributions in models used for the prediction. Since model calibrations were done directly on the scales of interest, the upscaling issue was automatically considered. On the other hand, joint use of data and the prior information in inversions can further increase the reliability of the developed parameters compared with those for the prior information.

Rock parameter sets were developed for both the site and drift scales because of the scale-dependent behavior of fracture permeability. Note that these parameter sets, except those for faults, were determined based on the 1-D assumption. Therefore, they cannot be directly used for modeling lateral flow because of perched water in the unsaturated zone of Yucca Mountain. Modification of the parameter sets to consider the perched water effects will be reported in a future AMR supporting the UZ Flow and Transport PMR.

As discussed above in Sections 6.1.4, 6.2, and 6.3.5, uncertainties for these calibrated properties are difficult if not impossible to accurately determine on account of the inaccuracy of simplified methods for this complex problem or to the extremely large computational expense of more rigorous methods. One estimate of uncertainty that may be useful to investigators using these properties is the uncertainty used for the prior information. In most cases, the inversions did not change the properties very much with respect to the prior information.

All TBV inputs are expected to be verified in their current form, so there will be no impact on this model from verification activities.

The calibrated properties documented in and submitted with this AMR represent the best estimates based on the available data. However, as has been repeatedly discussed, the number of parameters being estimated makes this a very complex problem, one that could only be improved by more data and/or increased discretization of the numerical model. Two recommendations are directly attributable to this. First, more data is needed at the repository level and below. Data on ambient flow in fractures is one of the most under-represented data types, and their inclusion would vastly improve the inversions. Second, increased discretization of the numerical models would allow comparison of model predictions to data on a much finer scale. However, the limits of computational speed are already being pushed for the UZ Model, so this avenue can only be pursued as faster computers become available.

Future validation exercises and/or sensitivity studies in support of the UZ Flow and Transport PMR should consider the use of Monte Carlo simulations to evaluate the appropriateness of using the prior information uncertainty for the calibrated properties.

This document may be affected by technical product input information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the DIRS database.

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SOFTWARE CITED

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Software Routine: factorOBJ V1.0. ACC: MOL.19991011.0223

Software Routine: inf V1.0. ACC: MOL.19991021.0465

Software Routine: TBgas3D V1.1. ACC: MOL.19991012.0222.

Software Routine: e9-3in V1.0. STN: 10126-1.0-00.

Software Code: infil2grid V1.6. STN: 10077-1.6-00.

Software Code: ITOUGH2 V3.2. STN: 10054-3.2-00.

Software Code: TOUGH2 V1.4. STN: 10007-1.4-01.

8.2 CODES, STANDARDS, REGULATIONS AND PROCEDURES

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8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

GS000399991221.001. Water Potential Data from Heat Dissipation Probes in ECRB Holes for the Topopah Spring Lower Nonlithophysal, Stations 23+50 to 25+85.7. Submittal Date: 03/09/2000.

GS000399991221.002. Rainfall/Runoff/Runon 1999 Simulations. Submittal date: 3/10/2000

GS000399991221.004. Preliminary Developed Matrix Properties. Submittal date: 3/10/2000.

GS950208312232.003. Data, Including Water Potential, Pressure and Temperature, Collected from Boreholes USW NRG-6 and USW NRG -7a from Instrumentation through March 31, 1995. Submittal date: 02/13/1995.

GS951108312232.008. Data, Including Water Potential, Pressure and Temperature, Collected from Boreholes UE-25 UZ#4 & UZ#5 from Instrumentation through September 30, 1995, and from USW NRG-6 & NRG-7a from April 1 through September 30, 1995. Submittal date: 11/21/1995.

GS960208312261.001. Shut-In Pressure Test Data from April 1995 to December 1995 from Select Wells and Boreholes at Yucca Mountain, NV. Submittal date: 02/07/1996.

GS960308312232.001. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, USW NRG-6, UE-25 UZ#4, UE-25 UZ#5, USW

UZ-7A, and USW SD-12 for the Time Period 10/01/95 through 3/31/96. Submittal date: 04/04/1996.

GS960808312232.004. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data for Boreholes USW NRG-7A, USW N RG-6, UE-25, UZ#4, UE-25 UZ#5, USW UZ-7A and USW SD-12 for the Time Period 4/1/96 through 8/15/96. Submittal date: 08/30/1996.

GS960908312261.004. Shut-in Pressure Test Data from UE-25 NRG#5 and USW SD-7 from November, 1995 to July, 1996. Submittal date: 09/24/1996.

GS970108312232.002. Deep Unsaturated Zone, Surface-Based Borehole Instrumentation Program - Raw Data Submittal for Boreholes USW NRG-7A, USW NRG-6, UE-25 UZ#4, UE-25 UZ#5, USW UZ-7A, and USW SD-12, for the Period 8/16/96 through 12/31/96. Submittal date: 01/22/1997.

GS970808312232.005. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ#4, UE-25 UZ#5, USW UZ-7A and USW SD-12 for the Time Period 1/1/97-6/30/97. Submittal date: 08/28/1997.

GS971108312232.007. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ #4, UE-25 UZ #5, USW UZ-7A and USW SD-12 for the Time Period 7/1/97-9/30/97. Submittal date: 11/18/1997.

GS980408312232.001. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ #4, USW NRG-6, UE-25 UZ #5, USW UZ-7A and USW SD-12 for the Time Period 10/01/97-03/31/98. Submittal date: 04/16/1998.

GS980708312242.010. Physical Properties of Borehole Core Samples, and Water Potential Measurements Using the Filter Paper Technique, for Borehole Samples from USW WT-24. Submittal date: 07/27/1998.

GS980808312242.014. Physical Properties of Borehole Core Samples and Water Potential Measurements Using the Filter Paper Technique for Borehole Samples from USW SD-6. Submittal date: 08/11/1998.

LB990501233129.001. Fracture Properties for the UZ Model Grids and Uncalibrated Fracture and Matrix Properties for the UZ Model Layers for AMR U0090, "Analysis of Hydrologic Properties Data." Submittal date: 08/25/1999.

LB990501233129.002. 1-D Grids for Hydrogeologic Property Set Inversions and Calibrations for AMR U0000, "Development of Numerical Grids for UZ Flow and Transport Modeling." Submittal date: 09/24/1999.

LB990501233129.003. 2-D East-West Cross-Sectional Grid for Borehole UZ-7a and Ghost Dance Fault for AMR U0000, "Development of Numerical Grids for UZ Flow and Transport Modeling." Submittal date: 09/24/1999.

LB991091233129.005. Hydrologic Properties Data - Number of Matrix Permeability Non Detects for AMR U0090, "Analysis of Hydrologic Properties Data." Submittal date: 10/22/1999.

8.4 OUTPUT DATA, LISTED BY DATA TRACKING NUMBER

LB997141233129.001. Calibrated Basecase Infiltration 1-D Parameter Set for the UZ Flow and Transport Model, FY99. Submittal date: 07/21/1999.

LB997141233129.002. Calibrated Upper-Bound Infiltration 1-D Parameter Set for the UZ Flow and Transport Model, FY99. Submittal date: 07/21/1999.

LB997141233129.003. Calibrated Lower-Bound Infiltration 1-D Parameter Set for the UZ Flow and Transport Model, FY99. Submittal date: 07/21/1999.

LB990861233129.001. Drift Scale Calibrated 1-D Property Set, FY99. Submittal date: 08/06/1999.

LB990861233129.002. Drift Scale Calibrated 1-D Property Set, FY99. Submittal date: 08/06/1999.

LB990861233129.003. Drift Scale Calibrated 1-D Property Set, FY99. Submittal date: 08/06/1999.

LB991091233129.001. One-Dimensional, Mountain-Scale Calibration for AMR U0035, "Calibrated Properties Model." Submittal date: 10/22/1999.

LB991091233129.002. One-Dimensional, Drift-Scale Calibration for AMR U0035, "Calibrated Properties Model." Submittal date: 10/22/1999.

LB991091233129.003. Two-Dimensional, Fault Calibration for AMR U0035, "Calibrated Properties Model." Submittal date: 10/22/1999.

LB991091233129.004. Calibrated Fault Properties for the UZ Flow and Transport Model for AMR U0035, "Calibrated Properties Model." Submittal date: 10/22/1999.t

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9. ATTACHMENTS

Attachment I - Document Input Reference Sheet

Attachment II - Technical Data Information Form

Attachment III - Input and Output Files used in the Modeling

Attachment IV - Software Routines

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ATTACHMENT I-DOCUMENT INPUT REFERENCE SHEET

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

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
2a									
1.	DTN: GS000399991221.001. Water Potential Data from Heat Dissipation Probes in ECRB Holes for the Topopah Spring Lower Nonlithophysal. Stations 23+50 to 25+85.7. Submittal Date: 03/09/2000.	Entire	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2	Water potential data from heat dissipation probes in the ECRB.	N/A	N/A	N/A	N/A
2.	DTN: GS000399991221.002. Rainfall/Runoff/Runon 1999 Simulations. Submittal date: 3/10/2000.	base-case, lower bound and upper bound present day simulation	N/A-Qualified-Verification Level 2	4.1.1 6.1.1 6.3.1	Infiltration data	N/A	N/A	N/A	N/A
3.	DTN: GS000399991221.004. Preliminary Developed Matrix Properties. Submittal date: 3/10/2000.	Saturation	N/A-Qualified-Verification Level 2	4.1.2.1 6.1.2 6.3.2	Saturation data from USW SD-7, USW SD-9, USW SD-12, USW UZ-14, UE-25 UZ-16, and USW UZ-7a	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
4.	DTN: GS950208312232.003. Data, including Water Potential, Pressure and Temperature, Collected from Boreholes USW NRG-6 and USW NRG -7a from Instrumentation through March 31, 1995. Submittal date: 02/13/1995.	Water potential and pressure	N/A-Qualified-Verification Level 2	4.1.2.2 4.1.2.3 6.1.1	Water potential from USW NRG-6 and USW NRG-7a; pressure from USW NRG-6 and USW NRG-7a	N/A	N/A	N/A	N/A
5.	DTN: GS951108312232.008. Data, including Water Potential, Pressure and Temperature, Collected from Boreholes UE-25 UZ#4 & UZ#5 from Instrumentation through September 30, 1995, and from USW NRG-6 & NRG-7a from April 1 through September 30, 1995. Submittal date: 11/21/1995.	Water potential and pressure	N/A-Qualified-Verification Level 2	4.1.2.2 4.1.2.3 6.1.1	Water potential from USW NRG-6 and USW NRG-7a; pressure from USW NRG-6 and USW NRG-7a	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
6.	DTN: GS960208312261.001. Shut-in Pressure Test Data from April 1995 to December 1995 from Select Wells and Boreholes at Yucca Mountain, NV. Submittal date: 02/07/1996.	UE-25 NRG#5 data	N/A-Qualified-Verification Level 2	4.1.2.3 6.1.2	Pressure from UE-25 NRG#5	N/A	N/A	N/A	N/A
7.	DTN: GS960308312232.001. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, USW NRG-6, UE-25 UZ#4, UE-25 UZ#5, USW UZ-7A, and USW SD-12 for the Time Period 10/01/95 through 3/31/96. Submittal date: 04/04/1996.	Water potential and pressure	N/A-Qualified-Verification Level 2	4.1.2.2 4.1.2.3 6.1.1 6.1.2 6.3.1 6.3.2	Water potential from USW NRG-6, USW NRG-7a, and UE-25 UZ#4; pressure from USW NRG-6, USW NRG-7a, USW SD-12, and USW UZ-7a	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
8.	DTN: GS960808312232.004. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data for Boreholes USW NRG-7A, USW N RG-6, UE-25, UZ#4, UE-25 UZ#5, USW UZ-7A and USW SD-12 for the Time Period 4/1/96 through 8/15/96. Submittal date: 08/30/1996.	Water potential	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2	Water potential from USW NRG-6, USW NRG-7a, UE-25 UZ#4, and USW SD-12	N/A	N/A	N/A	N/A
9.	DTN: GS960908312261.004. Shut-in Pressure Test Data from UE-25 NRG#5 and USW SD-7 from November, 1995 to July, 1996. Submittal date: 09/24/1996.	USW SD-7 data	N/A-Qualified-Verification Level 2	4.1.2.3 6.1.2	Pressure from USW SD-7	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
10.	DTN: GS970108312232.002. Deep Unsaturated Zone, Surface-Based Borehole Instrumentation Program - Raw Data Submittal for Boreholes USW NRG-7A, USW NRG-6, UE-25 UZ#4, UE-25 UZ#5, USW UZ-7A, and USW SD-12, for the Period 8/16/96 through 12/31/96. Submittal date: 01/22/1997.	Water potential	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2	Water potential from USW NRG-6, USW NRG-7a, UE-25 UZ#4, and USW SD-12	N/A	N/A	N/A	N/A
11.	DTN: GS970808312232.005. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ#4, UE-25 UZ#5, USW UZ-7A and USW SD-12 for the Time Period 1/1/97–6/30/97. Submittal date: 08/28/1997.	Water potential	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2 6.3.2	Water potential from USW NRG-6, USW NRG-7a, UE-25 UZ#4, USW SD-12, and USW UZ-7a	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
12.	DTN: GS971108312232.007. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ #4, UE-25 UZ #5, USW UZ-7A and USW SD-12 for the Time Period 7/1/97–9/30/97. Submittal date: 11/18/1997.	Water potential	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2 6.3.2	Water potential from USW NRG-6, USW NRG-7a, UE-25 UZ#4, USW SD-12, and USW UZ-7a	N/A	N/A	N/A	N/A
13.	DTN: GS980408312232.001. Deep Unsaturated Zone Surface-Based Borehole Instrumentation Program Data from Boreholes USW NRG-7A, UE-2 5 UZ #4, USW NRG-6, UE-25 UZ #5. USW UZ-7A and USW SD-12 for the Time Period 10/01/97–03/31/98. Submittal date: 04/16/1998.	Water potential	N/A-Qualified-Verification Level 2	4.1.2.2 6.1.2 6.3.2	Water potential from USW NRG-6, USW NRG-7a, UE-25 UZ#4, USW SD-12, and USW UZ-7a	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
14.	DTN: GS980708312242.010. Physical Properties of Borehole Core Samples, and Water Potential Measurements using the Filter Paper Technique, for Borehole Samples from USW WT-24. Submittal date: 07/27/1998.	Saturation	N/A-Qualified-Verification Level 2	4.1.2.1 6.1.2	Saturation from USW WT-24	N/A	N/A	N/A	N/A
15.	DTN: GS980808312242.014. Physical Properties of Borehole Core Samples and Water Potential Measurements using the Filter Paper Technique for Borehole Samples from USW SD-6. Submittal date: 08/11/1998.	Saturation	N/A-Qualified-Verification Level 2	4.1.2.1 6.1.2	Saturation from USW SD-6	N/A	N/A	N/A	N/A

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1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
16.	DTN: LB990501233129.001. Fracture Properties for the UZ Model Grids and Uncalibrated Fracture and Matrix Properties for the UZ Model Layers for AMR U0090, "Analysis of Hydrologic Properties Data." Submittal date: 08/25/1999.	Entire	TBV-3168	Table 3 Table 4 4.1.1 6 6.1.1 6.3.1	Fracture and matrix permeability, standard deviation of permeability data, number of permeability data, matrix porosity, fracture and matrix van Genuchten *a* and *m* parameters, standard error of matrix *m* parameter estimate, matrix residual and satiated saturation, fracture frequency, standard deviation of frequency data, number of frequency data	1	N/A	N/A	✓
17.	DTN: LB990501233129.002. 1-D Grids for Hydrogeologic Property Set Inversions and Calibrations for AMR U0000, "Development of Numerical Grids for UZ Flow and Transport Modeling." Submittal date: 09/24/1999.	Entire	TBV-	4.1.1 6.1 6.1.1 6.2	1-D grid for steady-state simulations (1doldstdyst.mesh) and for transient simulations (1doldtrans.mesh)	1	✓	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
18.	DTN: LB990501233129.003. 2-D East-West Cross-Sectional Grid for Borehole UZ-7a and Ghost Dance Fault for AMR U0000, "Development of Numerical Grids for UZ Flow and Transport Modeling." Submittal date: 09/24/1999.	Entire	TBV-	4.1.1 6.3.1	2-D grid for steady-state simulations (2d2kstdyst.mesh) and for transient simulations (2d2ktrans.mesh)	1	✓	N/A	N/A
19.	DTN: LB991091233129.005. Hydrologic Properties Data - Number of Matrix Permeability Non Detects For AMR U0090, "Analysis of Hydrologic Properties Data." These Data are also Associated with AMR U0035, "Calibrated Properties Model." Submittal date: 10/22/1999. Initial use.	Entire	TBV-3536	Table 3 6.2	Number of non detect permeability data	1	N/A	N/A	✓

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
20.	Ahlers, C.F.; Finsterle, S.; and Bodvarsson, G.S. 1998. "Characterization and Prediction of Subsurface Pneumatic Pressure Variations at Yucca Mountain, Nevada." *Proceedings of the TOUGH2 Workshop '98*, 222-227. Report LBNL-41995 . Berkeley, California: Lawrence Berkeley National Laboratory. ACC: MOL.19980713.0595.	p. 224	N/A-Reference only	5 6.1.1	30 day initialization period for pneumatic (barometric pumping) simulations	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
21.	Ahlers, C.F.; Finsterle, S.; and Bodvarsson, G.S. 1999. "Characterization and Prediction of Subsurface Pneumatic Pressure Variations at Yucca Mountain, Nevada." *Journal of Contaminant Hydrology, 38* (1–3), 47–68. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	Entire	N/A-Reference only	6.4	Yucca Mountain pneumatic data inversion	N/A	N/A	N/A	N/A
22.	Bandurraga, T.M. and Bodvarsson, G.S. 1999. "Calibrating Hydrogeologic Parameters for the 3-D Site-Scale Unsaturated Zone Model of Yucca Mountain, Nevada." *Journal Of Contaminant Hydrology, 38* (1–3), 25–46. Amsterdam, The Netherlands: Elsevier Science Publishers. TIC: 244160.	Entire	N/A-Reference only	6.4	Yucca Mountain UZ Model calibration	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
23.	Bird, R.B.; Stewart, W.E.; and Lightfoot, E.N. 1960. *Transport Phenomena*. New York, New York: John Wiley. TIC: 208957.	pp. 648–649, 505, 744	N/A – Reference only	6.1.2	Equations for evaporation from a spherical water drop, mass transfer coefficient of water in air, and effective binary diffusivity Molecular weight and critical temperature and pressure of air	N/A	N/A	N/A	N/A
24.	Brooks, R.H. and Corey, A.T. 1966. "Properties of Porous Media Affecting Fluid Flow." *Journal of Irrigation and Drainage Division: Proceedings of the American Society of Civil Engineers, 92* (IR2), 61–88. Washington, DC: American Society of Civil Engineers. TIC: 216867.	p. 71	N/A – Reference only	6	Equation for relative permeability of air	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
25.	CRWMS M&O (Civilian Radioactive Waste Management System Management & Operating Contractor) 1999a. *M&O Site Investigations.* Activity Evaluation, January 23, 1999. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990317.0330.	Entire	N/A – Reference only	2	Activity Evaluation	N/A	N/A	N/A	N/A
26.	CRWMS M&O 1999b. *M&O Site Investigations.* Activity Evaluation. September 28, 1999. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990928.0224.	Entire	N/A – Reference only	2	Activity Evaluation	N/A	N/A	N/A	N/A
27.	CRWMS M&O 1999c. *Analysis & Modeling Development Plan (DP) for U0035 Calibrated Properties Model Data, Rev 00.* TDP-NBS-HS-000004. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990830.0376.	Entire	N/A – Reference only	1 2	Plan	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
28.	CRWMS M&O 1999d. *Development of Numerical Grids for UZ Flow and Transport Modeling.* ANL-NBS-HS-000015. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990721.0517.	Table 10, Figure 1, attachments III and IV p. 48-52	N/A – Reference only	Table 5 Figure 1 6 6.1	FY99 UZ Model Layers and their relationship to other geologic and hydrogeologic layering definitions; borehole locations; grid generation documentation.	N/A	N/A	N/A	N/A
29.	CRWMS M&O 2000. *UZ Flow Models and Submodels.* MDL-NBS-HS-000006. Las Vegas, Nevada: CRWMS M&O. URN: 0030. ACC: MOL.19990721.0527.	Sec. 6.3 6.4 6.8.2 6.8.4	N/A-Reference only	6.4	Comparison of UZ Flow Model predictions to ambient geochemistry data, temperature data, *in situ* water potential data, and pneumatic pressure data.	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
30.	Dyer, J.R. 1999. "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada." Letter from J.R. Dyer (DOE) to D.R. Wilkins (CRWMS M&O), September 9, 1999, OL&RC: SB-1714, with enclosure, "Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Rev. 01)." ACC: MOL.19990910.0079.	Entire	N/A – Reference only	4.2	Interim Guidance	N/A	N/A	N/A	N/A
31.	Finsterle, S. 1998. *ITOUGH2 V3.2 Verification and Validation Report*. Report LBNL-42002. Berkeley, California: Lawrence Berkeley National Laboratory. ACC: MOL.19981008.0014.	Entire	N/A – Reference only	6 6.1.3.1	ITOUGH2 v.3.2 use	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
32.	Finsterle, S. 1999. *ITOUGH2 User's Guide.* Report LBNL-40040. Berkeley, California: Lawrence Berkeley National Laboratory. TIC: 243018.	Entire	N/A – Reference only	6 6.1.3.1	ITOUGH2 v.3.2 use	N/A	N/A	N/A	N/A
33.	Flint, L.E. 1998. *Characterization of Hydrogeologic Units Using Matrix Properties, Yucca Mountain, Nevada.* Water Resources Investigations Report 97-4243. Denver, Colorado: U.S. Geological Survey. TIC: 236515.	pp. 11, 17-19	N/A – Reference only	6.1 6.1.2	Description of measurement error for bulk properties, core dimensions, core handling time	N/A	N/A	N/A	N/A
34.	Liu, H.H.; Doughty, C.; and Bodvarsson, G.S. 1998. "An Active Fracture Model for Unsaturated Flow and Transport in Fractured Rocks." *Water Resources Research, 34* (10), 2633–2646. Washington, D.C.: American Geophysical Union. TIC: 243012.	Entire	N/A – Reference only	6	Active fracture model	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
35.	Neuman, S.P. 1994. "Generalized Scaling of Permeabilities: Validation and Effect of Support Scale." *Geophysical Research Letters, 21* (5), 349–352. Washington, D.C.: American Geophysical Union. TIC: 240142.	Entire	N/A – Reference only	6.2	Scale-dependent behavior of permeability	N/A	N/A	N/A	N/A
36.	Roberson, J.A.; and Crowe, C.T. 1990. *Engineering Fluid Mechanics*. Boston, Massachusetts: Houghton Mifflin Company. TIC: on order.	p. A-22	N/A – Reference only	6.1.2	Density and viscosity of air	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
37.	Rousseau, J.P.; Loskot, C.L.; Thamir, F.; and Lu, N. 1997. *Results of Borehole Monitoring in the Unsaturated Zone within the Main Drift Area of the Exploratory Studies Facility, Yucca Mountain, Nevada*. Milestone Report SPH22M3. Denver, Colorado: U.S. Geological Survey. TIC: 238150.	p. 31	N/A – Reference only	6.1.2	Lack of pneumatic isolation of instrument station C in USW SD-12	N/A	N/A	N/A	N/A
38.	Rousseau, J.P.; Kwicklis, E.M.; and Gillies, D.C., eds. 1999. *Hydrogeology of the Unsaturated Zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, Nevada*. Water Resources Investigations Report 98-4050. Denver, Colorado: U.S. Geological Survey. ACC: MOL.19990419.0335.	pp. 125, 143-151, 129-131	N/A – Reference only	4.1.2 6.1.2	Sources of error for measurements of saturation on core and measurements of water potential *in situ*	N/A	N/A	N/A	N/A

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DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
39.	van Genuchten, M. 1980. "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils." *Soil Science Society of America Journal, 44* (5), 892–898. Madison, Wisconsin: Soil Science Society of America. TIC: 217327.	pp. 892-893	N/A – Reference only	6	Relative permeability and water potential relationships; relationship of van Genuchten *m* parameter to Brooks Corey λ parameter	N/A	N/A	N/A	N/A
40.	Weast, R.C., ed. 1987. *CRC Handbook of Chemistry and Physics: 1987-1988 68th Edition.* Boca Raton, Florida: CRC Press. TIC: 245444.	pp. B-94, F-66, D-190	N/A – Reference only	6.1.2	Molecular weight, critical temperature and pressure, and vapor pressure of water	N/A	N/A	N/A	N/A
41.	Wemheuer, R.F. 1999. "First Issue of FY00 NEPO QAP-2-0 Activity Evaluations." Interoffice correspondence from R.F. Wemheuer (CRWMS M&O) to R.A. Morgan (CRWMS M&O), October 1, 1999, LV.NEPO.RTPS.TAG.10/99-155, with attachments, Activity Evaluation for Work Package #1401213UM1. ACC: MOL.19991028.0162.	Work Package #1401213UM1	N/A – Reference only	2	Activity Evaluation	N/A	N/A	N/A	N/A

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SHEET

1. Document Identifier No./Rev.: MDL-NBS-HS-000003/00			Change:	Title: Calibrated Properties Model					
Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBV Due To		
2. Technical Product Input Source Title and Identifier(s) with Version		3. Section					Unqual.	From Uncontrolled Source	Un-confirmed
42.	Software Routine: aversp_I V1.0. ACC: MOL.19991011.0222.	Entire	N/A-Qualified/ Verfied/ Confirmed	6.1.2	Software for averaging data	N/A	N/A	N/A	N/A
43.	Software Routine: factorOBJ V1.0. ACC: MOL.19991011.0223.	Entire	N/A-Qualified/ Verfied/ Confirmed	6.1.3.2	Comparison of pneumatic data with simulation results	N/A	N/A	N/A	N/A
44.	Software Routine: TBgas3D V1.1. ACC: MOL.19991012.0222.	Entire	N/A-Qualified/ Verfied/ Confirmed	6.3.1	Pneumatic boundary condition file generation	N/A	N/A	N/A	N/A
45.	Software Routine: e9-3in V1.0. STN: 10126-1.0-00.	Entire	N/A-Qualified/ Verfied/ Confirmed	6	Conversion of EOS9 format initial conditions to EOS3 format	N/A	N/A	N/A	N/A
46.	Software Code: infil2grid V1.6. STN: 10077-1.6-00.	Entire	N/A-Qualified/ Verfied/ Confirmed	6.3.1	Infiltration boundary condition file generation	N/A	N/A	N/A	N/A
47.	Software Code: ITOUGH2 V3.2. STN: 10054-3.2-00.	Entire	N/A-Qualified/ Verfied/ Confirmed	6	Multiphase flow simulation and data inversion	N/A	N/A	N/A	N/A
48.	Software Code: TOUGH2 V1.4. STN: 10007-1.4-01.	Entire	N/A-Qualified/ Verfied/ Confirmed	6	Multiphase flow simulation	N/A	N/A	N/A	N/A
49.	Software Routine: inf V1.0. ACC: MOL.19991021.0465	Entire	N/A-Qualified/ Verfied/ Confirmed	6.1.1	Infiltration boundary condition calculation	N/A	N/A	N/A	N/A

AP-3.15Q.1 Rev. 06/30/1999

ATTACHMENT II–TECHNICAL DATA INFORMATION FORM

308692

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION FORM

Page 1 of 2

☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB997141233129.001

Preliminary Data: ____

PART I Identification of Data

Title of Data: CALIBRATED BASECASE INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99.

Description of Data: CALIBRATED BASECASE INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99. (THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.001.)

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 7/14/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PARAMETER SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES. THIS PARAMETER SET IS ALSO BASED UPON TWO UPCOMING DATA SETS: LB990501233129.001 AND LB990501233129.002 AND DATA SETS FROM USGS WITH

Checked by: Suzanne M. Link July 21, 1999
Signature Date

AP-SIII.3Q

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YMP-023-R6
04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
CONTINUATION SHEET

Page 2 of 2

Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014

Comments (continued)

DATA TRACKING NUMBERS TO BE DETERMINED (TBD). THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.001; A CORRECTION WAS MADE TO THE DATA IN DTN LB990601233129.001, THUS NECESSITATING THIS SUPERSEDE.

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION FORM

Page 1 of 2

☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB997141233129.002

Preliminary Data: ____

PART I Identification of Data

Title of Data: CALIBRATED UPPER-BOUND INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99.

Description of Data: CALIBRATED UPPER-BOUND INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99. (THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.002.)

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 7/14/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PARAMETER SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES. THIS PARAMETER SET IS ALSO BASED UPON TWO UPCOMING DATA SETS: LB990501233129.001 AND LB990501233129.002 AND DATA SETS FROM USGS WITH

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Signature Date

AP-SIII.3Q

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
CONTINUATION SHEET

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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014

Comments (continued)

DATA TRACKING NUMBERS TO BE DETERMINED (TBD). THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.002; A CORRECTION WAS MADE TO THE DATA IN DTN LB990601233129.002, THUS NECESSITATING THIS SUPERSEDE.

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT TECHNICAL DATA INFORMATION FORM

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☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB997141233129.003

Preliminary Data: ____

PART I Identification of Data

Title of Data: CALIBRATED LOWER-BOUND INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99.

Description of Data: CALIBRATED LOWER-BOUND INFILTRATION 1-D PARAMETER SET FOR THE UZ FLOW AND TRANSPORT MODEL, FY99. (THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.003.)

Data Originator/Preparer: WU, Y S (Last Name / First and Middle Initials)

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 7/14/1999 (From: MM/DD/YY To: MM/DD/YY)

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PARAMETER SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES. THIS PARAMETER SET IS ALSO BASED UPON TWO UPCOMING DATA SETS: LB990501233129.001 AND LB990501233129.002 AND DATA SETS FROM USGS WITH

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
CONTINUATION SHEET

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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014

Comments (continued)

DATA TRACKING NUMBERS TO BE DETERMINED (TBD). THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB990601233129.003; A CORRECTION WAS MADE TO THE DATA IN DTN LB990601233129.003, THUS NECESSITATING THIS SUPERSEDE.

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION FORM

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☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB990861233129.001

Preliminary Data: ____

PART I Identification of Data

Title of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99.

Description of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99: BASECASE INFILTRATION. (THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.001.)

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 8/3/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PROPERTY SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES FOR BASECASE INFILTRATION. THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.001; A CORRECTION WAS MADE TO THE DATA IN

Checked by: Suzanne M. Link August 6, 1999
Signature Date

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014
LB997141233129.001

Comments (continued)

DTN LB997211233129.001, THUS NECESSITATING THIS SUPERSEDE.

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION FORM

Page 1 of 2

☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB990861233129.002

Preliminary Data: ____

PART I Identification of Data

Title of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99.

Description of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99: UPPER BOUND INFILTRATION.
(THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.002.)

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 8/3/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PROPERTY SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES FOR UPPER BOUND INFILTRATION. THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.002; A CORRECTION WAS MADE TO THE DATA

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Signature Date

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04/99

YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
CONTINUATION SHEET

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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014
LB997141233129.002

Comments (continued)

IN DTN LB997211233129.002, THUS NECESSITATING THIS SUPERSEDE.

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04/99

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Page 1 of 2

☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LB990861233129.003

Preliminary Data: ____

PART I Identification of Data

Title of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99.

Description of Data: DRIFT SCALE CALIBRATED 1-D PROPERTY SET, FY99: LOWER BOUND INFILTRATION. (THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.003.)

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☒ Q ☐ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: CALIBRATED PROPERTIES MODEL USING ITOUGH2, VERSION 3.2 SOFTWARE.

Location(s): LBNL

Period(s): 10/1/1998 to 8/3/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

THIS PROPERTY SET INCLUDES BOTH FRACTURE AND MATRIX PROPERTIES FOR LOWER BOUND INFILTRATION. THESE DATA SUPERSEDE DATA PREVIOUSLY IDENTIFIED BY DTN LB997211233129.003; A CORRECTION WAS MADE TO THE DATA

Checked by: Suzanne M. Link August 6, 1999
Signature Date

AP-SIII.3Q

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04/99

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TECHNICAL DATA INFORMATION
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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014
LB997211233129.003

Comments (continued)

IN DTN LB997211233129.003, THUS NECESSITATING THIS SUPERSEDE.

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04/99

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TECHNICAL DATA INFORMATION FORM

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☐ ACQUIRED DATA

☒ DEVELOPED DATA

DRAFT

DTN: LB$91091233129.001

Preliminary Data: ____

PART I Identification of Data

Title of Data: ONE-DIMENSIONAL, MOUNTAIN-SCALE CALIBRATION FOR AMR U0035, "CALIBRATED PROPERTIES MODEL."

Description of Data: FILES SUPPORTING 1-D, MOUNTAIN-SCALE CALIBRATION, AMR U0035, MDL-NBS-HS-000003, MOL.19990721.0520. SR/LA SUPPORTING DATA.

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☐ Q ☒ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: ITOUGH2, V.3.2

Location(s): LBNL

Period(s): 10/1/1998 to 9/1/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960308312232.001	GS970108312232.002
GS951108312232.008	GS960808312232.004	GS970808312232.005
GS960208312261.001	GS960908312261.004	GS971108312232.007

Comments

ADDITIONAL SOURCE DATA WERE ACQUIRED PER AP 3.14Q UNDER ITN: LBL-USG-99248.T; ITN: LBL-USG-99247.T; ITN: LBL-USG-99323.R.

Checked by: ____ ____
Signature Date

AP-SIII.3Q

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
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Source Data DTN(s) (continued)

GS980408312232.001
GS980708312242.010
GS980808312242.014
LB$91091233129.005
LB990501233129.001
LB990701233129.001

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT TECHNICAL DATA INFORMATION FORM

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☐ ACQUIRED DATA

☒ DEVELOPED DATA

DRAFT

DTN: LB$91091233129.002

Preliminary Data: ____

PART I Identification of Data

Title of Data: ONE-DIMENSIONAL, DRIFT-SCALE CALIBRATION FOR AMR U0035, "CALIBRATED PROPERTIES MODEL."

Description of Data: FILES SUPPORTING 1-D, DRIFT-SCALE CALIBRATION, AMR U0035, MDL-NBS-HS-000003. MOL.19990721.0520. SR/LA SUPPORTING DATA.

Data Originator/Preparer: WU, Y S (Last Name / First and Middle Initials)

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☐ Q ☒ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 1.2.3.3.1.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: ITOUGH2, V.3.2

Location(s): LBNL

Period(s): 10/1/1998 to 9/1/1999 (From: MM/DD/YY To: MM/DD/YY)

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS950208312232.003	GS960808312232.004	GS971108312232.007
GS951108312232.008	GS970108312232.002	GS980408312232.001
GS960308312232.001	GS970808312232.005	GS980708312242.010

Comments

ADDITIONAL SOURCE DATA WERE ACQUIRED PER AP 3.14Q UNDER ITN: LBL-USG-99248.T; ITN: LBL-USG-99247.T; LBL-USG-99323.R.

Checked by: ____ (Signature) ____ (Date)

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
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Source Data DTN(s) (continued)

GS980808312242.014
LB990501233129.001
LB990701233129.001

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DRAFT

☐ ACQUIRED DATA

☒ DEVELOPED DATA

DTN: LBS91091233129.003

Preliminary Data: ____

PART I Identification of Data

Title of Data: TWO-DIMENSIONAL FAULT CALIBRATION FOR AMR U0035, "CALIBRATED PROPERTIES MODEL."

Description of Data: FILES SUPPORTING 2-D FAULT CALIBRATION, AMR U0035, MDL-NBS-HS-000003, MOL.19990721.0520. SR/LA SUPPORTING DATA.

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☐ Q ☒ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: ITOUGH2, V.3.2

Location(s): LBNL

Period(s): 10/10/1998 to 9/1/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS960308312232.001	GS970808312232.005	LB990501233129.001
GS960808312232.004	GS971108312232.007	LB990701233129.001
GS970108312232.002	GS980408312232.001	

Comments

ADDITIONAL SOURCE DATA WERE ACQUIRED PER AP 3.14Q UNDER ITN: LBL-USG-99248.T AND ITN: LBL-USG-99247.T.

Checked by: ____ Signature ____ Date

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION FORM

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☐ ACQUIRED DATA

☒ DEVELOPED DATA

DRAFT

DTN: LB$91091233129.004

Preliminary Data: ____

PART I Identification of Data

Title of Data: CALIBRATED FAULT PROPERTIES FOR THE UZ FLOW AND TRANSPORT MODEL FOR AMR U0035, "CALIBRATED PROPERTIES MODEL."

Description of Data: CALIBRATED FAULT PROPERTIES FOR THE UZ FLOW AND TRANSPORT MODEL, AMR U0035, MDL-NBS-HS-000003, MOL.19990721.0520. SR/LA SUPPORTING DATA.

Data Originator/Preparer: WU, Y S
Last Name First and Middle Initials

Data Originator/Preparer Organization: LAWRENCE BERKELEY NATIONAL LABORATORY

Qualification Status: ☐ Q ☒ Un-Q ☐ Accepted Governing Plan: SCP

SCP Activity Number(s): 8.3.1.2.2.9

WBS Number(s): 1.2.3.3.1.2.9

PART II Data Acquisition/Development Information

Method: ITOUGH2, V.3.2

Location(s): LBNL

Period(s): 10/1/1998 to 9/1/1999
From: MM/DD/YY To: MM/DD/YY

Sample ID Number(s): ____

PART III Source Data DTN(s)

GS960308312232.001	GS970808312232.005	LB990501233129.001
GS960808312232.004	GS971108312232.007	LB9907G1233129.001
GS970108312232.002	GS980408312232.001	

Comments

ADDITIONAL SOURCE DATA WERE ACQUIRED PER AP 3.14Q UNDER ITN: LBL-USG-99248.T AND ITN: LBL-USG-99247.T. UNCALIBRATED HYDROLOGIC AND THERMAL PARAMETERS ARE AVAILABLE UNDER DTN: LB990501233129.001 AND DTN:

Checked by: ____ ____
Signature Date

AP-SIII.2Q

YMP-023-R6
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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT
TECHNICAL DATA INFORMATION
CONTINUATION SHEET

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Comments (continued)

LB991091233129.006.

DRAFT

ATTACHMENT III – INPUT AND OUTPUT FILES USED IN THE MODELING

Table 1. Files supporting the 1-D, mountain-scale, calibrated properties. Files are referenced to scientific notebook page(s) where documented.

File Name	Notebook Number	Notebook Page(s)
sd6sat.txt	YMP-LBNL-GSB-1.1.2	78
sd7sat.txt	YMP-LBNL-GSB-1.1.2	78
sd9sat.txt	YMP-LBNL-GSB-1.1.2	78
sd12sat.txt	YMP-LBNL-GSB-1.1.2	78
uz14sat2.txt	YMP-LBNL-GSB-1.1.2	89
uz16sat.txt	YMP-LBNL-GSB-1.1.2	78
wt24sat.txt	YMP-LBNL-GSB-1.1.2	78
sd6sat.out	YMP-LBNL-GSB-1.1.2	79
sd7sat.out	YMP-LBNL-GSB-1.1.2	79
sd9sat.out	YMP-LBNL-GSB-1.1.2	79
sd12sat.out	YMP-LBNL-GSB-1.1.2	79
uz14sat2.out	YMP-LBNL-GSB-1.1.2	89
uz16sat.out	YMP-LBNL-GSB-1.1.2	79
wt24sat.out	YMP-LBNL-GSB-1.1.2	79
layavsat.xls	YMP-LBNL-GSB-1.1.2	91
in_situ_pcap2.xls	YMP-LBNL-GSB-1.1.2	91
binfl0	YMP-LBNL-GSB-1.1.2	97
binfl0i	YMP-LBNL-GSB-1.1.2	98
binfl0i.out	YMP-LBNL-GSB-1.1.2	98
binfl1	YMP-LBNL-GSB-1.1.2	101
binfl1i	YMP-LBNL-GSB-1.1.2	101
binfl1.sav	YMP-LBNL-GSB-1.1.2	102
binfl1i.out	YMP-LBNL-GSB-1.1.2	102
binfl1i.par	YMP-LBNL-GSB-1.1.2	102
binfl2	YMP-LBNL-GSB-1.1.2	102
binfl2i	YMP-LBNL-GSB-1.1.2	102
binfl2i.out	YMP-LBNL-GSB-1.1.2	102
binfl2i.par	YMP-LBNL-GSB-1.1.2	102
NRG5_133_zone3.txt	YMP-LBNL-GSB-1.1.2	104
NRG5_187_zone4.txt	YMP-LBNL-GSB-1.1.2	104
NRG5_243_zone5.txt	YMP-LBNL-GSB-1.1.2	104
NRG5_298_zone6.txt	YMP-LBNL-GSB-1.1.2	104
NRG5_354_zone7.txt	YMP-LBNL-GSB-1.1.2	104
NRG5_799_zone13.txt	YMP-LBNL-GSB-1.1.2	104
NRG6_130_PT737.txt	YMP-LBNL-GSB-1.1.2	104
NRG6_180_PT731.txt	YMP-LBNL-GSB-1.1.2	104
NRG6_280_PT725.txt	YMP-LBNL-GSB-1.1.2	104

DTN: LB991091233129.001

Table 1. Files supporting the 1-D, mountain-scale, calibrated properties. Files are referenced to scientific notebook page(s) where documented. (Cont.)

File Name	Notebook Number	Notebook Page(s)
NRG6_720_PT701.txt	YMP-LBNL-GSB-1.1.2	104
nrg7a_18_PT425.txt	YMP-LBNL-GSB-1.1.2	104
nrg7a_153_PT420.txt	YMP-LBNL-GSB-1.1.2	104
nrg7a_388_PT413.txt	YMP-LBNL-GSB-1.1.2	104
nrg7a_668_PT401.txt	YMP-LBNL-GSB-1.1.2	104
sd7_300_zone1.txt	YMP-LBNL-GSB-1.1.2	104
sd7_350_zone2.txt	YMP-LBNL-GSB-1.1.2	104
sd7_400_zone3.txt	YMP-LBNL-GSB-1.1.2	104
sd7_800_zone11.txt	YMP-LBNL-GSB-1.1.2	104
SD12_214_PT1679.txt	YMP-LBNL-GSB-1.1.2	104
SD12_301_PT1667.txt	YMP-LBNL-GSB-1.1.2	104
SD12_350_PT1661.txt	YMP-LBNL-GSB-1.1.2	104
SD12_1058_PT1619.txt	YMP-LBNL-GSB-1.1.2	104
surfbc.xls	YMP-LBNL-GSB-1.1.2	105
timvsp.dat	YMP-LBNL-GSB-1.1.2	106
binfpJ0	YMP-LBNL-GSB-1.1.2	106
binfpJ1i	YMP-LBNL-GSB-1.1.2	107
binfpJ1i.out	YMP-LBNL-GSB-1.1.2	107
binfpJ1i.par	YMP-LBNL-GSB-1.1.2	107
binfL0	YMP-LBNL-GSB-1.1.2	108
binfL0i	YMP-LBNL-GSB-1.1.2	108
binfL0.out	YMP-LBNL-GSB-1.1.2	108
binfL0i.out	YMP-LBNL-GSB-1.1.2	108
binfL1	YMP-LBNL-GSB-1.1.2	109
binfL1i	YMP-LBNL-GSB-1.1.2	109
binfL1.out	YMP-LBNL-GSB-1.1.2	109
binfL1i.out	YMP-LBNL-GSB-1.1.2	109
binfL1i.par	YMP-LBNL-GSB-1.1.2	109
LINFI1	YMP-LBNL-GSB-LHH-2	41
LINFI1i	YMP-LBNL-GSB-LHH-2	41
LINFI1.out	YMP-LBNL-GSB-LHH-2	41
LINFI1i.out	YMP-LBNL-GSB-LHH-2	41
LINFI1i.par	YMP-LBNL-GSB-LHH-2	41
LINFI2	YMP-LBNL-GSB-LHH-2	42-43
LINFI2i	YMP-LBNL-GSB-LHH-2	42-43
LINFI2.out	YMP-LBNL-GSB-LHH-2	43
LINFI2i.out	YMP-LBNL-GSB-LHH-2	43
LINFI2i.par	YMP-LBNL-GSB-LHH-2	43

DTN: LB991091233129.001

Table 1. Files supporting the 1-D, mountain-scale, calibrated properties. Files are referenced to scientific notebook page(s) where documented. (Cont.)

File Name	Notebook Number	Notebook Page(s)
UINFI1	YMP-LBNL-GSB-LHH-2	43
UINFI1i	YMP-LBNL-GSB-LHH-2	43
UINFI2.out	YMP-LBNL-GSB-LHH-2	44
UINFI2i.out	YMP-LBNL-GSB-LHH-2	44
UINFI2i.par	YMP-LBNL-GSB-LHH-2	44
LINFJ2i	YMP-LBNL-GSB-LHH-2	46
UINFJ2i	YMP-LBNL-GSB-LHH-2	46
LINFJ2	YMP-LBNL-GSB-LHH-2	47
UINFJ2	YMP-LBNL-GSB-LHH-2	47
LINFJ2.out	YMP-LBNL-GSB-LHH-2	47
LINFJ2i.out	YMP-LBNL-GSB-LHH-2	47
LINFJ2i.par	YMP-LBNL-GSB-LHH-2	47
LINFJ2i.tec	YMP-LBNL-GSB-LHH-2	47
UINFJ2.out	YMP-LBNL-GSB-LHH-2	47
UINFJ2i.out	YMP-LBNL-GSB-LHH-2	47
UINFJ2i.par	YMP-LBNL-GSB-LHH-2	47
UINFJ2i.tec	YMP-LBNL-GSB-LHH-2	47
Nlinf1	YMP-LBNL-GSB-LHH-2	47-48
Ninf1i	YMP-LBNL-GSB-LHH-2	47-48
Nlinf1.out	YMP-LBNL-GSB-LHH-2	47-48
Nlinf1i.out	YMP-LBNL-GSB-LHH-2	47-48
Nlinf1i.par	YMP-LBNL-GSB-LHH-2	47-48
Nlinf1i.tec	YMP-LBNL-GSB-LHH-2	47-48
Nuinf1	YMP-LBNL-GSB-LHH-2	48
Nuinf1i	YMP-LBNL-GSB-LHH-2	48
Nuinf1.out	YMP-LBNL-GSB-LHH-2	48
Nuinf1i.out	YMP-LBNL-GSB-LHH-2	48
Nuinf1i.par	YMP-LBNL-GSB-LHH-2	48
Nuinf1i.tec	YMP-LBNL-GSB-LHH-2	48
Nbinf1	YMP-LBNL-GSB-LHH-2	48
Nbinf1i	YMP-LBNL-GSB-LHH-2	48
Nbinf1.out	YMP-LBNL-GSB-LHH-2	48
Nbinf1i.out	YMP-LBNL-GSB-LHH-2	48
Nbinf1i.par	YMP-LBNL-GSB-LHH-2	48
Nbinf1i.tec	YMP-LBNL-GSB-LHH-2	48
Linf_gas	YMP-LBNL-GSB-LHH-2	49
Linf_gasi	YMP-LBNL-GSB-LHH-2	49
Linf_gas.out	YMP-LBNL-GSB-LHH-2	49

DTN: LB991091233129.001

Table 1. Files supporting the 1-D, mountain-scale, calibrated properties. Files are referenced to scientific notebook page(s) where documented. (Cont.)

File Name	Notebook Number	Notebook Page(s)
Linf_gasi.out	YMP-LBNL-GSB-LHH-2	49
Linf_gasi.par	YMP-LBNL-GSB-LHH-2	49
Uinf_gas	YMP-LBNL-GSB-LHH-2	49
Uinf_gasi	YMP-LBNL-GSB-LHH-2	49-50
Uinf_gas.out	YMP-LBNL-GSB-LHH-2	49-50
Uinf_gasi.out	YMP-LBNL-GSB-LHH-2	49-50
Uinf_gasi.par	YMP-LBNL-GSB-LHH-2	49-50
Nlinf2	YMP-LBNL-GSB-LHH-2	50
Nlinf2i	YMP-LBNL-GSB-LHH-2	50
Nlinf2.out	YMP-LBNL-GSB-LHH-2	50
Nlinf2i.out	YMP-LBNL-GSB-LHH-2	50
Nlinf2i.par	YMP-LBNL-GSB-LHH-2	50
Nlinf2i.tec	YMP-LBNL-GSB-LHH-2	50
Nuinf2	YMP-LBNL-GSB-LHH-2	50
Nuinf2i	YMP-LBNL-GSB-LHH-2	50
Nuinf2.out	YMP-LBNL-GSB-LHH-2	50
Nuinf2i.out	YMP-LBNL-GSB-LHH-2	50
Nuinf2i.par	YMP-LBNL-GSB-LHH-2	50
Nuinf2i.tec	YMP-LBNL-GSB-LHH-2	50
UINFI1.out	YMP-LBNL-GSB-LHH-2	43
UINFI1i.out	YMP-LBNL-GSB-LHH-2	43
UINFI1i.par	YMP-LBNL-GSB-LHH-2	43
UINFI2	YMP-LBNL-GSB-LHH-2	44
UINFI2i	YMP-LBNL-GSB-LHH-2	44

DTN: LB991091233129.001

Table 2. Files supporting the 1-D, drift-scale, calibrated properties. Files are referenced to scientific notebook page where documented.

File Name	Notebook Number	Notebook Page
Binfd1	YMP-LBNL-GSB-LHH-2	53
Binfd1i	YMP-LBNL-GSB-LHH-2	53
Binfd1i.par	YMP-LBNL-GSB-LHH-2	54
Binfd1.out	YMP-LBNL-GSB-LHH-2	54
Binfd1i.out	YMP-LBNL-GSB-LHH-2	54
Linfd1	YMP-LBNL-GSB-LHH-2	55
Linfd1i	YMP-LBNL-GSB-LHH-2	55
Linfd1.out	YMP-LBNL-GSB-LHH-2	55
Linfd1i.out	YMP-LBNL-GSB-LHH-2	55
Linfd1i.par	YMP-LBNL-GSB-LHH-2	55
Uinfd1	YMP-LBNL-GSB-LHH-2	55
Uinfd1i	YMP-LBNL-GSB-LHH-2	55
Uinfd1.out	YMP-LBNL-GSB-LHH-2	55
Uinfd1i.out	YMP-LBNL-GSB-LHH-2	55
Uinfd1i.par	YMP-LBNL-GSB-LHH-2	55

DTN: LB991091233129.002

Table 3. Files supporting the 2-D, fault, calibrated properties. Files are referenced to scientific notebook page where documented.

File Name	Notebook Number	Notebook Page
gener	YMP-LBNL-GSB-1.1.2	130
generu	YMP-LBNL-GSB-1.1.2	144
generl	YMP-LBNL-GSB-1.1.2	144
UZ-7asat.xls	YMP-LBNL-GSB-1.1.2	131
UZ-7acap.xls	YMP-LBNL-GSB-1.1.2	134
fbinfA0t2.dat	YMP-LBNL-GSB-1.1.2	137
fbinfA0t2.out	YMP-LBNL-GSB-1.1.2	138
Save	YMP-LBNL-GSB-1.1.2	138
fbinfC0	YMP-LBNL-GSB-1.1.2	139
fbinfC0.out	YMP-LBNL-GSB-1.1.2	139
fbinfC0.sav	YMP-LBNL-GSB-1.1.2	139
fbinfC0i	YMP-LBNL-GSB-1.1.2	139
fbinfC0i.out	YMP-LBNL-GSB-1.1.2	139
fbinfC0i.par	YMP-LBNL-GSB-1.1.2	139
uz7a1343.prn	YMP-LBNL-GSB-1.1.2	140
uz7a1337.prn	YMP-LBNL-GSB-1.1.2	140
uz7a1331.prn	YMP-LBNL-GSB-1.1.2	140
uz7a1325.prn	YMP-LBNL-GSB-1.1.2	140
uz7a1319.prn	YMP-LBNL-GSB-1.1.2	140
fort.100	YMP-LBNL-GSB-1.1.2	140
fort.101	YMP-LBNL-GSB-1.1.2	140
save.es9	YMP-LBNL-GSB-1.1.2	141
save.es3	YMP-LBNL-GSB-1.1.2	141
save_p141[1]	YMP-LBNL-GSB-1.1.2	141
fort.300	YMP-LBNL-GSB-1.1.2	142
timvsp.dat	YMP-LBNL-GSB-1.1.2	142
gfbinfC1	YMP-LBNL-GSB-1.1.2	142
gfbinfC1i	YMP-LBNL-GSB-1.1.2	142
gfbinfC1i.out	YMP-LBNL-GSB-1.1.2	142
gfbinfC1i.par	YMP-LBNL-GSB-1.1.2	142
fbinfD1	YMP-LBNL-GSB-1.1.2	143
fbinfD1i	YMP-LBNL-GSB-1.1.2	143
fbinfD1i.out	YMP-LBNL-GSB-1.1.2	143
fbinfD1i.par	YMP-LBNL-GSB-1.1.2	143
gfbinfE2	YMP-LBNL-GSB-1.1.2	143

DTN: LB991091233129.003

NOTE: 1. Save_p141 is a copy of the file 'Save' documented on p. 141 of notebook YMP-LBNL-GSB-1.1.2.

Table 3. Files supporting the 2-D, fault, calibrated properties. Files are referenced to scientific notebook page where documented. (Cont.)

File Name	Notebook Number	Notebook Page
gfbinfE2i	YMP-LBNL-GSB-1.1.2	143
gfbinfE2i.out	YMP-LBNL-GSB-1.1.2	143
fbinfuA0t2.dat	YMP-LBNL-GSB-1.1.2	144-145
fbinfuA0t2.out	YMP-LBNL-GSB-1.1.2	144-145
Saveu	YMP-LBNL-GSB-1.1.2	144-145
fbinflA0t2.dat	YMP-LBNL-GSB-1.1.2	144-145
fbinflA0t2.out	YMP-LBNL-GSB-1.1.2	144-145
Savel	YMP-LBNL-GSB-1.1.2	144-145
fbinfuA0	YMP-LBNL-GSB-1.1.2	144-145
fbinfuA0i	YMP-LBNL-GSB-1.1.2	144-145
fbinfuA0i.out	YMP-LBNL-GSB-1.1.2	144-145
fbinflA0	YMP-LBNL-GSB-1.1.2	144-145
fbinflA0i	YMP-LBNL-GSB-1.1.2	144-145
fbinflA0i.out	YMP-LBNL-GSB-1.1.2	144-145

DTN: LB991091233129.003

NOTE: 1. Save_p141 is a copy of the file 'Save' documented on p. 141 of notebook YMP-LBNL-GSB-1.1.2.

ATTACHMENT IV

SOFTWARE ROUTINES

factorOBJ v1.0
Routine/Macro Documentation Form

The following information can be included in the scientific notebook. Attach and reference notebook pages and diskettes with files as needed when submitting routine/macro to records.

1. Name of routine/macro with version/OS/hardware environment:
   factorOBJ v.1.0 (routine) / UNIX SUNOS Solaris 5.5.1/Sun workstation

2. Name of commercial software with version/OS/hardware used to develop routine/macro:
   FORTRAN 77/UNIX SUNOS Solaris 5.5.1/Sun workstation

3. **Test Plan.**

   - Explain whether this is a routine or macro and describe what it does:
     This simple routine is used to calculate the F factor value as described on p. 45 of S/N YMP-LBNL-GSB-LHH-2. The F factor value is used to measure the degree of gas signal attenuation in the TSw unit.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     p. 45 (at bottom of page) S/N YMP-LBNL-GSB-LHH-2

   - Description of test(s) to be performed (be specific):
     The test will use a representative sample data set containing a small number of data points as in put. The code will apply the equation printed on p. 60 (bullet 2c), of S/N YMP-LBNL-GSB-LHH-2 using the sample input to give the F value test output. A hand calculation will be conducted to confirm that the output is correct to the significant figures given.

   - Specify the range of input values to be used and why the range is valid:
     This routine performs a simple calculation of the F factor value, and the range of input values is 0 to ∞. The specific test case input range is deemed valid because the routine's simple arithmetic changes can be inspected using only a small sampling of lines from the very large output file.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The routine output from the test is given on p. 60 (bullet 3) of S/N YMP-LBNL-GSB-LHH-2. The test case input range is deemed valid because the routine's calculation can be successfully checked using sample data that do not cover the full range.

   - Description of how the testing shows that the results are correct for the specified input:
     Hand calculation confirms that the output is correct to the significant figures given.

   - List limitations or assumptions to this test case and code in general:
     The data points in the input file must be consistent with the value of variable "nn" in the source code. The input values must be between 0 and ∞.

   - Electronic files identified by name and location (include disc if necessary):
     The routine code and test files are printed on p. 45 and p. 60 of S/N YMP-LBNL-GSB-LHH-2, respectively.

5. Supporting Information. Include background information, such as revision to a previous routine or macro, or explanation of the steps performed to run the software. Include listings of all

IV-2 JEH 3/31/00

electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated:

See attached pages for technical review forms, referenced scientific notebook pages and other supporting documentation

Note: All relevant scientific notebook (SN) pages are included in this package. In some instances, the included SN pages cross-reference other pages that are not included here because these were not essential to the documentation of this routine.

MAINTAIN PAGES IN THIS ORDER:
1) This 2-page Routine Documentation Form
2) pp. 45 and 60 for S/N YMP-LBNL-GSB-LHH-2
3) Review Forms

(d)

5-6-99 Determination of smallest factor for gas calibration

hwe 5-4-99

The little attenuation in the TSw unit is considered as an important feature showed by the gas pressure data, and the calibrated fracture permeabilities for the model layers in the TSw unit need to be consistent with this feature. Therefore, it is needed to determine fracture permeabilities in the TSw unit such that the simulated and observed gas pressure signals at the two sensor's locations in the TSw unit have the similar degrees of attenuation for the borehole SD-12. We concentrated on the borehole SD-12 because the distance between the two TSw sensors within this borehole is the largest. The degree of attenuation of gas flow through the TSw unit for SD-12, or the relative difference between gas signals at the two sensor's locations, was determined by

$$F = \frac{1}{N}\left\{\sum_{i=1}^{N}\{[P_u(t_i) - P_u(t_1)] - [P_b(t_i) - P_b(t_1)]\}^2\right\}^{1/2}$$

hhe 5-10-99

where N is the total number of calibration times t_i, P is the gas pressure, and subscripts, u and b, refer to the sensors in the upper and low portions of the TSw within the borehole SD-12. Obviously, if the gas signals from the two sensors are identical, F should be equal to zero. For the given gas signal data, the F value is 2.01E-3 ($kPa^{\frac{1}{2}}$). A single user macro, factorOBJ.f, was used for calculating F values. Theoretically, the F value from simulated gas signals at the two sensor's locations should approach to zero if the fracture permeabilities for the TSw unit approach to infinite values. In this study, we needed to determine the fracture permeabilities, which provide the similar F value as that calculated from the data, such that the simulated and observed gas pressure signals have the similar degrees of attenuation. Since the gas pressure data from the TSw unit are generally limited, fracture permeabilities for different model layers in this unit could not be reliably and independently estimated. Therefore, we assumed difference between log values of model layer fracture permeability and the corresponding uncalibrated permeability to be the same among all the related TSw model layers. F is a function of the difference d. For a given infiltration map and a number of d values between 1 and 2 with an interval of 0.1, we determined the d value resulting in the F value which is the closest to 2.01E-3 ($kPa^{\frac{1}{2}}$). The latter value corresponds to the data.

hhe 5-10-99

hhe 2-2-00

```
      real a(10000),b(10000)
      nn=121
c
      do i=1,nn
      read(100,*)t,a(i)
      enddo

      do i=1,nn
      read(100,*)t,b(i)
      enddo
c
      sum=0.
      do k=1,nn
      x=a(k)-a(1)
      y=b(k)-b(1)
      sum=sum+(x-y)**2.
      enddo
c
      sum=sqrt(sum)/real(nn)
      write(*,*)sum
c
      stop
      end
```

read (P) information for TPtrn of SD12

read (Pressure) information for tpt p/n of SD12

Calculate F

factorOBJ.f (Version) hhe 2-2-00

(~~fumo~~ /usr/users/hhtim/JG_99_Gas Cal. dir

hhe 6-1-99

Reviewed and acceptable G. L 5-10-99

See page 60 for testing

This is a fortran77 code (unix)

hhe 8-11-00 routine ~~macro~~ routine hhe 8-10-00

7-30-99 Testing of factor OBJ.f, a ~~single use macro~~.

① Description of code: (P45 of this notebook)

② plan of testing

ⓐ for testing with a small number of data; change "nn=121" to "nn=3" in the code

ⓑ Generate a input file (fort.100)

0. 0.
0. 0.
0. 0.
0. 0.

hhe 7-30-99

0. 0.
1. 0.
2. 0.
0. 0.
1. 1.
2. 1.

ⓒ According to the formulation on P.45 of this notebook

$$F = \frac{1}{3}\left\{0^2+1^2+1^2\right\}^{\frac{1}{2}} = 0.4714045$$

hhe 7-30-99 ③ ~~output from~~ hhe 7-30-99

③ Testing results:

Output from the code = 0.4714045

④ Acceptance Criteria

Difference between accurate value and that from the code should be less than 5%.

The results show that the code calculation is acceptable.

⑤ Valid input range:
no limitation, as long as the input formate and nnU are consistent with the code.

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of: 1

3. Originator: Hui-Hai Liu
4. Document Title: Routine factor OBJ v1.0 Documentation
5. Document Number: —
6. Revision/Mod.: —
7. Draft: —
8. Governing Procedure Number: AP-SI.1Q
9. Revision/Mod: Rev.2. ICN4

REVIEW CRITERIA

10. ☒ Standard Review Criteria N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☒ Source: AP-SI.1Q/Rev.2 ICN4 Sec 5.1.1 (or timeline)
☐ Attached:
☐ Scientific notebook/data associated with this review as noted on Attachment 3

12. Comment Documentation:
☒ Comment Sheets
☐ Review Copy Mark-up

13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson

14.

Reviewer	Org./Discipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
Guomin Li	LBNL	Technical			

COMMENTS DUE:

15. Due Date: 2/24/00

16. Originator/Review Coordinator: H.H. Liu
Print Name

REVIEW BY:

17. Guomin Li
Print Name

18. Signature Date 2-24-00

19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Print Name/Signature Date 2-24-00

CONCURRENCE:

21. Document Draft No: NA Date:

22. Reviewer: Signature Date 2/24/00

23. PM: Signature Date 2/3/00

DISPUTE RESOLUTION: (if applicable)

24. PM: Signature Date

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YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook YMP-LBNL-GSB-LHH-2 for Routine factor OBJ v1.0

Date of Document (or revision, draft revision number, as applicable):

Pertinent sections of scientific notebook(s) or other backup documents and/or data DTN# are identified below, supporting the document which is the subject of this review. These documents/data shall be included in the scope of this review.

Document(s) Title/Data	Relevant Sections/Pages
YMP-LBNL-GSB-LHH-2	P.76; P.45; P.60
Routine Documentation Form	pg 1 + 2

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YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine factorOBJ V1.0			2. Page 1 of 1
3. Document No. —	4. Revision/ Change/Mod: —	5. Draft —	6. ☒ Q ☐ NQ
7. Reviewer: Guomin Li			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		The previous comments were given on the corresponding pages of the Scientific Notebook. No error is found during this review. The documentation for this routine was reviewed and it was found to meet the requirements AP-SI.1Q/Rev.2/ICN4. The test case fully checked the routine for the input specified.		

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STANDARD REVIEW CRITERIA

Page 1 of 1

Routine/Macro Review Criteria, Option 1

NOTE: Where a checklist item does not apply to the software product, check "N/A".

	Yes	No	N/A	
R/M-1	X			**The information given below is to be documented in the technical product, in which the routine/macro is used to support. Does the routine/macro include:** Name of routine/macro with version/Operating System/hardware environment
R/M-2	X			Name of commercial software used to write the routine/macros with version/Operating System/hardware used to develop it
R/M-3	X			Test Plan • Explanation whether this is a routine or macro and a description of what it does • The source code (this section shall include equations or algorithms form software setup (Labview, Excel, etc.) • Description of test(s) to be performed (be specific) • Specified range of input values to be used and why the range is valid
R/M-4	X			Test Results • Output from test (explain difference between input range used and possible input) • Description of how the testing shows that the results are correct for the specified input • List of limitations or assumptions to this test case (s) and code in general • Electronic files identified by name and location (included if necessary to perform the tests)
R/M-5	X			Supporting Information. Include background information, such as revision to a previous routine or macro or explanation of the steps performed to run the software. Include listing of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated.

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inf v.1.0
Routine/Macro Documentation Form

The following information can be included in the scientific notebook. Attach and reference notebook pages and diskettes with files as needed when submitting routine/macro to records.

1. Name of routine/macro with version/OS/hardware environment:
   inf v.1.0 (routine) / UNIX SUNOS Solaris 5.5.1/Sun workstation

2. Name of commercial software with version/OS/hardware used to develop routine/macro:
   FORTRAN 77/UNIX SUNOS Solaris 5.5.1/Sun workstation

3. **Test Plan.**

   - Explain whether this is a routine or macro and describe what it does:
     This routine is used to calculate the average infiltration rates for borehole NRG#5, NRG-6, NRG-7a, SD-12, SD-7, SD6, SD9, UZ-14, UZ#16, UZ#4 and WT-24.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     The source code is printed on p.39 S/N YMP-LBNL-GSB-LHH-2

   - Description of test(s) to be performed (be specific):
     During the test, the routine will first read a simplified infiltration rate data set (p. 58, bullet 2b: Column 1-Easting(x), Column 2-Northing(y), Column 3- test infiltration value). Next it will calculate the average infiltration rate for each borehole by averaging given infiltration rates over a circular area with the center corresponding to a borehole location and radii of 100m, 200m and 300m, respectively. To facilitate verification by the hand calculation method, the number of iterations the code operates will be limited as explained on p. 58 (bullet 2a). The resulting output are compared and verified using hand calculation.

   - Specify the range of input values to be used and why the range is valid:
     In the input file for the test, two infiltration rate values adjacent to each borehole are included. Because the routine does the simple averaging calculation for each borehole and because any amount of numbers can be averaged using the equation, the use of two values is adequate for the test purpose. Because the average infiltration for a borehole is calculated using only infiltration rates near the bore, the sample input set range of infiltration values immediately adjacent to each borehole is valid.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The output from the test is given on p. 59 of S/N YMP-LBNL-GSB-LHH-2. Because the average infiltration for a borehole is calculated using only infiltration rates near the borehole, the sample input set range of infiltration values immediately adjacent to each borehole is valid.

   - Description of how the testing shows that the results are correct for the specified input:
     The output results are the same as those by hand calculation (see p. 59, bullet 4 of S/N YMP-LBNL-GSB-LHH-2).

   - List limitations or assumptions to this test case and code in general:
     In an input file, there must be at least one infiltration rate data point for each borehole over a circular area with a center corresponding to the borehole and a

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radius of 200m. The data points in a valid input file should be consistent with the value for the variable "nn" in the source code.

- Electronic files identified by name and location (include disc if necessary):
  The routine code and test files are printed on p.39 and pp.58-59, S/N YMP-LBNL-GSB-LHH-2.

5. Supporting Information. Include background information, such as revision to a previous routine or macro, or explanation of the steps performed to run the software. Include listings of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated:

   See attached pages for technical review forms, referenced scientific notebook pages and other supporting documentation

   Note: All relevant scientific notebook (SN) pages are included in this package. In some instances, the included SN pages cross-reference other pages that are not included here because these were not essential to the documentation of this routine.

   MAINTAIN PAGES IN THIS ORDER:
   1) This 2-page Routine Documentation Form
   2) pp. 39, 58-59 for S/N YMP-LBNL-GSB-LHH-2
   3) Review Forms

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infi.f ver1.0

Fortran 77 Code (Unix)


```
      real*8 xborehole(11),yborehole(11),R(3)
      real*8 x(140000),y(140000),z(140000)
      character*8 borehole(11)
c
      nn=137278
c
      R(1)=100.
      R(2)=200.
      R(3)=300.
c
      borehole(1)="nrg-6"
      xborehole(1)=171964.2
      yborehole(1)=233698.1
c
      borehole(2)="nrg-7a"
      xborehole(2)=171597.5
      yborehole(2)=234354.6
c
      borehole(3)="sd6"
      xborehole(3)=170276.5
      yborehole(3)=232424.6
c
      borehole(4)="sd7"
      xborehole(4)=171066.
      yborehole(4)=231328.
c
      borehole(5)="sd9"
      xborehole(5)=171242.1
      yborehole(5)=234085.8
c
      borehole(6)="SD12"
      xborehole(6)=171177.5
      yborehole(6)=232244.5
c
      borehole(7)="uz4"
      xborehole(7)=172559.5
      yborehole(7)=234304.6
c
      borehole(8)="uz14"
      xborehole(8)=170731.3
      yborehole(8)=235095.3
c
      borehole(9)="uz16"
      xborehole(9)=172168.4
      yborehole(9)=231811.1
c
      borehole(10)="WT24"
      xborehole(10)=171390.9
      yborehole(10)=236729.9
c
      borehole(11)="NRG-5"
      xborehole(11)=172141.9
      yborehole(11)=234052.9
c
      do i=1,nn
      read(100,*)x(i),y(i),z(i)
c
      enddo
c
      do i=1,3
      write(200,*)R(i)
        do j=1,11
         jj=0
c
         suminf=0.
          do k=1,nn
           xx=x(k)-xborehole(j)
           yy=y(k)-yborehole(j)
          rxy=sqrt(xx**2.+yy**2.)
          if(rxy.lt.R(i))then
            jj=jj+1
            suminf=suminf+z(k)
         endif
        enddo
c
        write(200,*)borehole(j),suminf/real(jj)
      enddo
c
      enddo
c
      stop
      end
```

See p.58 for testing

* This code is used to calculate infiltration rates for boreholes: nrg-6, nrg-7a, sd6, sd7, sd9, sd12, uz4, uz14, uz16, WT24 and NRG-5.

* The input formats must be consistent with the code

* If the input data points are different from 137278, the nn value needs to be changed.

Reviewed and acceptable

G.L

4-16-91

IV-12 JEH 3/31/06

hhl 8-10-00 ~~macro~~ routine routine hhl 8-10-00

7-30-99 Testing of inf.f, a ~~single user macro~~ (Pg of this notebook)

① Description of code (Pg of this notebook)

② plan of testing.

ⓐ for testing with a small number of data, change "nn = 17278" to "nn = 22"

ⓑ Near each borehole center, give two data points with inf rate of 1.0 and 0., respectively.

The input file for the testing is

y	x	z
171964.	233698.	1.
171963.	233698.	0.
171597.	234354.	1.
171596.	234354.	0.
170276.	232424.	1.
170275.	232424.	0.
171066.	231328.	1.
171065.	231328.	0.
171242.	234085.	1.
171241.	234085.	0.
171177.	232244.	1.
171176.	232244.	0.
172559.	234305.	1.
172558.	234305.	0.
170731.	235095.	1.
170730.	235095.	0.
172168.	231811.	1.
172167.	231811.	0.
171390.	236729.	1.
171389.	236720.	0.
172141.	234053.	1.
172140.	234053.	0.

hhl 7-30-99

ⓒ

③ Testing Results

ⓐ output files is given in the next page

ⓑ The accurate value should be 0.5 for each bore hole.

```
    100.000000000000
nrg-6        0.500000
nrg-7a       0.500000
sd6          0.500000
sd7          0.500000
sd9          0.500000
SD12         0.500000
uz4          0.500000
uz14         0.500000
uz16         0.500000
WT24         0.500000
NRG-5        0.500000
    200.00000000000
nrg-6        0.500000
nrg-7a       0.500000
sd6          0.500000
sd7          0.500000
sd9          0.500000
SD12         0.500000
uz4          0.500000
uz14         0.500000
uz16         0.500000
WT24         0.500000
NRG-5        0.500000
    300.00000000000
nrg-6        0.500000
nrg-7a       0.500000
sd6          0.500000
sd7          0.500000
sd9          0.500000
SD12         0.500000
uz4          0.500000
uz14         0.500000
uz16         0.500000
WT24         0.500000
NRG-5        0.500000
```

(4) Acceptance criteria for results of testing:

The difference between accurate value and calculate value should be less than 5%.

The accurate value = 0.5
The calculated value = 0.5

It is acceptable.

IV-14 JEH 3/31/00

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of: 1

3. Originator: H. H. Liu
4. Document Title: Routine inf V1.0 Documentation
5. Document Number: NA
6. Revision/Mod.: NA
7. Draft: NA
8. Governing Procedure Number: AP-SI.1Q
9. Revision/Mod: Rev2. ICN4

REVIEW CRITERIA

10. ☒ Standard Review Criteria NA (Taken from Attachment 5)
11. ☐ Specific Review Criteria:
☒ Source: AP-SI.1Q/Rev2. ICN4 Sec. 5.1.1 (one time use)
☐ Attached:
☐ Scientific notebook/data associated with this review as noted on Attachment 3
12. Comment Documentation:
☒ Comment Sheets
☐ Review Copy Mark-up
13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson
14. Reviewer: G. Li — Org./Discipline: LBNL — Review Criteria: Technical

Reviewer	Org./Discipline	Review Criteria

COMMENTS DUE:
15. Due Date: 2/24/00
16. Originator/Review Coordinator: H. H. Liu (Print Name)

REVIEW BY:
17. G. Li (Print Name)
18. [signature] 2-24-00 (Signature, Date)
19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. [signature] 2-24-00 (Print Name/Signature, Date)

CONCURRENCE:
21. Document Draft No: NA Date:
22. Reviewer: [signature] 2/24/00 (Signature, Date)
23. PM: [signature] 2/3/00 (Signature, Date)

DISPUTE RESOLUTION: (if applicable)
24. PM: (Signature, Date)

IV-15 EH 3/31/00

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine inf v1.0				2. Page 1 of 1
3. Document No. NA	4. Revision/ Change/Mod: NA	5. Draft NA	6. ☒ Q ☐ NQ	
7. Reviewer: G. Li				

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		The previous comments were given on the corresponding pages of the scientific notebook. No error is found during this review. The documentation for this routine was reviewed and it was found to meet the requirements of AP-SI.1Q/Rev.2/ICN4. The test case fully checks the routine for the input specified.		

11-16 #34 3/1/00

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Routine inf V1.0

Date of Document (or revision, draft revision number, as applicable):

Pertinent sections of scientific notebook(s) or other backup documents and/or data DTN# are identified below, supporting the document which is the subject of this review. These documents/data shall be included in the scope of this review.

Document(s) Title/Data	Relevant Sections/Pages
YMP-LBNL-GSB-LHH-2	P.74; P.39; pp.58-59
Routine Documentation Form	pp 1 & 2

IV-17 DEH 3/31/00

STANDARD REVIEW CRITERIA

Page 1 of 1

Routine/Macro Review Criteria, Option 1

NOTE: Where a checklist item does not apply to the software product, check "N/A".

	Yes	No	N/A	
R/M-1	X			**The information given below is to be documented in the technical product, in which the routine/macro is used to support. Does the routine/macro include:** Name of routine/macro with version/Operating System/hardware environment
R/M-2	X			Name of commercial software used to write the routine/macros with version/Operating System/hardware used to develop it
R/M-3	X			Test Plan • Explanation whether this is a routine or macro and a description of what it does • The source code (this section shall include equations or algorithms form software setup (Labview, Excel, etc.) • Description of test(s) to be performed (be specific) • Specified range of input values to be used and why the range is valid
R/M-4	X			Test Results • Output from test (explain difference between input range used and possible input) • Description of how the testing shows that the results are correct for the specified input • List of limitations or assumptions to this test case (s) and code in general • Electronic files identified by name and location (included if necessary to perform the tests)
R/M-5	X			Supporting Information. Include background information, such as revision to a previous routine or macro or explanation of the steps performed to run the software. Include listing of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated.

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TBgas3D v.1.0
Routine/Macro Documentation Form

The following information can be included in the scientific notebook. Attach and reference notebook pages and diskettes with files as needed when submitting routine/macro to records.

1. Name of routine/macro with version/OS/hardware environment:
   TBgas3D v.1.0 (routine) / UNIX SUNOS Solaris 5.5.1/Sun workstation

2. Name of commercial software with version/OS/hardware used to develop routine/macro:
   FORTRAN 77/UNIX SUNOS Solaris 5.5.1/Sun workstation

3. **Test Plan.**

   - Explain whether this is a routine or macro and describe what it does:
     This routine is used to prepare the input file (timvsp.dat) for the gas calibration from an EOS3 input file. timvsp.dat is the file specifying top gas pressure boundary condition for gas calibration.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     p. 61 S/N YMP-LBNL-GSB-LHH-2 (annotated with a description of what each step does)

   - Description of test(s) to be performed (be specific):
     During the test, the routine reads in top boundary element names and gas pressures from input file fort.101 (EOS3 output only containing top boundary elements), read in pressure values from file fort.100 containing needed gas pressure fluctuations, and calculate gas pressures for each top boundary element. To facilitate verification by the hand calculation method, the number of iterations the code operates will be limited as explained on p. 62 (bullet 2a). The resulting output are compared and verified using hand calculation.

   - Specify the range of input values to be used and why the range is valid:
     In the input file, a single top boundary element was used for simplicity. Because the routine does the same simple calculation repeatedly for each top boundary element, the use of one element is adequate for the test purpose.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The output from the test is given on pp. 62-63 of S/N YMP-LBNL-GSB-LHH-2. The specific test case input range is deemed valid because the routine's simple arithmetic changes can be inspected using only a small sampling of lines from the very large output file.

   - Description of how the testing shows that the results are correct for the specified input:
     The output results are the same as those by hand calculation.

   - List limitations or assumptions to this test case and code in general:
     The format of input file fort.101 should be the same as an EOS3 output file, and fort.101 only contains top boundary elements. The input values must be between 0 and ∞.

   - Electronic files identified by name and location (include disc if necessary):
     The routine and test files are printed on pp.61-63, S/N YMP-LBNL-GSB-LHH-2.

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TBgas3D v.1.0
Routine/Macro Documentation Form

5. Supporting Information. Include background information, such as revision to a previous routine or macro, or explanation of the steps performed to run the software. Include listings of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated:

See attached pages for technical review forms, referenced scientific notebook pages and other supporting documentation

Note: All relevant scientific notebook (SN) pages are included in this package. In some instances, the included SN pages cross-reference other pages that are not included here because these were not essential to the documentation of this routine.

MAINTAIN PAGES IN THIS ORDER:
1) This 2-page Routine Documentation Form
2) pp. 61-63 for S/N YMP-LBNL-GSB-LHH-2
3) Review Forms

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Test of TBgas3D.f, a ~~single use macro~~ ~~routine~~ macro routine 8-17-00 nnl 8-17-00

① Description of the code (Ver 1.0)

FORTRAN 77 (UNIX)

8-2-99

This code is used to determine an input file for the gas calibration from a EOS3 output. The detailed function of this code can be found from steps A through D given on pp 61 & 62.

```
      real*8 p(3000),pp(2000)
      character*8 Name(3000)
c n -- # of TP blocks
      n=29
      nn=324
c
c
      do i=1,n
      read(101,99)Name(i)
 99   format(A5)
      read(101,*)p(i),x1,x2,x3,x4
      write(102,*)Name(i),p(i)
      enddo
c
      do i=1,nn
      ii=1+(i-1)*4
      read(100,*)pp(ii),pp(ii+1),pp(ii+2),pp(ii+3)
      enddo
      read(100,*)pp(1297)
c
c
      sum=0.0
      do i=1,1297
      sum=sum+pp(i)
      enddo
c
      sum=sum/real(1297)
      write(*,*)sum
c
      do i=1,1297
      pp(i)=pp(i)-sum
      enddo
c
      do i=1,29
      write(300,10)Name(i)
 10   format(A5)
c
      do j=1,324
      ii=(j-1)*4+1
      write(300,20)pp(ii)+p(i),pp(ii+1)+p(i),
&     pp(ii+2)+p(i),pp(ii+3)+p(i)
      enddo
c
      write(300,20)p(i)+pp(1297)
      enddo
 20   format(7x,f7.1,7x,f7.1,7x,f7.1,7x,f7.1)

      stop
      end
```

Top Boundary

(n = # of TP blocks)

nn+1 = total lines for each element in file fort.100)

Fort.101 contains EOS3 output for TP block

Fort.100 contains a file with correct pressure fluctuation in TP elements

(1297 = nn × 4 + 1 for nn=324)

~~Remove~~ Remove mean from fort.100 8-2-99

n = 29

nn = 324

The code needs to do the following:

A: Read correct element names and gas pressures from fort.~~100~~ 101 which contains EOS3 outputs. 8-2-99

B. Read pressure values from file fort.100, which contains needed gas pressure fluctuation

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hnc/8-2-99

C Remove the mean for pressure ~~[illegible]~~ code reads from a file

D: For each element the code reads from fort.101, add the ~~pressure~~ hnc/8-2-99 pressure value from fort.101 to those calculated in step C.
The output file is fort.300

(2) plan of testing

(a) for testing with a small number of data, in the code
change "n=29" and "nn=324" to "n=1" and "nn=1";
change "1297" to "5"; (= nn×4+1)
change "29" to "1"; (= n)
change "324" to "1"; (= nn)

(b) input file

Fort.101

```
TPa 1
 0.8553300847658E+05 0.1080000001054E+02 0.2500000000000E+02 0.1999999894600E+00 0.199999
894600E+00 → a single line
```

Fort.100

```
87351.7
87307.0      87351.7      87223.4      87264.1
```

(c) hand calculation results (following steps A, B, C, D) pp. 61–62

TPa 1

85585.1 85585.1 85456.8 85497.5
85540.4

(3) testing results

output from the code fort.300

```
TPa 1
        85585.1        85585.1        85456.8        85497.5
        85540.4
```

(4) Acceptance criteria:

~~The differences between the simulated results and~~ ones calculated by hands are less than 1%.

The code is acceptable.

(5) Valid input range:

No limitation as long as the input formats and n, nn and other values are consistent with the code. (see plan of test (a)).

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Hui Hai Liu
4. Document Title: Documentation for Routine Tbgas3D V1.0 (Option 1 per AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1)
5. Document Number: N/A
6. Revision/Mod.: N/A
7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q
9. Revision/Mod: 2/4

REVIEW CRITERIA

10. ☒ Standard Review Criteria: YMP-LBNL-QIP-6.1, Attch. 5, p. 18 Routine Review Criteria (One time use Option 1) (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☒ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)

12. Comment Documentation:
☐ Comment Sheets
☐ Review Copy Mark-up
☐ Attached:
☒ Scientific notebook/data associated with this review as noted on Attachment 3

13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson

14.

Reviewer	Org./Discipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 1 MAR 2000

16. Originator/Review Coordinator: Hui Hai Liu
Print Name

REVIEW BY:
17. Randall F. Hedegaard
Print Name
18. [signature] iNAROO
Signature Date
19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Hui Hai Liu [signature] 3-1-00
Print Name/Signature Date

CONCURRENCE:
21. Document Draft No.: NA Date: –
22. Reviewer: [signature] iNAROO
Signature Date
23. PM: [signature] 3/1/00
Signature Date

DISPUTE RESOLUTION: (if applicable)
24. PM:
Signature Date

11-24 [signature] 3/1/00

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for Tbgas3D V1.0**			2. Page 1 of 1
3. Document No. **N/A**	4. Revision/ Change/Mod: **N/A**	5. Draft **N/A**	6. ☒ Q ☐ NQ
7. Reviewer: **Randall F. Hedegaard**			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		--NO COMMENTS— The documentation for this routine was reviewed and it was found to meet the requirements of AP-SI.1Q/Rev. 2/ICN4. The test case was checked by both hand calculation and by running the code as needed to fully check the test case. The test case fully checks the routine for the input specified and proves that the routine produces acceptable results.		

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YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Routine Documentation for **Tbgas3D v.10** per Option 1, AP-SI.1Q/Rev.2/ICN4, Sec. 5.5.1

Date of Document (or revision, draft revision number, as applicable):
NA

Pertinent sections of scientific notebook(s) or other backup documents and/or data DTN# are identified below, supporting the document which is the subject of this review. These documents/data shall be included in the scope of this review.

Document(s) Title/Data	Relevant Sections/Pages
Routine/Macro Documentation Form	pp. 1 and 2
YMP-LBNL-GSB-LHH-2 Scientific Notebook	pp. 61-63

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YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of: 1

3. Originator: H. H. Liu
4. Document Title: Routine TBgas3D V.1.0 Documentation
5. Document Number: —
6. Revision/Mod.: —
7. Draft: —
8. Governing Procedure Number: AP-SI.1Q
9. Revision/Mod: Rev 2. ICN 4

REVIEW CRITERIA

10. ☒ Standard Review Criteria NA (Taken from Attachment 5)
11. ☐ Specific Review Criteria:
    ☒ Source: AP-SI.1Q/Rev. 2, ICN4 Sec. 5.1.1 (one time use)
    ☐ Attached:
    ☐ Scientific notebook/data associated with this review as noted on Attachment 3
12. Comment Documentation:
    ☒ Comment Sheets
    ☐ Review Copy Mark-up
13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson
14. Reviewer

Reviewer	Org./Discipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
G. Li	LBNL	Technical			

COMMENTS DUE:

15. Due Date: 2-24-00
16. Originator/Review Coordinator: H.H. Liu (Print Name)

REVIEW BY:

17. G. Li (Print Name)
18. [signature] 2-24-00 (Signature, Date)
19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. [signature] 2-24-00 (Print Name/Signature, Date)

CONCURRENCE:

21. Document Draft No: NA Date:
22. Reviewer: [signature] 2/24/00 (Signature, Date)
23. PM: [signature] 3/3/00 (Signature, Date)

DISPUTE RESOLUTION: (if applicable)

24. PM: (Signature, Date)

N-27 Rev 3/31/00

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine TBgas3D V1.0			2. Page 1 of 1
3. Document No. NA	4. Revision/ Change/Mod: NA	5. Draft NA	6. ☒ Q ☐ NQ
7. Reviewer: G. Li			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		The previous comments were given on the corresponding pages on the Scientific Notebook. No error is found during this review. The documentation for this routine was reviewed and it was found to meet the requirement of AP-SI.1Q/Rev.2/1CN4. The test case fully checks the routine for the input specified.		

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YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Routine TBgas3D v1.0

Date of Document (or revision, draft revision number, as applicable):

Pertinent sections of scientific notebook(s) or other backup documents and/or data DTN# are identified below, supporting the document which is the subject of this review. These documents/data shall be included in the scope of this review.

Document(s) Title/Data	Relevant Sections/Pages
Ymp-LBNL-GSB-LHH-2	p.75; pp 61-63
Documentation for Routine Form	pp. 1 & 2

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STANDARD REVIEW CRITERIA

Page 1 of 1

Routine/Macro Review Criteria, Option 1

NOTE: Where a checklist item does not apply to the software product, check "N/A".

	Yes	No	N/A	
R/M-1	X			**The information given below is to be documented in the technical product, in which the routine/macro is used to support. Does the routine/macro include:** Name of routine/macro with version/Operating System/hardware environment
R/M-2	X			Name of commercial software used to write the routine/macros with version/Operating System/hardware used to develop it
R/M-3	X			Test Plan • Explanation whether this is a routine or macro and a description of what it does • The source code (this section shall include equations or algorithms form software setup (Labview, Excel, etc.) • Description of test(s) to be performed (be specific) • Specified range of input values to be used and why the range is valid
R/M-4	X			Test Results • Output from test (explain difference between input range used and possible input) • Description of how the testing shows that the results are correct for the specified input • List of limitations or assumptions to this test case (s) and code in general • Electronic files identified by name and location (included if necessary to perform the tests)
R/M-5	X			Supporting Information. Include background information, such as revision to a previous routine or macro or explanation of the steps performed to run the software. Include listing of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated.

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Routine/Macro Documentation Form

The following information can be included in the scientific notebook. Attach and reference notebook pages and diskettes with files as needed when submitting routine/macro to records.

1. Name of routine/macro with version/OS/hardware environment:
   aversp_1 V 1.0 (routine) / UNIX SUNOS Solaris 5.5.1/Sun workstation

2. Name of commercial software with version/OS/hardware used to develop routine/macro:
   FORTRAN 77/UNIX SUNOS Solaris 5.5.1/Sun workstation

3. Test Plan.

   - Explain whether this is a routine or macro and describe what it does:
     This routine groups saturation or water potential data from borehole core by depth (elevation) intervals and then calculates the center elevation, the number of data points, the data average (arithmetic for saturation and geometric for water potential), and standard deviations (standard deviation of the logarithm of water potential data) for each interval. The input file is structured as follows: the first line is the number of intervals plus 1 (*nz*); the next *nz*-1 lines are the elevations of the interval tops; the next line is the elevation of the bottom of the bottom interval; the next line has two numbers: the first indicates whether the data are saturation (1) or water potential (2) data, and the second indicates the number of data (*nsp*); the next line gives the borehole collar (ground surface) elevation; the next *nsp* lines are the depth of each data point from the borehole collar; the last *nsp* lines are the data values. Saturation values greater than 1.0 are changed to 1.0. Water potential values less than 0.1 are changed to 0.1, and values greater than 30 are discarded. Note that depth and elevation units should be consistent.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     See Attachment I

   - Description of test(s) to be performed (be specific):
     The two input files shown in Attachment II are processed by the routine, and the output is checked by hand calculation.

   - Specify the range of input values to be used and why the range is valid:
     The range of test input values are shown in attachment II. These test case input ranges are deemed valid because the routine's calculations can be successfully checked using sample data that do not cover the full range.

4. Test Results.

   - Output from test (explain difference between input range used and possible input):
     The output from the test is shown in Attachment III. These test case input ranges are deemed valid because the routine's calculations can be successfully checked using sample data that do not cover the full range.

   - Description of how the testing shows that the results are correct for the specified input:
     Hand calculation confirms that the output is correct to the significant figures given.

   - List limitations or assumptions to this test case and code in general:
     The test case and routine assume that saturation data are positive and normally distributed and water potential data are positive and lognormally distributed. There is

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a limitation of 10,000 data points and 9,999 intervals. Saturation values from 0 to ∞ may be used, but, as noted above, values greater than 1.0 will be changed to 1.0. Water potential values greater than zero may be used, but as noted above values less than 0.1 will be changed to 0.1 and values greater than 30 will be discarded.

- Electronic files identified by name and location (include disc if necessary):
  None

5. Supporting Information. Include background information, such as revision to a previous routine or macro, or explanation of the steps performed to run the software. Include listings of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated:
   Attachments include source code, test input and output files, and technical review forms.

```
real z(10000),sp(10000),zsp(10000)
c
c z - elevation (m)
c sp - core measurements of saturation or capillary pressure
c zsp --- depths of samples
c
      read(*,*)nz
c
c nz- # of interface elevations
c
      do i=1,nz
         read(*,*)z(i)
      enddo
c
      read(*,*)isp,nsp
c
c isp -- isp=1, saturation; 0, capillary pressure
c
c nsp --- # of measurements
c
      read(*,*)selev
c
c selev --- surface elevation
c
c
      do  i=1,nsp
         read(*,*)zsp(i)
         zsp(i)=selev-zsp(i)
      enddo
c
      do 20 i=1,nsp
         read(*,*)sp(i)
         write(102,*)sp(i),zsp(i)
         if(isp.eq.1.and.sp(i).gt.1.)sp(i)=1.
         if(isp.eq.0)then
            ii=0
            if(sp(i).gt.30.)then
               ii=1
               sp(i)=-10000.
            endif
            if(ii.eq.0) then
               if(sp(i).lt.0.1)sp(i)=0.1
               sp(i)=log(sp(i))/log(10.)
            endif
         endif
   20 continue
c
      do i=2,nz
         zz=0.5*(z(i)+z(i-1))
         ave=0.
         iave=0
         do j=1,nsp
            zx=(z(i)-zsp(j))*(z(i-1)-zsp(j))
            if(zx.le.0.)then
               if(sp(j).gt.-9000.)then
                  ave=ave+sp(j)
                  iave=iave+1
               endif
            endif
         enddo
c
         if(iave.eq.0)then
            write(*,*)zz,i-1,iave
            go to 100
         endif
         ave=ave/real(iave)
```

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```
c
          dev=0.
          iave1=0
          do j=1,nsp
             zx=(z(i)-zsp(j))*(z(i-1)-zsp(j))
             if(zx.le.0.)then
                if(sp(j).gt.-9000.)then
                   dev=dev+(sp(j)-ave)**2.
                   iave1=iave1+1
                endif
             endif
          enddo
c
c         dev=sqrt(dev/real(iave1))
          dev=sqrt(dev/(real(iave1)-1.))

          if(isp.eq.0)ave=10.**(ave)
c
             write(*,*)zz,i-1,iave,ave,dev
             write(101,*)zz,ave
  100     continue
       enddo
       stop
       end
```

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Test #1 Input File

```
2
1322.1000
1286.3500
1       30
1323.7
4.1
5.5
7.2
7.9
9.1
9.5
10.3
12.1
13.1
14.2
15.3
17.8
18.7
19.7
20.8
21.6
23.5
24.0
26.2
27.3
28.3
29.0
29.3
30.7
31.6
32.6
33.3
34.6
35.4
36.3
0.759
0.415
0.395
0.612
0.729
0.857
0.616
0.759
0.713
0.838
0.956
0.833
0.802
0.765
0.824
0.899
0.879
0.655
0.793
0.733
0.913
0.773
0.653
0.562
0.640
0.557
0.580
0.677
0.670
0.595
```

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Test #2 Input File

```
2
1347.7000
1308.9000
0        60
1363.1
15.4
16.5
18.3
19.3
20.4
22.6
23.0
25.6
26.2
27.4
28.4
29.3
30.3
30.9
31.9
33.1
33.6
34.7
35.9
36.5
37.3
38.4
39.3
40.1
41.1
42.0
43.1
43.9
44.8
45.6
47.4
47.6
48.3
49.3
50.0
51.1
52.7
53.0
53.9
55.3
56.3
56.7
57.5
59.2
59.8
61.1
61.3
62.1
63.0
64.1
65.1
65.7
67.7
68.6
70.1
70.4
71.4
72.4
73.2
73.9
```

0.1
1.4
2.8
0.1
4.2
4.1
1.4
9.7
0.1
4.1
6.9
5.6
5.5
2.8
4.2
11.1
0.1
8.2
5.6
8.3
2.8
7.0
6.9
4.1
4.2
2.8
6.9
13.8
2.8
5.5
8.3
6.9
8.3
8.3
9.7
4.2
4.2
5.5
4.1
8.3
5.5
2.8
4.2
4.1
11.1
15.3
13.9
20.9
25.1
37.7
11.1
36.4
33.6
12.5
15.3
32.1
29.4
48.1
16.7
15.1

Routine/Macro Documentation Form
Attachment III

Test #1 Output File

```
1304.22  1  30   0.715067   0.138140
```

Test #2 Output File

```
1328.30  1  39   3.40695   0.568464
```

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YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of: 2

3. Originator: C. Fredrik (Rick) Ahlers
4. Document Title: Routine/Macro Documentation Form for routine aversp_1
5. Document Number: N/A
6. Revision/Mod.: N/A
7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q
9. Revision/Mod: REV. 2, ICN 4

REVIEW CRITERIA

10. ☒ Standard Review Criteria YMP-LBNL-QIP-6.1, p18 (Taken from Attachment 5) Attch.5
11. ☐ Specific Review Criteria:
☐ Source:
12. Comment Documentation:
☒ Comment Sheets
☐ Review Copy Mark-up
☐ Attached:
☒ Scientific notebook/data associated with this review as noted on Attachment 3
no scientific notebook pages associated with this review CFA 3/7/00
13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson

14. Reviewer	Org./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
Hui-Hai Liu	LBNL	Technical			

COMMENTS DUE:

15. Due Date: 2/24/00
16. Originator/Review Coordinator: C. Fredrik Ahlers
Print Name

REVIEW BY:

17. Hui-Hai Liu
Print Name
18. 2-24-00
Signature Date
19. Mandatory Comments: ☐ Yes ☒ No

CONCURRENCE:

21. Document Draft No: NA Date:
22. Reviewer: 3/3/00
Signature Date
23. PM: 2-24-00
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. 2/24/00
Print Name/Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

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YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine/Macro Documentation Form for routine aversp_1			2. Page 2 of 2
3. Document No. N/A	4. Revision/ Change/Mod: N/A	5. Draft N/A	6. ☒ Q ☐ NQ
7. Reviewer: Hui-Hai Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
1		The Previous Review Comments were given in the note book. Rechecked the routine including the input and output files for the test and found no errors.		

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INSTRUCTIONS FOR COMMENT SHEET

REVIEWER

1. Record title of reviewed document.
2. Identify the total number of pages of Comment Sheets.
3. Record number of reviewed document.
4. Record proposed revision/change indicator, as applicable. Mark "N/A" if there is no revision/change indicator.
5. Record the draft of document to be reviewed.
6. Identify if QARD applies to document.
7. Print the name of the document reviewer.
8. Number comments sequentially. Mark mandatory comments with an "M" and non-mandatory comments with a "NM".
9. Identify the section or paragraph and page number to which comment applies.
10. Record comment. Include explanation of the basis for comment, if necessary, and suggested change when possible.

ORIGINATOR

11. Document response adjacent to each technical mandatory or non-mandatory comment.

REVIEWER

12. Initial and date adjacent to each mandatory comment when the response is accepted. Leave blank if not accepted. Acceptance of responses to non-mandatory comments is not required.

PROJECT MANAGER ACCEPTING DISPUTED ISSUE (complete if Document Reviewer does not accept comment resolution)

13. Initial and date adjacent to comment after resolution of disputed issue and documentation of final response by Originator or Review Coordinator.

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STANDARD REVIEW CRITERIA

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Routine/Macro Review Criteria, Option 1

NOTE: Where a checklist item does not apply to the software product, check "N/A".

	Yes	No	N/A	
R/M-1	X			**The information given below is to be documented in the technical product, in which the routine/macro is used to support. Does the routine/macro include:** Name of routine/macro with version/Operating System/hardware environment
R/M-2	X			Name of commercial software used to write the routine/macros with version/Operating System/hardware used to develop it
R/M-3	X			Test Plan • Explanation whether this is a routine or macro and a description of what it does • The source code (this section shall include equations or algorithms form software setup (Labview, Excel, etc.) • Description of test(s) to be performed (be specific) • Specified range of input values to be used and why the range is valid
R/M-4	X			Test Results • Output from test (explain difference between input range used and possible input) • Description of how the testing shows that the results are correct for the specified input • List of limitations or assumptions to this test case (s) and code in general • Electronic files identified by name and location (included if necessary to perform the tests)
R/M-5	X			Supporting Information. Include background information, such as revision to a previous routine or macro or explanation of the steps performed to run the software. Include listing of all electronic files and codes used. Attach Scientific Notebook pages with appropriate information annotated.

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