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

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; ☒ Mathematical Model; ☐ System Model; ☒ Process Model
Intended Use of Analysis: ☐ Input to Calculation; ☐ Input to another Analysis or Model; ☐ Input to Technical Document; ☐ Input to other Technical Products	**Intended Use of Model:** ☐ Input to Calculation; ☒ Input to another Model or Analysis; ☐ Input to Technical Document; ☐ Input to other Technical Products
Describe use:	Describe use: Used by Performance Assessment to develop probability distribution of water seepage into drifts.

4. Title:

Seepage Model for PA Including Drift Collapse

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

MDL-NBS-HS-000002 REV01

6. Total Attachments:	7. Attachment Numbers - No. of Pages in Each:
3	Attachment I-7 Attachment II-160 Attachment III-3

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2. Analysis or Model Title:

Seepage Model fro PA Including Drift Collapse

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

MDL-NBS-HS-000002 REV01

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue
01	The Seepage Model for PA Including Drift Collapse has been revised using updated parameter sets from the Seepage Calibration Model (MDL-NBS-HS-000004 REV01). The entire model documentation was revised according to AP-3.10Q, Rev 2, ICN 3, Step 5.9)2); the changes were too extensive to use revision tracking of individual modifications.

CONTENTS

FIGURES

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TABLES

TABLES (Continued)

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ACRONYMS

1D	One-dimensional, one-dimension
2D	Two-dimensional, two-dimensions
3D	Three-dimensional, three-dimensions
ACC	Accession Number
AMR	Analysis/Model Report
AP	Administrative Procedure
CRWMS	Civilian Radioactive Waste Management System
DFNM	Discrete Fracture Network Model
DIRS	Document Input Reference System
DOE	Department of Energy
DST	Drift Scale Test
DTN	Data Tracking Number
EBS	Engineered Barrier System
ESF	Exploratory Studies Facility
LBNL	Lawrence Berkeley National Laboratory
M&O	Management and Operating Contractor
OCRWM	Office of Civilian Radioactive Waste Management
PA	Performance Assessment
QAP	Quality Assurance Procedure
QARD	Quality Assurance Requirements and Description
QIP	Quality Implementing Procedure
R1, R2, R3	Three Realizations of 3D Heterogeneous Fracture Continuum Blocks
SCM	Seepage Calibration Model
SHT	Single Heater Test
SMPA	Seepage Model for Performance Assessment
STN	Software Tracking Number
TBV	To Be Verified
Tptpmn	Topopah Spring middle nonlithophysal unit
Tptpll	Topopah Spring lower lithophysal unit
TSw	Topopah Spring welded hydrogeologic unit
TDMS	Technical Data Management System
UZ	Unsaturated Zone
YMP	Yucca Mountain Site Characterization Project

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1. PURPOSE

The purpose of this Analysis/Model Report (AMR) is to document the predictions and analysis performed using the Seepage Model for Performance Assessment (PA) and the Disturbed Drift Seepage Submodel for both the Topopah Spring middle nonlithophysal and lower lithophysal lithostratigraphic units at Yucca Mountain. These results will be used by PA to develop the probability distribution of water seepage into waste-emplacement drifts at Yucca Mountain, Nevada, as part of the evaluation of the long term performance of the potential repository. This AMR is in accordance with the *Technical Work Plan for Unsaturated Zone (UZ) Flow and Transport Process Model Report* (CRWMS M&O 2000 [153447]). This purpose is accomplished by performing numerical simulations with stochastic representations of hydrological properties, using the Seepage Model for PA, and evaluating the effects of an alternative drift geometry representing a partially collapsed drift using the Disturbed Drift Seepage Submodel. Seepage of water into waste-emplacement drifts is considered one of the principal factors having the greatest impact of long-term safety of the repository system (CRWMS M&O 2000 [153225], Table 4-1). This AMR supports the analysis and simulation that are used by PA to develop the probability distribution of water seepage into drift, and is therefore a model of primary (Level 1) importance (AP-3.15Q, *Managing Technical Product Inputs*). The intended purpose of the Seepage Model for PA is to support:

- PA
- Abstraction of Drift-Scale Seepage
- Unsaturated Zone (UZ) Flow and Transport Process Model Report (PMR)

Seepage into drifts is evaluated by applying numerical models with stochastic representations of hydrological properties and performing flow simulations with multiple realizations of the permeability field around the drift. The Seepage Model for PA uses the distribution of permeabilities derived from air injection testing in niches and in the cross drift to stochastically simulate the 3D flow of water in the fractured host rock (in the vicinity of potential emplacement drifts) under ambient conditions. The Disturbed Drift Seepage Submodel evaluates the impact of the partial collapse of a drift on seepage. Drainage in rock below the emplacement drift is also evaluated.

The work scope of this AMR is to:

(1) establish a Seepage Model for Performance Assessment (SMPA),

(2) evaluate percolation flux predictions from the UZ Site Scale Flow and Transport Model (UZ model) to develop a range of flux rates for the upper boundary of the drift seepage model,

(1) use the calibrated parameter sets developed using the Seepage Calibration Model to develop ranges of permeability and van Genuchten parameters for SMPA,

(2) design a set of simulations for evaluating drift seepage,

(3) perform multiple realizations of heterogeneous rock properties and subsequent simulations of drift seepage using the Seepage Model for PA and provide input for evaluating the distribution probability of water dripping onto waste packages,

(4) evaluate dependence of predictions on the effective local correlation length and the degree of heterogeneity of hydrologic parameters,

(5) evaluate existing models of tunnel or drift collapse provided by the Engineered Barrier System (EBS) group for representation as an alternative drift geometry and develop a simplified representation of partial drift collapse, and

(6) perform simulations using this simplified representation.

This AMR is classified as a scientific model/analysis because it documents predictions and analyses for seepage into drifts for use in the evaluation of the performance of natural barriers. The terms "model" and "analysis" are used interchangeably throughout this AMR and refer to predictions and evaluation of seepage and not necessarily to the classification of this AMR per AP-3.10Q, *Analyses and Models*.

The primary caveats and limitations in the scope of this AMR and the results from the Seepage Model for PA are that its basis is limited to the current repository design and available site data. This includes the drift configuration defined by the current design, available hydrologic properties data from the site, limitations reported in the AMRs that directly support this AMR, and consideration of seepage under ambient conditions only. Thus thermal-hydrological and thermal-hydrological-mechanical effects are not considered in this AMR.

Note that the purpose of this AMR is to document the predictions from the Seepage Model for PA and not to draw conclusions about final PA predictions. Thus, it forms a vital link between field data and calibrated-model parameters and the PA effort. The AMR establishes trends of seepage over ranges of parameter values with a state-of-the-art understanding of the processes involved. The PA calculations will be discussed under a separate AMR, in which probability weighting factors will be developed for parameter values and scenarios that are appropriate to the potential repository horizon at Yucca Mountain. Hence, for this AMR, the data that have been surveyed are not used directly, but rather as corroborative information to establish the limits of the parameter ranges to be used. Similarly, the scenarios (such as rockfalls) are taken to indicate trends and potential values of the results. In other words, this AMR does not utilize a particular parameter set, but considers ranges of possible values for these input parameters. Indeed, in PA any combination of input values can be selected for its analyses.

2. QUALITY ASSURANCE

The activities documented in this AMR were evaluated under AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance 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 2000 [149540]). This evaluation is documented in the Technical Work Plan (CRWMS M&O 2000 [153447], Addendum D, Attachment 9). Electronic management of information was evaluated (CRWMS M&O 2000 [153447], Addendum D. Attachment 8) in accordance with AP-SV-IQ, *Control of the Electronic Management of Information*, and is controlled under YMP-LBNL-QIP-SV.0, *Management of YMP-LBNL Electronic Data.*

This AMR reports on a natural barrier that has been included in the Q-list (CRWMS M&O 2000 [149733]) as an item important to waste isolation. This AMR contributes to the analyses and modeling data used to support performance assessment. The conclusions of this AMR do not affect the repository design or permanent items as discussed in QAP-2-3, *Classification of Permanent Items.*

The modeling activities documented in this AMR were conducted in accordance with the quality assurance program of the Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O), using OCRWM Administrative Procedures (APs) and Yucca Mountain Site Characterization Project (YMP) Quality Implementing Procedures (QIPs) for the Lawrence Berkeley National Laboratory (LBNL) as identified in the AMR Technical Work Plan (CRWMS M&O 2000 [153447]). This AMR was developed based on the Technical Work Plan (CRWMS M&O 2000 [153447]) and in accordance with procedure AP-3.10Q, *Analyses and Models.*

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3. COMPUTER SOFTWARE AND MODEL USAGE

The software codes, routines and macros used in this study are listed in Table 1 and were documented, verified, and used in accordance with AP-SI.1Q, *Software Management.* These are appropriate for the intended application and were used only within the range of software validation. The software were submitted to and obtained from software configuration management. The qualification status of this software is given in the Document Input Reference System (DIRS) and in the DIRS database.

Table 1. Computer Software, Routines and Macros

Software Name and Version		Software Tracking Number (STN)	Computer Used*
ITOUGH2 [112757]	V3.2_drift	10055-3.2_DRIFT-00	1
GSLIB [146609]	V2.0MSISIMV2.0	10098-2.0MSISIMV2.0-00	1
AMESH [153216]	V1.0	10045-1.0-00	1
Routines and Macros:			
frac_calc	V1.1	(see Attachment II)	2
Read_TDB	V1.0	(see Attachment II)	2
Meshbd.f	V1.0	(see Attachment II)	1
mininipresf.f	V1.0	(see Attachment II)	1
mddf.f	V1.0	(see Attachment II)	1
mk_gener.f	V1.0	(see Attachment II)	1
mk_scale_k.f	V1.0	(see Attachment II)	1
mininipresf_ir.f	V1.0	(see Attachment II)	1
mddf_cc8.f	V1.0	(see Attachment II)	1
mddf_cs8.f	V1.0	(see Attachment II)	1
mddf_cc.f	V1.0	(see Attachment II)	1
minrefine3df.f	V1.0	(see Attachment II)	1

* Platform with operating system and computer ID:
1: SUN Ultrasparc with Unix 0S, Computer ID - LBNL DOE #6332537
2: PC with DOS, Computer ID - LBNL DOE #6362015

The AMESH V1.0 code is used in the analysis to generate numerical grids for modeling simulations of the undisturbed and partially collapsed drifts. GSLIB V2.0MSISIMV2.0 generates stochastic representations of the permeability fields in the host rock surrounding the drifts, using the air permeability data obtained from niche studies. ITOUGH2 V3.2_drift is used to perform forward simulations during the analyses.

The first two routines (frac_calc and Read_TDB) in Table 1 were used for pre-processing of data from the Technical Data Management System (TDMS) and calculating fracture spacing for the discussion of alternative conceptual models in Section 6.7. The other routines and macros listed in Table 1 were used for pre-processing and preparing input files for ITOUGH2 V3.2_drift. All the routines and macros are documented in Attachment II of this AMR in accordance with AP-SI.1Q.

This AMR documents the analysis using the Seepage Model for PA. The input and output files for the model runs presented in this AMR are listed in Attachment II.

4. INPUTS

The inputs to the models were obtained from the Technical Data Management System (TDMS), and their development is documented in other AMRs, such as CRWMS M&O, 2000 [153045] and [151554] (specific references will be given in the rest of the document as such inputs are needed). The acquired and developed data used to characterize seepage conditions in the models are discussed below.

4.1 DATA AND PARAMETERS

The input data used for the development of the Seepage Model for PA are described below, while specific DTNs associated with the data are presented in Table 2. The data contained in the DTNs discussed in this section were collected in the lithostratigraphic units, Tptpmn and Tptpll, which are the units where the seepage model is applied. The data sets used in the model are the sets most important for the calculation of seepage into drifts. The current Q-status of these data are provided in the DIRS database.

- *Drift geometry and waste package length and spacing.* These data are appropriate for use for proposed drift and waste package configuration because they have been developed for use in TSPA-SR modeling (see Table 2, Row 1)

- *Mountain-scale, calibrated parameter sets for base-case infiltration.* These data are appropriate for use in corroborating fracture properties (frequency and calibrated van Genuchten α and n parameters) for the potential repository host rock to establish parameter ranges (see Table 2, Row 2)

- *Drift-scale, calibrated parameter sets for base-case infiltration.* These data are appropriate for use in corroborating calibrated drift-scale properties to establish parameter ranges (see Table 2, Row 3)

- *Air permeability data from Niches 3107 and 4788.* These data are appropriate for use in corroborating fracture permeabilities from air-permeability niche test results (see Table 2, Row 5)

- *Air permeability data from ECRB borehole SYBT-ECRB-LA#2.* These data are appropriate for use in corroborating the range of fracture permeabilities from air-permeability niche test results (see Table 2, Row 6)

- *Pre- and post-excavation air- permeability data from Niche 3650.* These data are appropriate for use in corroborating fracture permeabilities from air-permeability niche test results (see Table 2, Row 7)

- *Pneumatic pressure data from air injection tests in the SHT and DST areas used for air permeability estimates.* These data are appropriate for use in corroborating pneumatic pressure data used for estimating air permeability from the Single Heater Test (SHT) (Table 2, Row 8) and Drift Scale Test (DST) (Table 2, Row 8)

- *Fracture type (location, strike, dip, length) Sta. 26+00 to 30+00.* These data are appropriate for use in determining fracture spacing and fracture length in the Topopah Spring middle nonlithophysal lithostratigraphic unit along the Exploratory Studies Facility (ESF) Main Drift, corroborating the use of the fracture continuum approach (see Table 2, Row 9)

- *Fracture type (location, strike, dip, length) Sta. 30+00 to 35+00.* These data are appropriate for use in determining fracture spacing and fracture length in the Topopah Spring middle nonlithophysal lithostratigraphic unit along the Exploratory Studies Facility (ESF) Main Drift, corroborating the use of the fracture continuum approach (see Table 2, Row 10)

- *Fracture type (location, strike, dip, length) Sta. 35+00 to 40+00.* These data are appropriate for use in determining fracture spacing and fracture length in the Topopah Spring middle nonlithophysal lithostratigraphic unit along the Exploratory Studies Facility (ESF) Main Drift, corroborating the use of the fracture continuum approach (see Table 2, Row 11)

- *Drift geometry and waste package length and spacing.* These data are appropriate for use for determining the general drift shape (*Drift Degradation Analysis,* CRWMS M&O 2000 [151554]) (see Table 2, Row 1).

- *Estimates of log-air-permeabilities and van Genuchten capillary-strength parameters $1/\alpha$.* These data are appropriate for use for estimates of log-air-permeabilities and van Genuchten capillary-strength parameters $1/\alpha$ to determine the choice of parameter sets A and B (see Table 2, Row 4)

- *Geology maps of ECRB cross drift.* This data is appropriate for use as the only available source of detailed fracture mapping data in the ECRB cross drift used in corroborating fracture spacing and fracture length (see Table 2, Row 12)

4.2 CRITERIA

This AMR complies with the DOE interim guidance (Dyer 1999 [105655]). Subparts of the interim guidance that apply to this analysis or modeling activity are those pertaining to the characterization of the Yucca Mountain Site (Subpart B, Section 15), the compilation of information regarding hydrology of the site in support of the License Application (Subpart B, Section 21(c)(1)(ii)), and the definition of hydrologic parameters and conceptual models used in performance assessment (Subpart E, Section 114(a)).

4.3 CODES AND STANDARDS

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

Table 2. Input Data Used

Row	DTN	Data Description
1	SN9908T0872799.004 [108437]	Drift geometry and waste package length and spacing
2*	LB997141233129.001 [104055]	Mountain-scale, calibrated parameter sets for base-case infiltration
3*	LB990861233129.001 [110226]	Drift-scale, calibrated parameter sets for base-case infiltration
4	LB0010SCMREV01.002 [153393]	Estimates of log-air-permeabilities and van Genuchten capillary-strength parameters $1/\alpha$
5*	LB990601233124.001 [105888]	Air permeability data from Niches 3107 and 4788
6*	LB00090012213U.001 [153141]	Air permeability data from ECRB borehole SYBT-ECRB-LA#2
7*	LB0011AIRKTEST.001 [153155]	Pre- and post-excavation air-permeability data from Niche 3650
8*	LB960500834244.001 [105587] LB970600123142.001 [105589]	Pneumatic pressure data from air injection tests in the SHT and DST areas used for air permeability estimates
9	GS971108314224.025 [106025]	Fracture type (location, strike, dip, length) Sta. 26+00 to 30+00
10	GS960708314224.008 [105617]	Fracture type (location, strike, dip, length) Sta. 30+00 to 35+00
11	GS00060831224.004 [152573]	Fracture type (location, strike, dip, length) Sta. 35+00 to 40+00
12*	GS990908314224.010 [152631]	Geology maps of ECRB cross drift

NOTE: * indicates data used as corroborative inputs to this AMR

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5. ASSUMPTIONS

The Seepage Model for PA (SMPA) follows the approach and modeling framework described in Birkholzer et al. (1999 [105170], pp. 358–362) and is based on the Seepage Calibration Model (SCM) presented in CRWMS M&O (2000 [153045], Sections 5 and 6). These documents provide the necessary scientific and technical background for the readers to understand this AMR. In particular, SMPA uses parameters determined in the SCM and is consistent with the SCM.

The general model assumptions and justifications are the same as those of the SCM presented in CRWMS M&O (2000 [153045], Section 5). The applicable assumptions are essentially reproduced below.

5.1 CONTINUUM APPROACH

Assumption: It is assumed that the continuum approach is a valid concept to calculate percolation flux and drift seepage at Yucca Mountain.

Rationale: The continuum approach can be considered appropriate for seepage studies if it is capable of predicting seepage threshold and seepage percentages for a drift in a fractured formation. The appropriateness of using the continuum approach to simulate flow through fractured rock was studied by Jackson et al. (2000 [141523], pp. 189–202) using synthetic and actual field data. They concluded that heterogeneous continuum representations of fractured media are self-consistent, i.e., appropriately estimated effective continuum parameters are able to represent the underlying fracture-network characteristics. Furthermore, Finsterle (2000 [151875], pp. 2055–2066) demonstrated that simulating seepage into underground openings excavated from a highly fractured formation could be performed using a model based on the continuum assumption, provided that the model is calibrated against seepage-relevant data (such as data from liquid-release tests). Synthetically generated data from a model that exhibits discrete flow and seepage behavior were used to calibrate a simplified fracture continuum model. Seepage predictions for low percolation fluxes made with the calibrated fracture continuum model were consistent with the synthetically generated data from the discrete feature model.

The continuum approach is considered applicable for seepage studies if applied within the framework described in this AMR. Inverse modeling should be used for the estimation of process-specific, model-related, and scale-dependent parameters, and the same or similar conceptual model should be used for the subsequent seepage predictions (i.e., the Seepage Model for PA). Under these conditions, this assumption does not require confirmation.

5.2 UNSATURATED FLOW

Assumption: Adopting the continuum approach, water flow under unsaturated conditions is assumed to be governed by Richards' equation (Richards 1931 [104252], pp. 318–333).

Rationale: Richard's equation states that isothermal flow of water in a porous medium occurs under the combined effect of gravitational and capillary forces, that flow resistance is a function of saturation, and that, for the purposes of this representation, movement of the nonwetting air phase can be neglected. This general concept is believed reasonable for unsaturated water flow through both porous matrix and fractures and does not require confirmation.

5.3 AIR PERMEABILITIES

Assumption: Permeabilities determined from air-injection tests are assumed representative of the hydraulic conductivity of the excavation-disturbed zone around the opening.

Rationale: A detailed discussion of this assumption is given in CRWMS M&O (2000 [141400], Sections 5.1 and 5.2.1). The assumption holds for the purposes of the current application, where postexcavation air-injection tests were conducted in a dry fracture network. Air-permeability estimates are used to condition the generation of a spatially correlated, random permeability field. Potential inaccuracies in this assumption are compensated for by the estimation of the van Genuchten $1/\alpha$ parameter (Luckner et al. 1989 [100590], pp. 2191–2192). Air-injection tests are a standard method to obtain drift-scale permeability values (CRWMS M&O 2000 [141400], Section 6.1). The use of these values during calibration and prediction of seepage ensures consistency.

Excavation effects increase the permeabilities around the niches and the Cross Drift (Wang and Elsworth 1999 [104366], pp. 751–757; CRWMC M&O 2000 [141400], Section 6.1.2.2). Since seepage is determined by the formation properties within the boundary layer in the immediate vicinity of the opening, it is reasonable to use postexcavation air-permeability data for seepage calculations.

This assumption does not require confirmation.

5.4 CHARACTERISTIC CURVES

Assumption: Relative permeability and capillary pressure are assumed to be described as continuous functions of effective liquid saturation, following the expressions given by the van Genuchten-Mualem model (Luckner et al. 1989 [100590], pp. 2191–2192) as implemented in the iTOUGH2 code (Finsterle 1997 [104043], p. 224). Capillary strength (represented by the $1/\alpha$ parameter) and permeability are not correlated.

Rationale: The van Genuchten-Mualem model is the standard model used in the suite of UZ flow and transport models; it was chosen here for consistency. Furthermore, the applicability of relative permeability and capillary pressure functions is consistent with the continuum assumption (see Section 5.1) and is appropriate to represent fractures that are rough and/or partially filled with porous material. The functional relationship describing the potential correlation between permeability and capillary strength is unknown. An increase in permeability may be attributed to larger fracture apertures (which would reduce capillary strength) or to an increase in fracture density (which would not affect capillary strength). The capillary strength parameter $1/\alpha$ is taken to be constant and will be subjected to estimation by inverse modeling. The calibration process and the consistent conceptualization in the downstream models (specifically the Seepage Model for PA) make this assumption a valid approach.

This assumption does not require confirmation.

5.5 MATRIX IMBIBITION

Assumption: The transient effects from matrix imbibition in a fracture-matrix system are assumed to be small and do not need to be modeled explicitly in the SCM (CRWMS M&O 2000 [153045]). Further, the imbibition and flow into the matrix continuum is not considered in the SMPA.

Rationale: Matrix permeability is low, and the potential for matrix imbibition is limited because of relatively low porosity and relatively high liquid saturation. In a fracture-matrix system, the transient effects from matrix imbibition are restricted to intermediate times, i.e., they are insignificant (1) for a short-term liquid-release test with insufficient time for matrix imbibition, and (2) for a long-term seepage experiment, when near-steady late-time data are no longer affected by matrix imbibition. To match intermediate times during a long-term test, an effective porosity is estimated by inverse modeling to account for the storage capacity of both the fracture system and the matrix. Porosity estimates are irrelevant in the subsequent simulations of seepage under natural flow conditions, which are near steady state.

For SMPA, the imbibition and flow into the matrix continuum is not considered. The rationale is that in the current AMR, except for the episodic percolation flux case (Sections 6.5 and 6.6.6), we are calculating steady-state flow conditions over long time frames. At steady-state, the flow exchange between fracture and matrix continua will settle to a small amount with the matrix close to full saturation. The flow partitions between the fracture and matrix continua according to their effective permeabilities and porosities, and it follows that the matrix with its five to six orders-of-magnitude lower permeability would not have significant effects on seepage into drift, which would be controlled by the flow in the fracture continuum. For the episodic percolation flux case (Sections 6.5 and 6.6.6), the matrix continuum provides a damping effect on seepage in the fracture continuum, and neglecting it represents a conservative case.

5.6 EVAPORATION

Assumption: The effect of evaporation on the observed seepage rates is insignificant, i.e., water removal from the formation, at the drift surface, and from the capture system by evaporation and vapor diffusion is assumed to be small.

Rationale: Under isothermal conditions, potential evaporation at the drift wall or in the capture system is small compared to the amount of water being released. Seepage experiments in the middle nonlithophysal zone of the Topopah Spring welded unit were conducted in niches that were closed off by a bulkhead, which leads to comparatively high relative humidity and low air circulation. Moreover, a humidifier was used in some of the experiments to ensure high relative humidity. For these conditions, Ho (1997 [141521], pp. 2665–2671) and Or and Ghezzehei (2000 [144773], pp. 381–393) provide a detailed description of evaporation mechanisms on the scale of individual water droplets within fractures or emerging from fractured formations. The evapo-infiltration thresholds calculated by Ho (1997 [141521], p. 2670) are significantly lower than the applied injection rates, suggesting a very minor influence of evaporation on measured seepage rates in experiments conducted in the niches.

Evaporation from a large surface of free or nearly free water, however, may be significant. As injected water reaches the opening, it spreads along the surface on account of capillarity within the rough surface. As a result, water potentially seeping into the opening may not only form droplets with a small surface area, but may be spread over a large area, providing a large surface for evaporation. Depending on the evaporation potential of the air in the opening, the water film covering the wall of the opening may evaporate at a rate comparable to the injection or seepage rates.

Moreover, evaporation may be significant during periods of active ventilation with high airflows in the drift in combination with low injection rates. Under these specific conditions, the evaporation rate may exceed the potential seepage rate, preventing the development of liquid droplets that drip into the opening. Ventilation effects are evident from the seepage data collected in the Cross Drift (see Section 6.3.3.3). To reduce the impact from ventilation effects, calibration of the SCM was restricted to seepage rate data collected during nighttime and weekends, when ventilation was turned off.

Currently, no quantitative estimates of evaporation potential under the conditions of the seepage experiments are available. The simplified assumption that evaporation rates are small compared to the injection rates is non-conservative if used for inverse modeling and is therefore an assumption that needs to be verified (TBV-4951 [153049]).

It is important to realize that a non-conservative assumption made in an inverse model is a conservative assumption when used for seepage predictions in a forward model. Specifically, neglecting evaporation effects by prescribing a 100% relative-humidity boundary condition in a forward seepage prediction model (such as the SMPA) is a conservative assumption. While such a model underestimates vapor flow, it yields the maximum liquid-phase influx, which is defined here as drift seepage. The underestimation of vapor flow is irrelevant, since the assumption of 100% relative humidity already implies that the moisture content in the drift environment is as high as possible, maximizing the amount of moisture that can condense within the waste-emplacement drift. In a ventilated drift, the development of a dry-out zone increases the capillary pressure and local storage volume and thus reduces the risk of reaching seepage conditions; the assumption of 100% relative humidity in the drift is again conservative. The assumption is also reasonable for the time when ventilation is stopped and the waste-emplacement drift is closed. A repository design that includes ventilation yields reduced seepage.

5.7 PERCOLATION FLUX RANGE USED IN THIS AMR

Assumption: It is assumed that the range of values for percolation flux used in simulations in this AMR is appropriate.

Rationale: For SMPA calculations, five values for Q_p are used, ranging from 5 to 500 mm/yr; more specifically Q_p = 5, 14.6, 73.2, 213 and 500 mm/yr. The justification for the choice of this range is so that the range covers various estimates of percolation fluxes. Wu et al. (1999 [117161], p. 210) calculated the percolation flux expected at the repository level, based on a 3D UZ model of Yucca Mountain. They obtained an average fracture flow of 4 to 5 mm/yr at the repository level under present climate conditions. Ritcey and Wu (1999 [139174], p. 262) found that under a climate scenario simulating the most recent glacial period, the percolation flux ranges from 0 to 120 mm/yr, with the peak of the probability distribution to be around 20 mm/yr. The upper limit of 500 mm/yr is chosen to accommodate potential flow focusing in the geologic layers above the drift and to safely bracket an uncertainty range more than four times the high flux value of 120 mm/yr. In cases where seepage is very low or zero, even larger Q_p values are also used to find when seepage might occur.

This assumption does not require confirmation.

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6. ANALYSIS/MODEL

6.1 OBJECTIVES AND OUTLINE

In this AMR, we model drift seepage under long-term, steady-state, and episodic conditions for a range of parameters and conditions (such as drift collapse scenarios). Seepage of water into waste emplacement drifts is considered one of the principal factors having the greatest impact of long-term safety of the repository system (CRWMS M&O 2000 [148713], Table 4-1). The model SMPA follows the SCM presented in CRWMS M&O (2000 [153045], Sections 5 and 6) and is also described in Birkholzer et al. (1999 [105170], pp. 358-362). The physical framework and mathematical construct of this model is identical to that of SCM (CRWMS M&O, 2000 [153045], Sections 5 and 6) with the only difference being the manipulation of the output data to obtain seepage results. The objectives of SMPA are to calculate seepage values for different values of percolation flux down to the drift, to discuss the effect on seepage resulting from various processes such as excavation-induced drift degradation (i.e., drift collapse), and to provide results as input to PA.

This section will first discuss the validity of this analysis for its intended purpose. Then, the geometry used, the ranges of parameters, and the choice of conditions will be presented and rationalized. Next, results will be given. Finally, the AMR will conclude with discussions of alternative models and conclusions.

Key scientific notebooks (with relevant page numbers) used for modeling activities described in this AMR are listed in Table 3.

Table 3. Scientific Notebooks

LBNL Scientific Notebook ID	Author/year	M&O Scientific Notebook Register ID	Page Numbers
YMP-LBNL-CFT-GL-1	Li, G./2000 [153480]	SN-LBNL-SCI-033-V1	71–72, 86–89, 125–156
YMP-LBNL-CFT-GL-2	Bodvarsson, G./2000 [153484]	SN-LBNL-SCI-189-V1	7–21
YMP-LBNL-DSM-MC-1	Cushey, M./2000 [153481]	SN-LBNL-SCI-052-V1	1–42

Note that the results in the current AMR Rev 01 are very different from those of the earlier version Rev 00. This is because we have made use of the new results from the SCM (CRWMS M&O 2000 [153045], Sections 5 and 6), with the following significant changes:

(1) At the drift wall, the last vertical connection between the drift surface and the gridblock in the rock next to it is set equal to 0.05 m, implying a direct gravity-controlled vertical flow with no horizontal diversion within this 0.05 m distance (Section 6.3).

(2) There is no correlation between k and $1/\alpha$ (Sections 5.4 and 6.8).

Both these two points are made to make the SMPA consistent with the SCM (CRWMS M&O 2000 [153045] Sections 5 and 6). Further, the SCM also provides results for the Topopah Spring lower lithophysal (Tptpll) unit, which were not available at the time of Rev00.

6.2 MODEL VALIDATION

Validation of a model normally requires testing model results against relevant data that were not used in the original development of the model and that are appropriate to the intended use of the model. For the Seepage Model for PA, these data should include percolation flux at low flow rates over periods of years, even hundreds of years, in many locations in the repository block (for proper statistical representation). No such data are available. Further, data for adequate validation would need to cover the wide range of conditions (such as drift degradation and collapse with time) studied in this AMR. Those are not available either. This lack of data results in the use of alternative approaches for model validation as described in Section 5.3c of AP-3.10Q. First, the relevant physics of the problem as represented by Richards' equation (Richards 1931 [104252], pp. 318–333), the van Genuchten-Mualem model (Luckner et al. 1989 [100590], pp. 2191–2192), Philip's studies (Philip et al. 1989 [105743], pp. 16–28), and effects of flow channelization resulting from heterogeneity and ponding (Birkholzer and Tsang 1997 [119397], pp. 2221–2224; Birkholzer et al. 1999 [105170], pp. 370–379) are used. These are all in the open literature and have gone through proper technical peer review and have withstood scrutiny of the scientific community since their dates of publication (AP-3.10Q, Section 5.3.c.2). Further, as stated in Section 6.1, the physical framework and mathematical construct of the SMPA is identical to that of the SCM; thus the validation of the SCM, documented in CRWMS M&O 2000 [153045] Section 6.3.4 is applicable to the validation of the SMPA in that, the SCM model is consistent with results from niche seepage tests in the ESF (Wang et al. 1999 [106146], pp. 332–338). These data were used in the SCM on which the seepage model is based (AP-3.10Q, Section 5.3.c.5), as described in CRWMS M&O (2000 [153045], Section 6).

In summary, the model validation for SMPA is supported by the following:

- The physical framework and mathematical construct of the SMPA and SCM are identical, except for manipulation of output data to obtain seepage results. Thus, the testing of SCM against field data directly supports the validation of SMPA;
- Parameters used are reasonable and consistent with all relevant data as discussed in Section 6.3;
- The basic physics used in the SMPA and particularly the SMPA have been published in the open literature (Birkholzer et al. 1999 [105170], pp. 349–384) and have gone through peer review and public scientific scrutiny. Thus, based on these external pieces of evidence, the analysis and predictions using the SMPA presented here, with proper uncertainty ranges assigned to these predictions, is an acceptable representation of the process system.

6.3 THE SMPA AND SELECTION OF CASES

The SMPA follows the SCM (CRWMS M&O, 2000 [153045], Section 6) and is also described in Birkholzer et al. (1999 [105170], pp. 358–362), which provide the scientific and technical background for this AMR. The conceptual model is a heterogeneous permeability field for the fracture continuum generated with parameters discussed below, using the SISIM module of the GSLIB package (GSLIB V2.0, 10098-2.0MSISIMV2.0-00 [146609]). The 3D field is 20 m vertical, 15 m wide normal to drift axis and 5.23 m along the drift axis. With the drift of 5.5 m diameter (see Section 6.3.1) an overlying thickness of 9.75 m, an underlying thickness of 4.75 m, and the distance to either side boundary of 4.75 m, the vertical cross section dimensions were chosen to be wide enough to capture the main flow feature, i.e. flow diversion around the drift (Philip et al. 1989 [105743], p. 21, Figure 1). The distance along the drift axis is defined by the waste package length being 5.13 m (see below), with 0.1 m between the waste packages (DTN: SN9908T0872799.004 [108437]). The side boundary conditions are no-flow, the lower boundary condition is gravity drainage, and the upper boundary surface is simulated by an extra grid cell with constant percolation flux connected to all the grid cells in the first row. Flow is thus free to move into these cells according to local property parameters. Regarding the no-flow boundary condition on the two planes at the end of the waste package normal to the drift axis: for a homogeneous, constant-property medium, these planes are symmetry planes between successive waste packages, and a no-flow boundary condition is justified. For a heterogeneous system, the issue is the length of the flow domain versus the spatial correlation length λ. From Section 6.3.6 below, $\lambda = 0.5$ m so that the length of the domain is about 10 correlation lengths and the effect of the no-flow boundary should not have a significant effect on the flow results.

The mesh is generated using the AMESH V1.0 code (AMESH V1.0, 10045-1.0-00 [153216]), with grid cell dimension of 0.5 m $\times$ 0.5 m $\times$ 0.5 m, chosen as a compromise between being fine enough to include the main flow feature and being coarse enough to allow the feasibility of about 1000 3D stochastic simulations. As discussed in Section 6.7 of this AMR, the choice of grid size is not related to Philip's boundary layer at the drift crown (Philip et al. 1989 [105743], p. 21, Figure 1), but to heterogeneity field characteristics. A numerical study (Li 2000 [153480], pp. 86–89) has shown that 0.5 m is an adequate grid size for our calculations (discussed in Section 6.7).

Except for the cases involving the effect of large correlation length values (λ=1 or 4 m), the spatial correlation length λ is chosen to be equal to the grid size of 0.5 m. This choice implies an uncorrelated spatial distribution of permeability values. This is consistent with CRWMS M&O (2000 [153045], Section 6.3.2.1) where λ is 0.2 m, which is smaller than our grid size for the case of the lower lithophysal zone. CRWMS M&O (2000 [153045], Section 6.4.2.1, Figure 9) also shows that, for the middle nonlithophysal zone, the nugget and sill values in the semivariograms are similar to each other, indicating an uncorrelated structure.

At the drift wall, the nodal distance between the drift surface and the grid cell representing the drift is set to be very small, so that the boundary condition can be applied directly at the drift wall. The length of the last vertical connection between the drift wall and the neighboring gridblocks representing the formation is set equal to 0.05 m. This is done to make our model consistent with the Seepage Calibration Model SCM (CRWMS M&O 2000 [153045], Sections 6.3.2.2 and 6.4.2.2), whose parameter values are used in the current calculations. The choice of this 0.05 m vertical connection to the drift wall implies a direct gravity-controlled vertical flow, with no horizontal diversion within this 0.05 m distance. (This is sometimes called a "needle" or "discrete surface fracture" effect.) Because of this 0.05 m vertical gravity flow at the drift wall, a capillary pressure that is higher (less negative) than -490 Pa at the grid cells in the formation next to the drift wall will induce seepage into the drift. This is because the -490 Pa is insufficient to balance the hydrostatic pressure that develops along the 0.05 m vertical connection (CRWMS M&O 2000 [153045], Sections 6.3.2.2 and 6.4.2.2). For $1/\alpha$ values of 870 Pa (see Section 6.3.5

below), this means that seepage occurs when saturation in the grid cell next to the drift wall exceeds 90%.

A comment needs to be added here. The SCM uses a grid size of 0.1 m, whereas in SMPA a grid size of 0.5 m is used, because, for the latter, a large number of simulation needs to be made and a finer mesh is impractical in terms of computational effort. The inaccuracy introduced by a coarser mesh (grid size from 0.5 m to 0.25 m) is discussed in Section 6.7. In general, so long as the vertical connection of the last grid block in the drift ceiling and the drift wall is set at 0.05 m (see last paragraph), the grid size dependence is probably similar to or less than the spread between multiple realizations of the heterogeneous field.

Flow calculation was performed using ITOUGH2 V3.2_drift (ITOUGH V3.2_drift, 10055-3.2_DRIFT-00 [112757]). A number of routines were also used for pre-processing of inputs for ITOUGH2 V3.2_drift. These are listed in Table 1, documented in Li 2000 [153480], pp. 128–129, 145–149, and provided in Attachment II.

The selection of parameter ranges and particular cases to be modeled is presented in this subsection together with the rationale for the selection. For the most part, a drift emplaced in the Topopah Spring middle nonlithophysal zone (UZ model layer tsw34, lithostratigraphic unit Tptpmn) is considered. The discussion of parameter values below mainly refers to this unit. However, additional data from the lower lithophysal unit have also been analyzed in the SCM (CRWMS M&O 2000 [153045], Section 6.3); the parameter values for this unit are also covered by the selected range of parameters. Figure 1 is a sketch summarizing the modeling cases, which can be used as a guide to the discussions below. The top part of Figure 1 shows a 3D space, defined by the three parameters that are expected to be most sensitive in affecting drift seepage, namely, fracture continuum permeability k_{FC}, van Genuchten $1/\alpha$ value, and the standard deviation σ of ln k_{FC}, which is a measure of heterogeneity of the permeability field. For each combination of these three parameters (i.e., at each grid point), seepage model calculations will be made for three realizations, using a range of values for percolation flux Q_p at the repository level. Five values of k_{FC}, four values of $1/\alpha$, three values of σ_{lnk}, and five values of percolation flux are examined, for each of three realizations, for a total of 900 cases. Two particular combinations of parameters, Set A and Set B, are selected for additional studies. These correspond to the calibrated parameters from the SCM (CRWMS M&O 2000 [153045], Sections 6.3 and 6.4) for the middle nonlithophysal and lower lithophysal zones, respectively. Their values are discussed in Section 6.3.6.

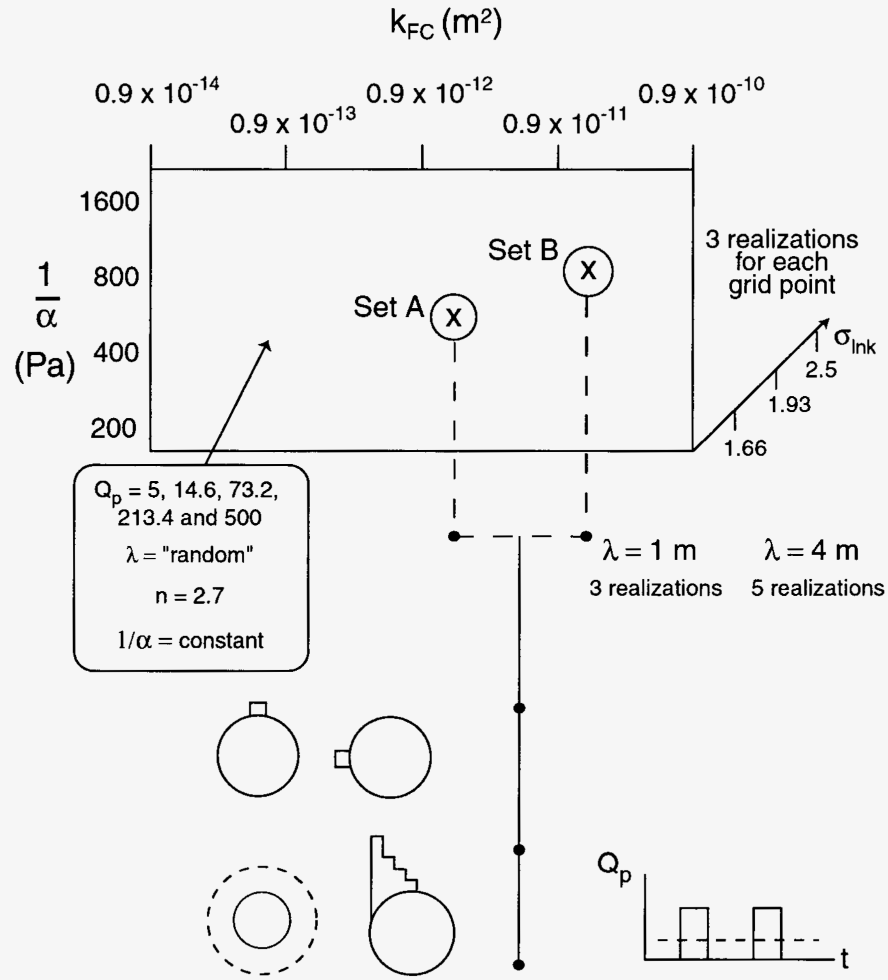


Figure 1. Cases Studied.

The middle-right part of Figure 1 indicates a study of drift seepage for three alternative permeability spatial correlation lengths λ. This allows an evaluation of the effect of this important parameter, which is difficult to determine in the field. The minimum set of parameters that describe a simple heterogeneous field can be the two parameters σ and λ (based on a spherical semi-variagram model). Thus, the study will indicate how seepage depends on the heterogeneity of the permeability field.

The lower left part of Figure 1 shows the disturbed drift seepage submodel. Based on a review of current information, alternative drift degradation modes are evaluated (see below) and four scenarios are identified for seepage model studies as indicated. The lower right part of Figure 1 shows a comparison of the constant-flux case with a case in which the percolation flux above the drift is episodic rather than at a constant average value, so that all the flux comes within a short period of time, with no flux between such pulses. Both episodic and constant average value cases will also be evaluated.

All the cases are computed on 3D heterogeneous unsaturated systems. Because some cases involve more than one run, altogether more than 1,000 runs were made. What follows below, after the specification of drift geometry, are the choices of parameter ranges on which seepage calculations are performed. These choices are based on a comprehensive review of available relevant data. However, the data are not used directly to produce a single set of simulation results, but rather as references to establish parameter ranges.

6.3.1 Geometry

As provided in DTN: SN9908T0872799.004 [108437], the drift diameter is 5.5 m and the drift section under study has the same length as that of a waste package, with half the spacing to the next waste packages on its two ends. Since the waste package length is 5.13 m and the spacing between the waste packages is 0.1 m, the drift section modeled is 5.23 m. This drift section is emplaced in a heterogeneous fracture continuum of dimensions 15 m wide and 20 m high, following Birkholzer et al. (1999 [105170], p. 360).

6.3.2 Fracture Continuum Permeability k_{FC}

As shown in Figure 1, the range of permeability chosen for the fracture continuum k_{FC} is from 0.9×10^{-14} m^2 to 0.9×10^{-10} m^2. This subsection reviews field measurements to show that this range is necessary and adequate. The upper limit of this choice of range is set to cover the mean permeability values measured in Niche 3107, Niche 3650, Niche 4788 and borehole SYBT-ECRB-LA#2 (CRWMS M&O 2000 [153045], Table 4). The three niches are situated in the Tptpmn middle nonlithophysal zone. The SYBT-ECRB-LA#2 tests were made in the Topopah Spring lower lithophysal unit (Tptpll). Note that the parameter value is based on field air-permeability data (see Table 2, Row 7 for DTN), which were collected around niche 3650 that has been impacted by excavation. Air permeability represents mainly permeability of the fractures, whose permeability is much larger and whose water capillary effect is much smaller than those of the rock matrix. The excavation is a coupled hydromechanical process in which the fracture apertures may be made larger in the immediate neighborhood of the opening. Permeability changes associated with these aperture changes can be as much as two orders of magnitude (Wang et al. 1999 [106146], p. 328, Figure 3; DTN: LB0011AIRKTEST.001 [153155]).

Because only one borehole was available the lower limit of the range of air permeability before excavation is taken from Wang et al. (1999 [106146], p.328) but is corroborated with data from SYBT-ECRB-LA#2 (LB000900122134.001 [153141]). The geometric mean value of air permeability is 6.6×10^{-14} m^2. This is based on their tests in boreholes at niche 3650, with a packer interval of 0.3 m (Wang et al. 1999 [106146], p. 325). Air-injection tests were also carried out in the SHT area in the ESF. There, the packer intervals are typically 3 to 7 m, and the mean permeability was found to be 5.8×10^{-14} m^2 (Tsang and Birkholzer 1999 [137577], p. 393). Air-permeability measurements were also carried out in the DST block in the ESF, where the geometric mean permeability was found to be 10^{-13} m^2, with a standard deviation in ln k_{FC} of 2 (Birkholzer et al. 1999 [105170], p. 359). Here, the packer intervals are mainly between 10–20 m in length. The DTNs for these data are provided in Table 2, Rows 4 and 5.

The mean air-permeability values without excavation effects, for the three sources mentioned in the last paragraph, are 0.7×10^{-13} m^2, 0.6×10^{-13} m^2 and 10^{-13} m^2 (Table 2, Rows 5 and 7) after being rounded to one significant figure. They are quite consistent with each other, even though the packer intervals used in the tests ranged from 0.3 m to ~20 m. These values are somewhat more than one order of magnitude smaller than post-excavation values (geometric mean $k = 1.4 \times 10^{-12}$ m^2). For seepage into drifts, the permeability of rock near the drift (i.e., the post-excavation value) is the relevant value. Thus, the weighting of seepage results in this table should be at this larger permeability value. On the other hand, the excavation effect on permeability depends on local fracture orientation, distribution, and density (as well as on excavation methods). All these factors carry sufficient uncertainty to require computing seepage percentages over the full range of fracture continuum permeability, 0.9×10^{-14} m^2 to 0.9×10^{-10} m^2, as shown in Figure 1.

Note that Ahlers et al. (1999 [109715], p. 66), from their analysis of pneumatic data in surface-based boreholes, give air permeability for the TSw units as 4×10^{-12} m^2 vertical, and 8×10^{-13} m^2 horizontal. Also, air-injection tests in four surface-based deep boreholes, UE–25 UZ#16, USW SD–12, USW NRG–6, and USW NRG–7a (LeCain 1997 [100153], pp. 2, 11–14), give permeability for the Tptpmn unit as ranging from $\sim 2.5 \times 10^{-14}$ to $\sim 1 \times 10^{-11}$ m^2, based on measurements with packer intervals of 3.5–4.9 m. These results are all covered by the range of values in Figure 1.

6.3.3 Standard Deviation of ln k_{FC}

For the three Niches in the middle nonlithophysal zone, CRWMS M&O (2000 [153045], Table 4, DTN: LB0010SCREV01.002 [153393]) gives values for the standard deviation of fracture continuum permeability in log base 10 varying from 0.72 to 0.84, which translates to a standard deviation σ (in ln k_{FC}) of 1.66 to 1.93. For comparison, Birkholzer et al. (1999 [105170], p. 359), used $\sigma = 2.1$. For the lower lithophysal unit, output from CRWMS M&O (2000 [153045]; DTN: LB0010SCREV01.002 [153393]) gives a log base 10 standard deviation of 0.21, corresponding to σ in ln k_{FC} of 0.48. This is, however, based on six measurements in one borehole only.

In a numerical study of seepage from a heterogeneous fracture continuum into a drift, Birkholzer et al. (1999 [105170], p. 371, Figure 14) found that drift seepage tracks the probability for finding local ponding in the heterogeneous field and, further, the ponding probability is smaller for smaller permeability standard deviations (Birkholzer et al. 1999 [105170], p. 375, Figure 17). Hence less seepage is expected for smaller σ values. Thus, in this AMR the dependence on σ is studied by calculating all cases for three alternatives, $\sigma = 1.66$, 1.93, and 2.5. The first two values represent the smallest and largest values found in niche studies in the Tptpmn unit (CRWMS M&O 2000 [153045], Table 4). Detailed results are presented using these two values in Section 6.6.1. The last σ value is a higher value used to explore the effect of higher σ.

6.3.4 Special Cases for Sensitivity Studies

For each combination of k_{FC}, $1/\alpha$ and σ values (see top part of Figure 1), calculations for three realizations were done to obtain an estimate of the variation range as a result of geostatistical variability. These multiple-realization results give a preliminary lower estimate of the spread of seepage predictions resulting from the geostatistical variability.

For further sensitivity studies on parameters (see below), two particular parameter sets out of the 3D table of (k_{FC}, $1/\alpha$, σ) values (see Figure 1) were selected. The first Set A is the set of calibrated mean parameters for the middle nonlithophysal zone given by the SCM (DTN: LB0010SCMREV01.002 [153393]):

$$\left.\begin{aligned} k_{FC} &= 1.38\times10^{-12}\ m^2 \\ 1/\alpha &= 589\ Pa \\ n &= 2.55 \\ \sigma &= 1.93 \end{aligned}\right\} \quad \text{Set A}$$

and the second parameter set, Set B, is chosen to be the set of mean calibrated parameters for the lower lithophysal unit (DTN: LB0010SCMREV01.002 [153393]):

$$\left.\begin{aligned} k_{FC} &= 1.86\times10^{-11}\ m^2 \\ 1/\alpha &= 871\ Pa \\ n &= 2.57 \\ \sigma &= 1.93 \end{aligned}\right\} \quad \text{Set B}$$

Here σ=1.93 is used for both sets as a more conservative value (i.e., the highest value for three niches, as discussed above under Section 6.3.3).

An additional parameter set, Set B′, is also considered and presented in Attachment III. Set B′ is identical to Set B except it uses a $1/\alpha$ value of 537 Pa. Set B′ is intended to compensate for the effect of lithophysal cavities which tend to increase seepage.

6.3.5 van Genuchten Parameters

The van Genuchten n parameter used by Birkholzer et al. (1999 [105170], p. 354, Table 1) has a value of 2.7, simply calculated as n=1/(1-m), from the m parameter value of 0.63 (DTN: LB990861233129.001 [110226]). CRWMS M&O (2000 [153045], Tables 6 and 8), on the other hand, uses the values n = 2.57 and 2.55 for the lower lithophysal and the middle nonlithophysal zone, respectively (DTN: LB0010SCMREV01.002 [153393]). In that calibration study, n is not varied, since it is not as sensitive a parameter as the van Genuchten α parameter and the effective porosity, which were indeed varied in the calibration (CRWMS M&O 2000 [153045], Sections 6.3.3 and 6.4.3). Considering these studies, the one single value for n = 2.7 is used, as it is based on fracture information in the ESF. Then a sensitivity study is made by running cases of Parameter Set A and Set B, with n = 2.55 and n = 2.57 respectively. As will be shown below (Section 6.6.3), the differences in seepage results are insignificant.

For the range of $1/\alpha$ values, CRWMS M&O (2000, Section 6.3.3.3 and Figure 6) provides a calibrated mean of 871 Pa for the lower lithophysal unit, with the interval from 740 to 1020 Pa containing 2/3 of the $1/\alpha$ values from their multiple realization studies. Birkholzer et al. (1999 [105170], p. 354, Table 1), on the other hand, used an α value of $9.73\times10^{-4}\ Pa^{-1}$, which translates to $1/\alpha = 1028$ Pa. For the middle nonlithophysal zone, CRWMS M&O (2000

[153045], Table 9, DTN: D010SCMREV01.002 [153393]) provides a calibrated mean for $\log_{10}$ $(1/\alpha)$ of 2.77 and standard deviation of 0.05, which translates to a mean for $1/\alpha$ of 589 Pa and the values at one standard deviation above and below the mean for $1/\alpha$ of 525 Pa to 660 Pa respectively. To cover all these values, four $1/\alpha$ values, namely 200, 400, 800, and 1600 Pa, are chosen, as shown in Figure 1.

6.3.6 Additional Special Cases for Sensitivity Studies on Spatial Correlation Length λ of k_{FC}

The analysis of air injection tests in the AMR (CRWMS M&O 2000 [153045], Section 6.4.2.1) suggests that "the permeability is essentially random without a noticeable or significant spatial correlation" for the middle nonlithophysal zone. Note that though the results show λ=0.61–3.87 m (CRWMS M&O 2000 [153045], Table 7), in their curves the correlation length is small or the nugget values are close to the sill values, in which case the precision of determining λ is very poor. In fact, if the nugget and sill values are equal, λ is undefined. The results can be taken to indicate spatially uncorrelated structure. Thus, for the main set of calculations covered in this report, heterogeneous fields with neglecting spatial correlation are generated, corresponding to no spatial correlation. This is also consistent with the SCM for the lower lithophysal zone, where CRWMS M&O (2000 [153045], Section 6.3.2.1) takes λ=0.2 m, which is smaller than the grid size used in this AMR.

Since λ is in general not an easily-determined parameter *in situ*, cases with alternative λ values were calculated to investigate its sensitivity. For the two parameter sets, Set A and Set B, the alternatives of $\lambda = 1$ m and $\lambda = 4$ m are studied. For the former, again three realizations are considered, while for the latter, because of the relatively large λ value as compared with the drift diameter, large variations in results are expected and five realizations are evaluated. While the many calculations made in this AMR aim towards understanding the trends of seepage results, Set A and Set B are established to be closest in representing actual field properties for the middle nonlithophysal and lower lithophysal zones, respectively.

6.3.7 Percolation Flux, Q_p

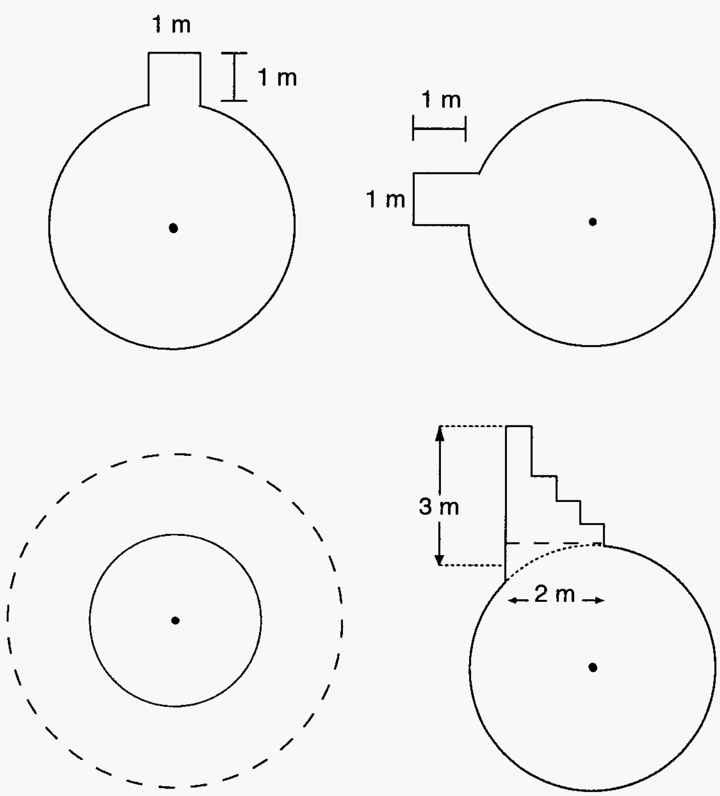
For SMPA calculations, five values for Q_p are used, ranging from 5 to 500 mm/yr; more specifically $Q_p = 5$, 14.6, 73.2, 213 and 500 mm/yr. The range is chosen to cover various estimates of percolation fluxes. Wu et al. (1999 [117161], p. 210) calculated the percolation flux expected at the repository level, based on a 3D UZ model of Yucca Mountain. They obtained an average fracture flow of 4 to 5 mm/yr at the repository level under present climate conditions. Ritcey and Wu (1999 [139174], p. 262) found that under a climate scenario simulating the most recent glacial period, the percolation flux ranges from 0 to 120 mm/yr, with the peak of the probability distribution to be around 20 mm/yr. The upper limit of 500 mm/yr is chosen to accommodate potential flow focusing in the geologic layers above the drift and to safely bracket an uncertainty range more than four times the high flux value of 120 mm/yr. In cases where seepage is very low, even larger Q_p values are also used to find when seepage might occur.

6.4 IMPACT OF DRIFT DEGRADATION ON SEEPAGE

Drift degradation may occur in three ways:

1. Loosening of rock blocks and hence wider fracture aperture (fracture dilation) (Section 6.4.1)
2. Rock fall from the ceiling of the drift (Section 6.4.2)
3. Extended rock failure in drift roof (Section 6.4.3)

These are discussed below. Based on these discussions, a drift degradation submodel was designed to evaluate the impact of drift degradation on seepage, and it is shown in Figure 2 as four alternative scenarios.



NOTE: Top two sub-figures are discussed in Section 6.4.2; lower left figure is discussed in Section 6.4.1 and lower right figure discussed in Section 6.4.3.

Figure 2. Drift Degradation Submodel Scenarios.

6.4.1 Fracture Dilation

Because of excavation, stress is relieved at the drift, and fractures are expected to dilate at certain areas around the drift (see lower left part of Figure 2). Such fracture dilation depends on the orientation of the fracture set and generally occurs within one drift radius (Brekke et al. 1999 [119404], Figures E-5, E-11 and E-13). An increase in fracture aperture generally causes an increase in fracture permeability and a decrease in $1/\alpha$ value. The measured increase in permeability from the pre-excavation to the post-excavation values (Wang et al. 1999 [106146],

p. 328, DTN: LB0011AIRKTEST.001 [153155]) is a result of this effect. In this sense, both Parameter Set A and Set B, Section 6.3.6 (see also Figure 1), which are based on *in situ* post-excavation calibration results, already have taken this into account. This means that the rock properties already represent the total effect of the near-field disturbed zone and the far field as shown in Figure 2, lower-left. Results are given in Tables 4–8, and no further calculations are necessary.

The possibility exists that new fractures may be formed during stress relief. In general, an increase in k_{FC} could be due to either an increase in the number of fractures or an increase in apertures. It is only with the latter case that $1/\alpha$ will be decreased. Thus the part of increase of k_{FC} due to the creation of new fractures will be accompanied by a decrease in $1/\alpha$ values. In this case, k_{FC} will be increased with a relatively smaller decrease in the $1/\alpha$ value. This conservative scenario is, however, not studied because it would lead to less seepage.

6.4.2 Rockfall from Drift Ceiling

CRWMS M&O (2000 [151554], Tables 20–21, 26–27, 35–36, 41–42) used the key block theory to calculate rockfall probability in the drifts, under various scenarios, based on fracture maps in the ESF. For the Topopah Spring middle nonlithophysal zone, the number of key blocks per kilometer of the drift was calculated to be less than 44 over these scenarios, and the volume of total rockfall per kilometer to be less than 36 m^3. This implies that rockfall occurs on the average of one block every 23 m and that the mean size of the block is about 0.8 m^3. This is confirmed by the result that 80% of the blocks are smaller than 1 m^3 (CRWMS M&O 2000 [151554], Figures 19–20, 27–28, 32–33, 36–37). Hart in Brekke et al. (1999 [119404], p. E-12) used a 2D discrete-element method and found rockfall to occur at the spring line of the drift and the size of the block to depend on the assumed fracture spacing. To study the effect of rockfall on seepage, two calculations were made, one in which a 1.0 m^3 block is taken out from the crown of the drift and the second in which the 1.0 m^3 block is taken out at the spring line (see Figure 2).

6.4.3 Extended Rock Failure at the Drift Roof

Over time, extended rock failure may also occur at the roof of the drift. Kaiser (Brekke et al. 1999 [119404], pp. D-11, D-12) estimated the failure at the roof to be 0.1–1 m in depth, and it would be 0.4–1.2 m in depth if seismic effects were included. Generally, Kaiser expected that stress-induced failure at the drift crown to be over a distance of 1/2 drift radius, i.e., ~1.375 m. CRWMS M&O (2000 [151554], Figures 39–40) used a discrete-region key-block analysis, which shows a more extended failure region up to one drift radius above the drift roof. In the seepage study, a case is designed in which an extended cavity is found in the drift roof with a step shape of 0.5 m at the crown, 1 m depth at 0.5 m to one side, and so on, reaching 3 m depth at 2 m laterally from the drift crown (see Figure 2, lower left). This shape is similar to that shown as a worst case profile in CRWMS M&O (2000 [151554], Figure 40). Further, the step-shaped failure is 1 m thick.

6.5 EPISODIC PERCOLATION FLUX

The cases discussed up to now use a steady-state percolation flux, ranging from 5 to 500 mm/yr. To study the sensitivity of seepage to episodic flux, a transient calculation for seepage percentage is done by assuming that, every year, the total flux over the year is concentrated in the first two months and no flux occurs in the other 10 months. The results are compared with the cases using steady-state percolation.

6.6 RESULTS

Seepage percentage is defined as the ratio of liquid that seeped into the drift to the total liquid arriving on a cross-sectional area corresponding to the footprint of the drift. (Note that this term is defined differently in the SCM (CRWMS M&O 2000 [153045], Section 6.1.2), where it is defined in reference to the total water released in the liquid release tests). All results and the input/output files for the model computation are submitted to TDMS under DTN: LB0011SMDCREV1.001 and described as in Attachment I (Bodvarsson 2000 [153484], YMP-LBNL-CFT-GL-2, pp.7–21).

6.6.1 Seepage Over (k_{FC}, $1/\alpha$) Space

For values of $k_{FC} = 0.9 \times 10^{-14}$, 0.9×10^{-13}, 0.9×10^{-12}, 0.9×10^{-11} m^2, and 0.9×10^{-10} m^2, $1/\alpha = 200$, 400, 800, and 1600 Pa, and $\lambda = 0.5$ m, Tables 4–8 give the seepage percentages in a matrix form of k_{FC} and $1/\alpha$ coordinates. Within each table are three subtables giving results of three realizations of the heterogeneous field (R1, R2, and R3), indicating the spread of geostatistical variability. Generally, to calculate the spread of geostatistical variability, many more realizations than three are needed. However, because of the need to keep computations within reasonable limits, three realizations are used to indicate the lower bound of the spread of this variability. The tables show a definite decrease of seepage percentage with increasing $1/\alpha$ or k_{FC}.

Tables 4–8 present the results for σ=1.66 and 1.93 corresponding to the largest and smallest values obtained for the niche tests in Tptpmn zone (CRWMS M&O 2000 [153045], Table 4). The corresponding results for σ = 2.5 are also available and have been submitted within DTN LB0011SMDCREV1.001.

Table 4a. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.66 and Q_p = 5 mm/yr.

Realizations	**1/α (Pa)**	**k_{FC} (m²)**				
		0.9×10^{-14}	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	0.0	0.0	0.0	0.0	0.0
	800	0.0	0.0	0.0	0.0	0.0
	400	69	1.7	0.0	0.0	0.0
	200	93	86	49	0.0	0.0
R2	1600	0.0	0.0	0.0	0.0	0.0
	800	0.16	0.0	0.0	0.0	0.0
	400	61	2.4	0.0	0.0	0.0
	200	90	83	43	0.0	0.0
R3	1600	0.0	0.0	0.0	0.0	0.0
	800	0.68	0.0	0.0	0.0	0.0
	400	70	5.6	0.0	0.0	0.0
	200	93	88	49	0.0	0.0

DTN: LB0011SMDCREV1.002

Table 4b. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.93 and Q_p = 5 mm/yr.

		k_{FC} (m²)				
Realizations	**1/α (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	0.0	0.0	0.0	0.0	0.0
	800	0.0	0.0	0.0	0.0	0.0
	400	68	3.2	0.0	0.0	0.0
	200	93	86	49	0.0	0.0
R2	1600	0.0	0.0	0.0	0.0	0.0
	800	0.18	0.0	0.0	0.0	0.0
	400	61	2.6	0.0	0.0	0.0
	200	90	82	43	0.0	0.0
R3	1600	0.0	0.0	0.0	0.0	0.0
	800	2.7	0.0	0.0	0.0	0.0
	400	70	7.5	0.0	0.0	0.0
	200	93	88	49	0.0	0.0

DTN: LB0011SMDCREV1.002

Tables 5a–b through Tables 8a–b give results for $Q_p = 14.6$, 73.2, 213 and 500 mm/yr, respectively. The corresponding results for $\sigma = 2.5$ are also available and have been submitted within DTN LB0011SMDCREV1.001.

Table 5a. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for $\sigma = 1.66$ and Qp = 14.6 mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	0.0	0.0	0.0	0.0	0.0
	800	22	0.0	0.0	0.0	0.0
	400	84	35	0.0	0.0	0.0
	200	94	91	73	0.0	0.0
R2	1600	0.0	0.0	0.0	0.0	0.0
	800	20	0.0	0.0	0.0	0.0
	400	79	31	0.0	0.0	0.0
	200	90	88	66	0.0	0.0
R3	1600	0.0	0.0	0.0	0.0	0.0
	800	27	0.0	0.0	0.0	0.0
	400	85	37	0.0	0.0	0.0
	200	93	92	73	0.0	0.0

DTN: LB0011SMDCREV1.002

Table 5b. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for $\sigma = 1.93$ and Qp = 14.6 mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	0.0	0.0	0.0	0.0	0.0
	800	23	0.0	0.0	0.0	0.0
	400	83	35	0.0	0.0	0.0
	200	94	91	72	0.0	0.0
R2	1600	0.0	0.0	0.0	0.0	0.0
	800	19	0.0	0.0	0.0	0.0
	400	79	30	0.0	0.0	0.0
	200	91	88	65	0.0	0.0
R3	1600	0.0	0.0	0.0	0.0	0.0
	800	27	0.0	0.0	0.0	0.0
	400	85	38	0.0	0.0	0.0
	200	93	92	73	0.0	0.0

DTN: LB0011SMDCREV1.002

Table 6a. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.66 and Q_p = 73.2 mm/yr.

		k_{FC} (m^2)				
Realizations	**1/α (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	29	0.0	0.0	0.0	0.0
	800	72	2.7	0.0	0.0	0.0
	400	92	75	9.2	0.0	0.0
	200	94	93	89	0.0	0.0
R2	1600	24	0.0	0.0	0.0	0.0
	800	65	3.2	0.0	0.0	0.0
	400	89	69	9.2	0.0	0.0
	200	91	90	85	0.04	0.0
R3	1600	34	0.0	0.0	0.0	0.0
	800	74	7.2	0.0	0.0	0.0
	400	93	76	14	0.0	0.0
	200	93	93	90	0.0	0.0

DTN: LB0011SMDCREV1.002

Table 6b. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.93 and Q_p = 73.2 mm/yr.

		k_{FC} (m^2)				
Realizations	**1/α (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	29	0.0	0.0	0.0	0.0
	800	71	4.0	0.0	0.0	0.0
	400	92	75	10	0.0	0.0
	200	94	93	88	0.0	0.0
R2	1600	23	0.0	0.0	0.0	0.0
	800	64	3.5	0.0	0.0	0.0
	400	89	68	9.6	0.0	0.0
	200	91	90	85	0.08	0.0
R3	1600	34	0.0	0.0	0.0	0.0
	800	74	8.9	0.0	0.0	0.0
	400	93	76	15	0.0	0.0
	200	94	93	90	1.3	0.0

DTN: LB0011SMDCREV1.002

Table 7a. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for $\sigma = 1.66$ and $Q_p = 213$ mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	65	0.0	0.0	0.0	0.0
	800	86	38	0.0	0.0	0.0
	400	94	87	48	0.0	0.0
	200	95	94	92	18	0.0
R2	1600	57	0.07	0.0	0.0	0.0
	800	82	33	0.0	0.0	0.0
	400	91	83	43	0.0	0.0
	200	91	90	89	17	0.0
R3	1600	68	0.48	0.0	0.0	0.0
	800	89	41	0.0	0.0	0.0
	400	95	89	48	0.0	0.0
	200	96	93	93	22	0.0

DTN: LB0011SMDCREV1.002

Table 7b. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for $\sigma = 1.93$ and $Q_p = 213$ mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	64	0.0	0.0	0.0	0.0
	800	86	38	0.0	0.0	0.0
	400	94	86	48	0.0	0.0
	200	95	94	92	18	0.0
R2	1600	56	0.05	0.0	0.0	0.0
	800	81	33	0.0	0.0	0.0
	400	91	83	43	0.0	0.0
	200	91	91	89	16	0.0
R3	1600	68	2.4	0.0	0.0	0.0
	800	89	41	0.0	0.0	0.0
	400	95	89	48	0.0	0.0
	200	96	93	93	22	0.0

DTN: LB0011SMDCREV1.002

Table 8a. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.66 and Q_p = 500 mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	82	14	0.0	0.0	0.0
	800	92	63	0.0	0.0	0.0
	400	96	91	69	0.0	0.0
	200	97	94	93	49	0.0
R2	1600	75	12	0.0	0.0	0.0
	800	88	56	0.16	0.0	0.0
	400	93	88	61	0.0	0.0
	200	94	91	90	43	0.0
R3	1600	86	18	0.0	0.0	0.0
	800	95	65	0.68	0.0	0.0
	400	97	92	70	0.0	0.0
	200	97	93	93	49	0.0

DTN: LB0011SMDCREV1.002

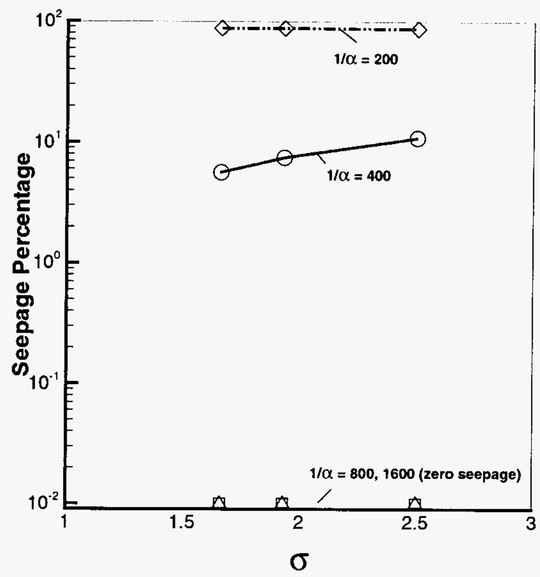
Table 8b. Seepage Percentage as a Function of k_{FC} and $1/\alpha$ for σ = 1.93 and Q_p = 500 mm/yr.

		k_{FC} (m^2)				
Realizations	**$1/\alpha$ (Pa)**	**0.9×10^{-14}**	**0.9×10^{-13}**	**0.9×10^{-12}**	**0.9×10^{-11}**	**0.9×10^{-10}**
R1	1600	82	14	0.0	0.0	0.0
	800	92	63	0.0	0.0	0.0
	400	96	91	68	0.0	0.0
	200	97	94	93	49	0.0
R2	1600	74	11	0.0	0.0	0.0
	800	88	56	0.003	0.0	0.0
	400	93	88	61	0.0	0.0
	200	95	91	90	43	0.0
R3	1600	87	18	0.0	0.0	0.0
	800	96	65	2.7	0.0	0.0
	400	98	92	70	0.0	0.0
	200	98	93	93	49	0.0

DTN: LB0011SMDCREV1.002

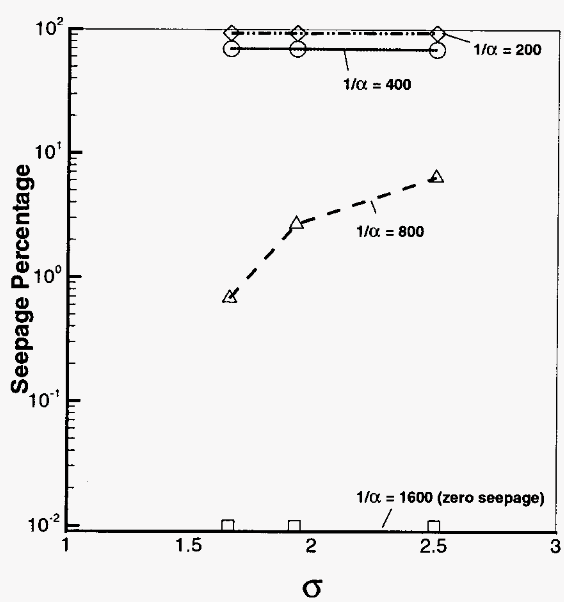
At Q_p = 5 mm/yr, seepage is essentially zero, except for cases with the very low permeability value of 0.9×10^{-14} m^2 and low values of $1/\alpha$. Generally, seepage is larger for lower permeability and lower $1/\alpha$ values. Though the extensive required computations make it impractical to obtain the full geostatistical distribution of seepage, results of three realizations are given for each case, giving an indication of the spread of the results. Note also that these results are all for $\lambda < 0.5$ m and, as shown in the next section, they are smaller than the corresponding results for larger λ values.

The dependence of seepage percentage as a function of σ is illustrated in Figure 3a and b. For high seepage cases, the dependence on σ is quite weak, but for low seepage cases seepage increases with σ, as expected (Birkholzer et al. 1999 [105170], pp. 372–376, Figure 17).



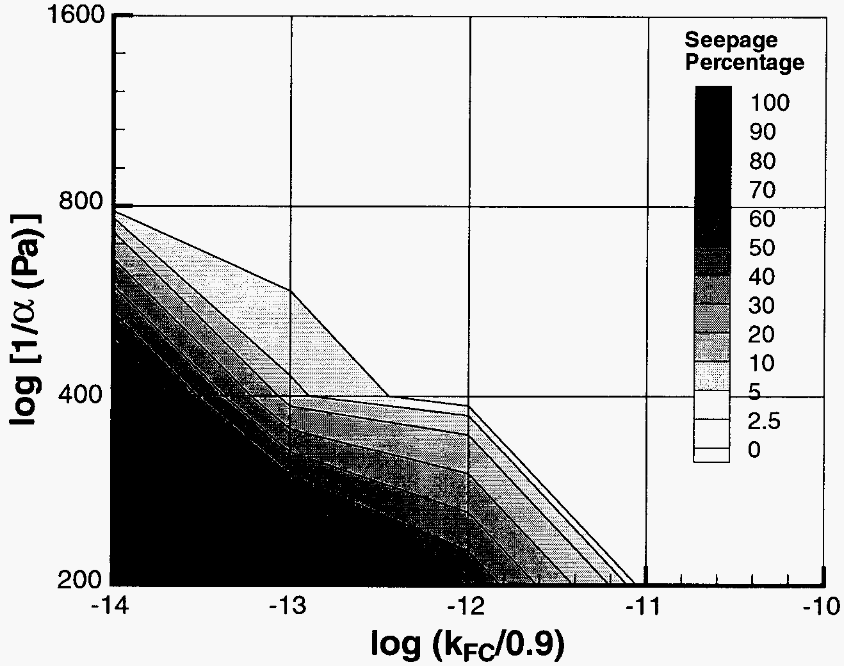
DTN: LB0011SMDCREV1.002
NOTE: This plot corresponds to Table 4a, $k = 0.9 \times 10^{-13}$ m^2, realization R3.

Figure 3a. Seepage percentage versus σ for various 1/α values, Q_P=5 mm/yr.



DTN: LB0011SMDCREV1.002
NOTE: This plot corresponds to Table 8a, $k = 0.9 \times 10^{-13}$ m^2, realization R3.

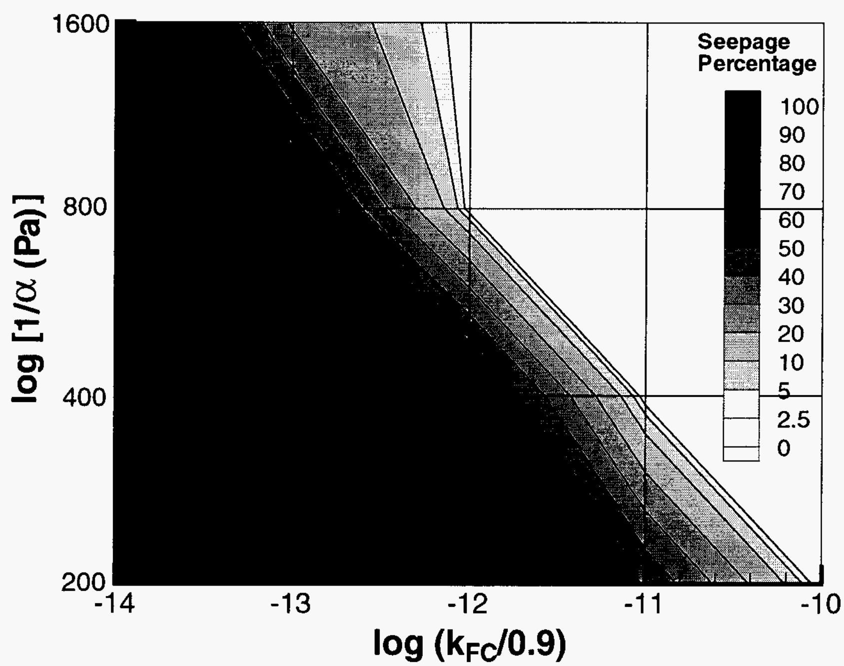
Figure 3b. Seepage percentage versus σ for various 1/α values, Q_P=500 mm/yr.



DTN: LB0011SMDCREV1.002

NOTE: This plot corresponds to Table 4a, $k = 0.9 \times 10^{-13}$ m^2, realization R3.

Figure 4a. Contour plot of seepage percentage over $k_{FC} - 1/\alpha$ space, Q_P=5 mm/yr.



DTN: LB0011SMDCREV1.002

NOTE: This plot corresponds to Table 8a, $k = 0.9 \times 10^{-13}$ m^2, realization R3.

Figure 4b. Contour plot of seepage percentage over $k_{FC} - 1/\alpha$ space, Q_P=500 mm/yr.

To illustrate the trends given in Table 4–8, contour plots for two particular cases are shown in Figures 4a and b, which give seepage percentages as contour in k_{FC} – $1/\alpha$ space. The two cases shown corresponds to realization R3 in Tables 4a (Q_P=5 mm/yr) and 8a (Q_P=500 mm/yr) respectively. These figures show "straight-line contour" joining results at grid points where the calculations were made. Zero-seepage line lies in the lightest gray area, which represents an interval with seepage from 0 to 2.5%.

6.6.2 Seepage for Alternative λ Values

Table 9 gives results for parameter Set A defined in Section 6.3.6 (see also Figure 1). For the four Q_p values from 14.6 to 500 mm/yr, seepage percentages are given for three realizations of the λ = 1 m case and for five realizations of the λ = 4 m case. Seepage was not calculated for Q_p = 5 mm/yr because, from Table 9, the results are expected to be zero. Appropriate results for λ = 0.5 m from Tables 5 through 8 are included for comparison. Table 10 gives the results for Set B, which indicates zero seepage in nearly all the cases. Note that seepage increases with λ, with the geostatistical spread of predictions also increasing with λ. While the results in Tables 9 and 10 provide an understanding of the trends, the field data collected to date (CRWMS M&O 2000 [153045], Section 6.4.2.1) indicate no spatial correlation, so that neglecting spatial correlation may be the most appropriate value to use.

Table 9. Seepage Percentage as a Function of Q_p for Alternative λ Values for Set A

		Q_p (mm/yr)			
λ		**14.6**	**73.2**	**213.4**	**500**
Uncorrelated λ = 0.5 m	R1	0.0	0.0	0.0	7.1
	R2	0.0	0.0	0.0	7.1
	R3	0.0	0.0	0.0	13
λ = 1.0 m	R1a	0.0	0.0	3.8	11
	R2a	0.0	0.0	0.0	5.2
	R3a	0.0	0.0	0.36	5.9
λ = 4.0 m	R1b	0.0	0.0	0.0	1.5
	R2b	0.0	2.3	8.1	12
	R3b	0.0	0.0	0.0	0.60
	R4b	0.0	0.0	0.0	7.1
	R5b	0.0	0.0	4.5	22

DTN: LB0011SMDCREV1.002

NOTE: Three realizations are calculated for each of the λ = 0.5 m and λ = 1 m cases and five realizations are calculated for the λ = 4 m case.

Table 10. Seepage Percentage as a Function of Q_p for Alternative λ Values for Set B

		Q_p (mm/yr)				
λ		213	500	1000	2000	3000
Uncorrelated λ = 0.5 m	R1	0.0	0.0	0.0	0.0	0.0
	R2	0.0	0.0	0.0	0.0	0.0
	R3	0.0	0.0	0.0	0.0	0.0
λ = 1 m	R1c	0.0	0.0	0.0	0.0	0.0
	R2c	0.0	0.0	0.0	0.0	0.0
	R3c	0.0	0.0	0.0	0.0	0.0
λ = 4 m	R1d	0.0	0.0	0.0	0.0	0.0
	R2d	0.0	0.0	0.0	0.33	1.9
	R3d	0.0	0.0	0.0	0.0	0.0
	R4d	0.0	0.0	0.0	0.0	0.0
	R5d	0.0	0.0	0.0	1.4	3.1

DTN: LB0011SMDCREV1.002

NOTE: Three realizations are calculated for each of the λ = 0.5 m and λ = 1 m cases and five realizations are calculated for the λ = 4 m case.

6.6.3 Sensitivity to n Value

As discussed in Section 6.3.5, van Genuchten n = 2.7 in all calculations. However the SCM suggests that n = 2.55 and 2.57 for the middle nonlithophysal and lower lithophysal units respectively (DTN: LB0010SCMREV01.002, [153393]). To study the impact of using n = 2.55 or n = 2.57 for parameter sets A and B, respectively, results for the two cases are compared against n = 2.7 using realization R1. The results are shown in Table 11, which indicates that the results are insensitive to n values over the range. Thus, in subsequent calculations, n = 2.55 and n = 2.57 are used for Set A and Set B respectively.

Table 11. Sensitivity to n Value. Seepage is given as percentage realization R1

Parameter Set A (varying 1/α) with Q_p = 213.4 mm/yr

1/α (Pa)	800	589	400	200
n = 2.7	0.0	0.0	34	91
n = 2.55	0.0	0.0	31	90

Parameter Set B (varying 1/α) with Q_p = 3000 mm/yr

1/α (Pa)	1600	871	400	200
n = 2.7	0.0	0.0	35	91
n = 2.57	0.0	0.0	33	90

DTN: LB0011SMDCREV1.002

6.6.4 Effects of Drift Degradation

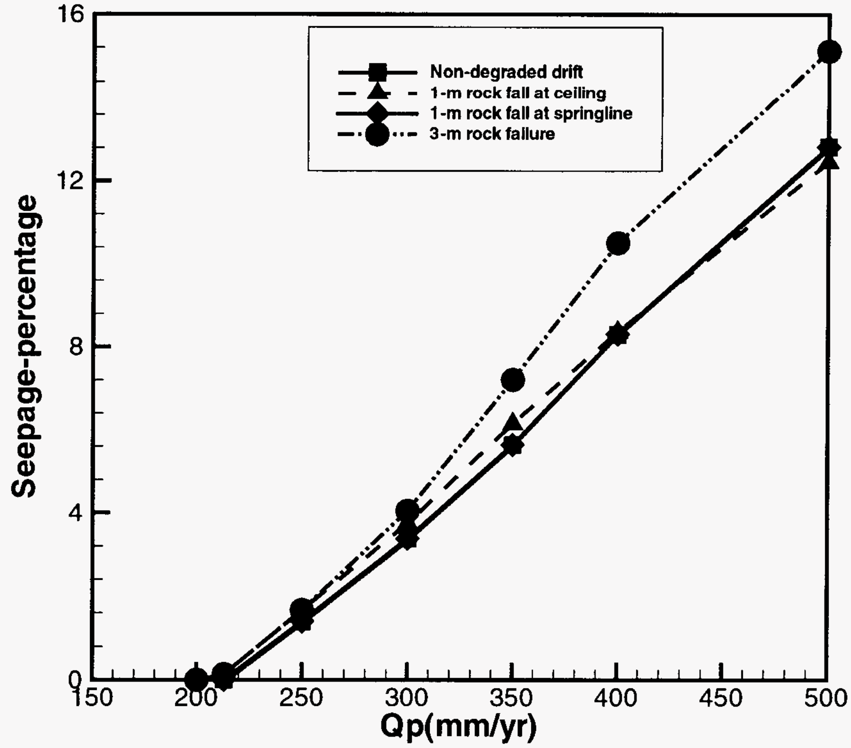
Table 12 presents the seepage percentages for parameter Set A (Section 6.3.6) for the three realizations (R1, R2 and R3) with drift degradation modes as defined in Section 6.4 (Figure 2), and compares them with the no-degradation case. Only the Q_p = 500 mm/yr cases are shown.

Table 12. Seepage Percentage (%) for Alternative Drift Degradation Scenarios, for Q_p = 500 mm/yr and parameter Set A

Condition	Seepage Percentage		
	R1	R2	R3
No-degradation case	7.1	7.1	13
1-m rock fall from crown of drift	7.2	7.3	12
1-m rock fall from springline of drift	7.1	7.1	13
3-m rock failure in drift roof	9.0	11	15

DTN: LB0011SMDCREV1.002

The results show that the effect of a single rockfall is not significant for seepage. A deeper rock failure in the drift roof increases seepage. Calculations were also made with parameter Set B with the results of zero seepage for all cases, with or without drift degradation.



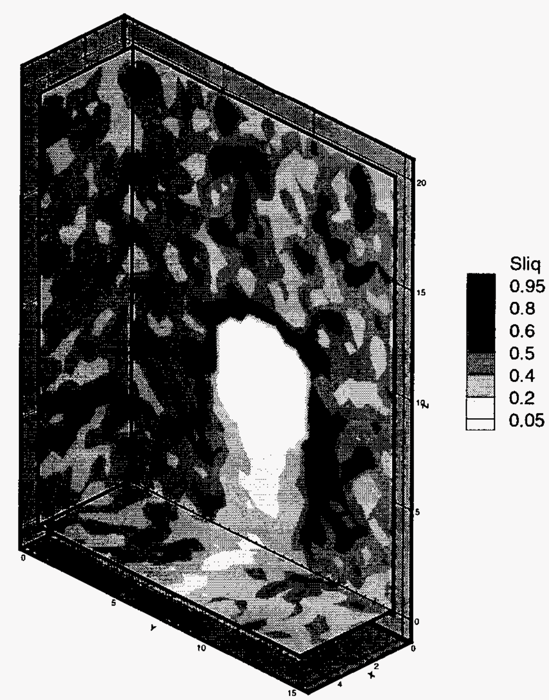
DTN: LB0011SMDCREV1.002

Figure 5. Seepage percentage as a function of percolation flux Q_P for the three drift degradation scenarios for parameter Set A

The results in Table 12 are for Q_p = 500 mm/yr. Additional simulations were done for other Q_p values to explore the effect of drift degradation on seepage threshold. Figure 5 shows the calculated seepage percentage as a function of percolation flux Q_p for realization R3. It is seen in this figure that the effect of drift degradation for the three scenarios as defined in Section 6.4 decreases with decreasing Q_p, so that its impact on seepage threshold is relatively small. This can perhaps be explained by the fact that, under vertical percolation flux, the seepage threshold depends significantly on the horizontal cross section (footprint) of the drift, so that, if the cross-section area does not change very much, the seepage threshold also will not change very much.

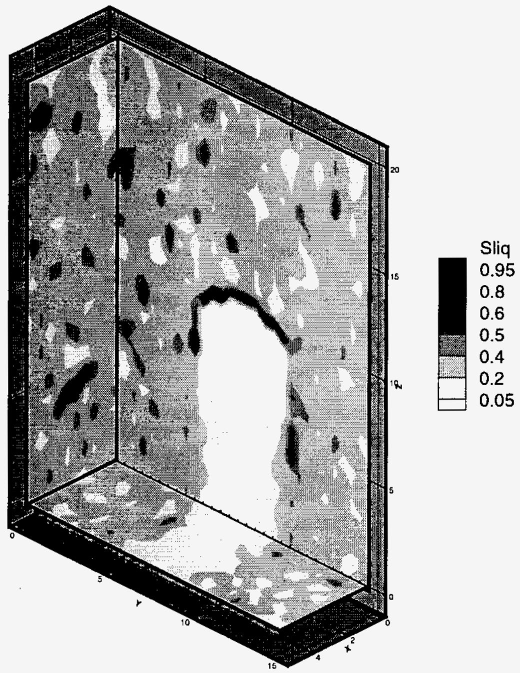
6.6.5 Drainage Below the Drift

The drift provides a partial barrier to downward percolation flux. Water moves around the drift or seeps into it. For the case that the water seeped into the drift is removed through an engineered drainage system, directly below the drift will be a shadow of dryer zone. This dryer zone will decrease in width with depth below the drift. The vertical extent of the shadow zone depends on both k_{FC} and $1/\alpha$ values (Philip et al. 1989 [105743], pp. 16–28). Figures 6 and 7 illustrate the saturation profiles one drift diameter below the drift for Parameter Sets A and B, with Q_p=500 mm/yr. The figures clearly show the shadow effect. Philip et al. (1989 [105743], pp. 21–23) also provide an approximate analytical solution to define the shadow zone, a solution that may be useful for practical applications.



DTN: LB0011SMDCREV1.002

Figure 6. Saturation Distribution around a Drift with Parameter Set A.



DTN: LB0011SMDCREV1.002

Figure 7. Saturation Distribution around a Drift with Parameter Set B.

6.6.6 Effects of Episodic Percolation

Episodic percolation is simulated for a drift without degradation. Table 13 shows the seepage results if, every year, the percolation flux over the year is concentrated in the first two months (representing a wet period) and then zero flux occurs for the remaining 10 months. These results are compared with the case where the flux is constant over the whole year. In both alternatives, the average flux over the year is 73.2 mm/yr. The seepage percentage at the end of the wet period (after the first two months) for the episodic scenario stabilizes very quickly after the first year. Calculations were performed for parameter Set A and Set B, with results for Set B being zero in all cases.

Generally, the seepage percentages for episodic scenarios are expected to be higher than those for the constant seepage scenario. Note that the percolation flux in the two wet months is 6 × 73.2 mm/yr, or 439.2 mm/yr. In Tables 7 and 8, calculated seepage percentages for Q_p = 213 and 500 mm/yr can be found. If an interpolation is made between these cases to obtain the seepage percentages for 439.2 mm/yr, they are found to be approximately equal to the seepage percentage for the episodic scenario. Thus for the sets of parameters used, the memory effect between percolation pulses separated by 10 months appears to be small, and each pulse can be treated independently at the high percolation rate of the wet period. The seepage rate over this period increases with time and its peak value at the end of the two wet months may be roughly estimated by interpolation from Tables 4–8 or calculated directly as been done here.

Table 13. Effects of Episodic Percolation. Q_p = 73.2 mm/yr

Parameters	Seepage % at end of wet period*	Seepage % if flux is constant over the year
Set A	5.1	0.0
Set B	0.0	0.0

DTN: LB0011SMDCREV1.002

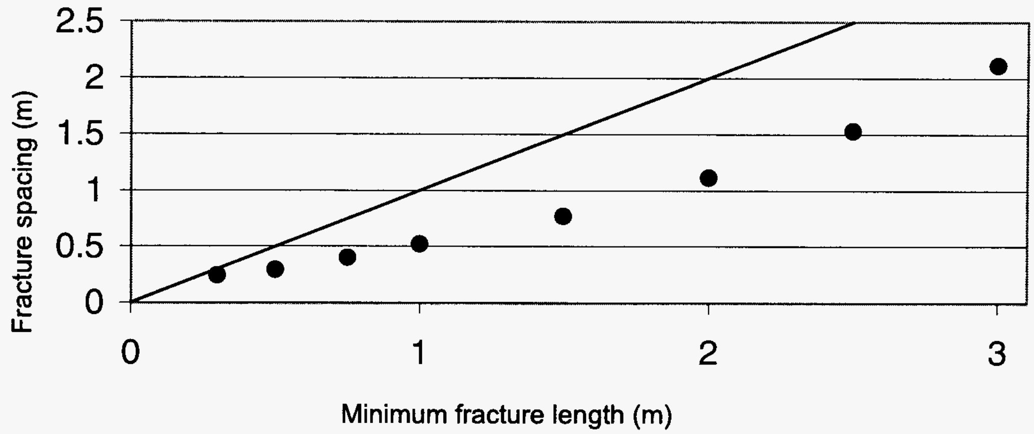
NOTE: *This value is the seepage rate at the end of the wet period divided by the percolation flux of the wet period, which is six times the average flux rate. For each year, the total percolation is all in the first two months and no flux in the remaining 10 months. Results are the same every year after the first year. Heterogeneous field used is Realization R1.

The results for Set A show the possible importance of the appropriate episodic percolation flux profile at the repository level, including effects of all the possible flow dissipation and diversion in the lithostratigraphic units above. In this case seepage may occur even though there is no seepage if the percolation is averaged out over the total period.

6.7 ALTERNATIVE CONCEPTUAL MODELS AND SENSITIVITY ANALYSIS

Sensitivity analyses are part of the scope of this AMR and are presented in the above subsections (6.6.2 through 6.6.6). The main alternative conceptual model is the discrete fracture-network model (DFNM). This is thoroughly discussed in CRWMS M&O (2000 [153045], Section 6.5.1) and will not be repeated here. Note further that the rock in the ESF is highly fractured and the fractures are well connected, so that the fracture continuum model is a reasonable representation. This is shown in Figure 8, in which fracture data from the ESF main drift from Station 27+20 to 37+80 were plotted as the average fracture spacing (calculated using the software routine frac_calc V1.1) against the minimum fracture length for groups of fractures that contain all fractures longer or equal to the minimum length selected (Cushey 2000 [153481], pp. 40–42). The figure shows that the spacing is consistently less than fracture lengths for all the fracture groupings. Further, Kicker in CRWMS M&O (2000 [151554], Fig. 5) shows that the major fracture sets in the Tptpmn unit are in three almost orthogonal planes, with strike/dip angles given by 131/84, 209/83, and 329/09. The result is thus a well-connected fracture network that can be represented by a fracture continuum. Note, however, that the fracture continuum is very heterogeneous (see Section 6.3.3), so that flow through it is highly channelized (Birkholzer and Tsang 1997 [119397], pp. 2229–2231).

As explained in Birkholzer et al. (1999 [105170], pp. 358–384), seepage into drift under conditions discussed in the AMR is controlled by heterogeneity-induced channeling and local ponding. It occurs much earlier than in the results of the conceptual model of a drift in homogeneous constant-property medium (Philip et al. 1989 [105743], pp. 17–21). In other words, Philip et al. would predict seepage to occur at a threshold that is orders of magnitude larger. In this sense, Philip's approach is not relevant, and Philip's boundary layer flow regime near the drift crown (Philip et al. 1989 [105743], p. 21, Figure 1) should not be used to define the required grid size. The sensitivity of seepage results to grid size was studied by calculating seepage into drift using grid sizes 0.5 m and 0.25 m while maintaining all other conditions, and comparing their results (Li 2000 [153480], pp. 86–89). The change in seepage into drift resulting from the change in grid size is of the same order as changes resulting from the different realizations, with an increase of 0–3% for the finer mesh for the case calculated.



DTN: GS971108314224.025 [106025], GS960708314224.008 [105617] and GS00060831224.004 [152573]

NOTE: Straight line indicates a 1:1 correspondence

Figure 8. Average Fracture Spacing for Topopah Spring Middle Nonlithophysal Lithostratigraphic Unit in the ESF from Stations 27+20 to 37+80.

The drift seepage problem involves the accumulation of unsaturated flow at the location near the drift wall. This accumulation continues until the local saturation is large and capillary suction is small. Then seepage into drift occurs. This problem is intrinsically a 3D problem, because flow accumulation at a location in 2D could easily disappear if it is allowed to flow away in the third dimension. Two-dimensional models would consequently overestimate seepage.

The present AMR considers alternative spatial correlation lengths, using a spherical correlation structure and a Gaussian field. There have been suggestions to use alternative geostatistical methods, such as nonparametric representations of the heterogeneity field and multiple-scale correlation structures. However, for a specific problem with a particular scale of a drift, such complications are not needed so long as the parameters used are appropriate to this scale. The reason is that structures much smaller than the drift diameter can be approximated by an average property parameter, except near the drift wall (see below for the "surface needle" effect). Structures with correlation lengths much larger than the drift diameter should be handled deterministically in each case, and do not need to be handled statistically.

What is of more interest and importance is the question of the appropriate parameter values to be used in the seepage-prediction model. This depends on an interplay between seepage-model grid-element scale, calibration-model grid-element scale, and having field data appropriate to those scales. It is shown in this AMR that the air (fracture) permeabilities without excavation effects seems to have quite consistent values when the data support scale ranges from 0.3 to ~20 m. However, no similar information on $1/\alpha$ and other parameters are available. Further study of the interplay among the three scales for the purpose of deriving appropriate parameter values for predictive modeling would be very useful to enhance confidence in these values. However, they will probably still be in the ranges shown in Figure 1.

One issue of great concern that may have a significant adverse impact on seepage is the "surface needle" effect. This refers to the possibility that 1D pathways exist from within the rock above the drift to the drift ceiling, from which there are no effective lateral intersecting fractures to divert water away. These 1D pathways or needles will then act as special conduits through which seepage can occur. The increase in seepage due to their presence could be very significant and needs to be carefully evaluated. One example of such "needles" is the rock bolts used to stabilize the drift roof. Whether rock bolts would form such special seepage pathways depends on the leakage around the bolts and how it develops as the bolt cement degrades and the bolts corrode with time. A very preliminary estimate has been made on the needles effect (Li 2000 [153480], pp. 71–72) for a special parameter set, $k_{FC} = 10^{-13}$ m^2, $1/\alpha = 1000$ Pa, $\lambda = 2$ m and no gravity drainage at the drift ceiling. Seepage increases are calculated as a function of needle length and the number of needles in the section. With increasing needle length, the seepage increase stabilizes to a constant value after the length exceeds 0.15–0.25 m. For a 16.5-m section of the drift (approximately three waste-package lengths), the seepage increase is found (Li 2000 [153480], p. 72) to be about 3% when there are three needles present in the drift ceiling (i.e. needle spacing 5 m); about 40% when there are 33 needles (i.e. needle spacing 1.5 m); and 70% when there are 330 needles (i.e. needle spacing 0.5 m).

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7. CONCLUSIONS

The present AMR is based on the Seepage Calibration Model AMR (CRWMS M&O 2000 [153045]) and Birkholzer et al. (1999 [105170]). By reviewing available information (Section 6.3 and 6.4), a range of parameters and possible scenarios (Figure 1) were selected, over which seepage calculations were conducted. Tabulated results (Tables 4–13) show the impact of various factors on seepage and provide data for PA to develop probability distributions (DTN: LB011SMDCREV1.001). Generally, seepage is calculated to be larger for smaller fracture continuum permeability (k_{FC}), smaller van Genuchten parameter ($1/\alpha$) and larger percolation flux (Q_p) values (Tables 4–8). It is insensitive to the van Genuchten n parameter (Table 11). Results in this AMR are based on SCM calibration results and a review of available *in situ* field results appropriate to the Tptpmn lithostratigraphic unit and one set of data for the Tptpll unit. As more data from these units (where the potential repository resides) are obtained in field measurements, parameter values with their uncertainties and probability weightings should be developed and then seepage predictions from tables in this AMR can be used in PA to obtain the best estimates (with uncertainty ranges) for Yucca Mountain.

Uncertainty associated with geostatistics is evaluated through calculations of three realizations for each case (five for a case of large spatial correlation length). Results are shown in Tables 4 through 8 and Table 10. In general, establishing geostatistical probability requires many more realizations than three, but the great number of simulations (over 1,000) in this AMR make it impractical to do more realizations. Nevertheless, the spread of results from the three realizations should give an indication of geostatistical variation. In general, the spread is expected to be larger for large spatial correlation length λ and more limited if λ is much smaller than the drift diameter.

This report demonstrates that the impact of mechanical effects such as rock falls and fracture dilation can be evaluated (Sections 6.4 and 6.6.4). This work builds on CRWMS M&O 2000 [151554] and Brekke et al. 1999 [119404], which includes fracture dilation scoping analyses. These reports also considered thermal and seismic effects on drift degradation in a schematic way. As further mechanical studies are made on drift degradation, seepage calculations should follow to update the assessment of their impact.

As mentioned in Section 1, analysis on the impact of coupled thermal-hydrological-mechanical effects on seepage is not within the scope of this AMR.

In summary, the present AMR identifies the following issues that could have a significant effect on seepage:

1. Drift degradation–disturbed-zone scenario and extended failure scenario (Section 6.6.5)

2. Episodic percolation flux (Section 6.6.7).

3. "Surface Needles" effect; in particular, the impact of rock bolts over the long time frame (Section 6.7)

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 technical product input information quality may be confirmed by review of the DIRS database.

Most of the input data and information (such as the 2nd, 3rd, 5th to 8th row of Table 2) are used to establish ranges of parameter values used in the systematic calculations presented in this AMR. Reasonable changes in the input data do not affect the choice of these ranges. For example, the permeability data are used to establish a range of values for the simulations. These permeability data could change by an order of magnitude and still be in the selected range and not affect these results. Thus, generally, the verification and confirmation of these permeability data should not affect this AMR. The only other essential data value used is the drift diameter of 5.5 m, which is verified. In general, smaller diameter drifts would result in less seepage or less conservative results. The other data (4th row of Table 2, DTN: LB0010SCMREV01.002 [153393]) are used for selecting special cases for sensitivity studies. These data are dependent on the "evaporation" assumption of CRWMS M&O 2000 [153045], which is to be verified.

8. INPUTS AND REFERENCES

The following is a list of the references cited in this document. Column 1 represents the unique six digit numerical identifier, which is placed in the text following the reference callout (e.g., CRWMS M&O 2000 [144054]). The purpose of these numbers is to assist the reader in locating a specific reference. Within the reference list, multiple sources by the same author (e.g., CRWMS M&O 2000) are ordered numerically by the unique identifier.

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8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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8.3 SOURCE DATA,LISTED BY DATA TRACKING NUMBER

152573 GS000608314224.004. Provisional Results: Geotechnical Data for Station 35+00 to Station 40+00, Main Drift of the ESF. Submittal date: 06/20/2000.

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8.4 OUTPUT DATA, LISTED BY DATA TRACKING NUMBER

LB0011SMDCREV1.001. Seepage Model for PA including Drift Collapse: 1. Model Input/Output Files AMR U0075 (MDL-NBS-HS-000002 REV01. Submittal date: Submitted with this AMR.

LB0011SMDCREV1.002. Seepage Model for PA including Drift Collapse: 2. Tables of Seepage Percentage AMR U0075 (MDL-NBS-HS-000002 REV01. Submittal date: Submitted with this AMR.

LB0012SMDCATT3.001. Seepage Model for PA Including Drift Collapse: 1. Model Input/Output Files AMR U0075 Attachment III (MDL-NBS-HS-000002 REV01). Submittal Date: 12/15/2000.

LB0012SMDCATT3.002. Seepage Model for PA Including Drift Collapse: 2. Seepage Percentage vs. Percolation Flux for Parameter Sets A and B' AMR U0075 Attachment III (MDL-NBS-HS-000002 REV01). Submittal Date: 12/15/2000.

9. ATTACHMENTS

Attachment I - Model Input and Output Files

Attachment II - Software Routine Code Listing

Attachment III - Additional Cases with Parameter Set B′

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ATTACHMENT I—MODEL INPUT AND OUTPUT FILES

Below are the descriptions of the directory paths and the input and output files submitted under DTN: LB0011SMDCREV1.001 for this AMR and the attachment LB0012SMDCATT3.001. The Table numbers refer to the tables in DTN: LB0011SNDCREV1.002.doc. For Attachment III (LB0012SMDCATT3.002), the file naming system corresponds to that for Tables 9—10, as described below.

Tables 4-8

Directories

/ad5k#@_r&/ (includes subpaths and data files)

- ad5 indicates that the correlation length is 0.5 meter.
- # 10,11,12,13 and 14 corresponding to the mean permeability at 0.9×10^{-10}, 0.9×10^{-11}, 0.9×10^{-12}, 0.9×10^{-13} m^2, and 0.9×10^{-14} m^2.
- @ standard deviation: s means the value of standard deviation is 1.66; l means the value is 2.50; otherwise the value is 1.93.
- & realization number.

For example, /ad5k13s_r1/ identifies the root directory for simulations where the correlation length is 0.5 meter and the mean permeability of realization 1 is 0.9×10^{-13} m^2 with a standard deviation of 1.66.

Mesh filename

MESHGR05 input file of mesh generation for a 5.5 m diameter drift.

Initial Condition Filenames

INCON@&_%

- @ standard deviation: s means the value of standard deviation is 1.66; l means the value is 2.50; otherwise the value is 1.93.
- & realization number. If the realization number is missing the file is generated for the realization number of the directory given above.
- % value of $1/\alpha$.

For example, INCONs1_200 identifies the initial condition file for realization 1 with standard deviation of 1.66 and $1/\alpha$ of 200 Pa. /ad5k13s_r1/INCONo_200 is generated for realization 1.

Subdirectories

/*_a%/

- * is the percolation flux (mm/yr).
- % is the value of $1/\alpha$.

For example, /500_a200/ is a subdirectory containing the files for a simulation with a percolation flux of 500 mm/yr and $1/\alpha$ of 200 Pa.

ITOUGH2 Input files

*_a^

- * is the percolation flux.
- ^ value of 1/α.

For example, 500_a200 is a input file for a flux of 500 mm/yr and 1/α of 200 Pa.

Output files

*_a^.out	output file for ITOUGH2.
*_a^.sav	ITOUGH2 .sav file with output conditions
outq	file containing seepage results
t2.msg	ITOUGH2 message file providing simulation status

Steps to rerun an example case corresponding to Tables 4 through 8

In table 4a, realization 3 and 1/α 200Pa with the mean permeability of 0.9×10^{-14} m^2 (the seepage percentage is 93).

Step 1: go to directory ad5k14s_r3, where the correlation length is 0.5 meter (ad5), σ = 1.66, the realization is 3 and the mean permeability is 0.9×10^{-14} m^2;

Step 2: go to directory 5_a200, where the percolation flux is 5 mm/yr and the 1/α is 200 Pa;

Step 3: Type rund and enter to run ITOUGH2v3.2_drift with the input file 5_a200;

Step 4: Calculate the seepage percentage from the output file outq.

Tables 9-10

Root directory

/lamda!_?/ includes subdirectories and data files.

- ! d5,1 or 4 is the value of the correlation length.d5 means the value of the correction length is 0.5 meter.
- ? a means Parameter Set A and b means Set B.

For example, /lamdad5_a/ indicates that the correlation length is 0.5 meter with Parameter Set A.

Mesh filename

MESHGR05 input file of mesh for a 5.5 m diameter drift.

Initial Condition Filenames

INCONl**a!_&_%**

- **!** d5,1 or 4 is the value of the correlation length. d5 means the value of the correction length is 0.5 meter.
- **&** realization number.
- **%** value of 1/α.

For example, INCONl1_1_589 indicates that it is for realization 1 with a standard deviation of 1.93, correlation length of 1 meter and 1/α of 589 Pa.

Subdirectories

/*_l!_&/

subpaths under /lamda!_? /.

- * is the percolation flux (mm/yr).
- ! d5, 1 or 4 is the value of the correlation length. d5 means the value of the correction length is 0.5 meter.
- & realization number (1 through 5 for correlation length 4).

For example, /500_l1_1/ indicates that the correlation length of realization 1 is 1 meter, and the percolation flux is 500 mm/yr.

ITOUGH2 Input files

*_l!

- * is the percolation flux.
- ! d5, 1 or 4 is the value of the correlation length. d5 means the value of the correction length is 0.5 meter.

For example, 500_l1 is a input file for a flux of 500 mm/yr and correlation length 1 meter.

Output files

*_l!.out	output file for ITOUGH2.
*_l!.sav	ITOUGH2 .sav file with output conditions
outq	file containing seepage results
t2.msg	ITOUGH2 message file providing simulation status

Steps to rerun an example case corresponding to the tables 9-10

In table 10, use Parameter Set B, alternative λ value of 4, realization 2, flux 3000 mm/yr (the seepage percentage is 1.9).

Step 1: go to directory lamda4_b, where the correlation length is 4 meter ;

Step 2: go to directory 3000_l4_2, where the percolation flux is 213 mm/yr, 1/α is 100 Pa, correlation length 4, realization 2;

Step 3: type rund and enter to run ITOUGH2v3.2_drift with the input file 3000_l4 ;

Step 4: calculate the seepage percentage from the output file outq.

Table 11

Root directory
/vangn_a/213_**nn**_%/
/vangn_b/213_**nn**_%/
includes subdirectories and data files.

nn means the van Genuchten parameter n.
% value of $1/\alpha$.

For example, /213_n255_200/ indicates that the correlation length is 0.5 meter, van Genuchten n is 2.55 with the standard deviation of 1.66.

Mesh filename
MESHGR05 input file of mesh generation for a 5.5 m diameter drift.

Initial Condition Filenames
INCON**&_%**
& realization number.
% value of $1/\alpha$.

For example, INCON_1_200 identifies the initial condition file for realization 1 with standard deviation of 1.93 and $1/\alpha$ of 200 Pa.

Subdirectories
/*/ subpaths under /213_nn_%/
* is the percolation flux (mm/yr).

For example, /500 / a subdirectory containing the files for a simulation with a percolation flux of 500 mm/yr .

ITOUGH2 Input files
*
* is the percolation flux.

For example, 500 is a input file for a flux of 500 mm/yr.

Output files

*.out output file for ITOUGH2.
*.sav ITOUGH2 .sav file with output conditions
outq file containing seepage results
t2.msg ITOUGH2 message file providing simulation status

Steps to rerun an example case corresponding to the table 11

In Table 11, use the file with a van Genuchten n of 2.55, and 1/α 300 Pa, and Parameter Set A (the seepage percentage is 90).

Step 1: go to directory /vangn_a/213_n255_200, where the correlation length is 0.5 meter (ad5), σ = 1.93, realization 1, the percolation flux is 500 mm/yr and the 1/α is 200 Pa;

Step 2: type rund and enter to run ITOUGH2v3.2_drift with the input file 500;

Step 3: calculate the seepage percentage from the output file outq.

Table 12

Root directory
/drift_geo/ includes subpaths and files for drift collapse models

Subdirectories
/drift_cc/drift_cc_r&/ files for the model cut out 3m depth and 2m width at the drift roof.
/drift_cc8/drift_cc8_r&/ files for the model cut out 1 m^3 rock-fall from the drift crown.
/drift_cs8/drift_cs8_r&/ files for the model cut out 1 m^3 rock-fall from the drift springline

Mesh names MESHGR_cc; MESHGR_cc8; MESHGR_cs8

Initial Condition Filenames
INCONcc_a_r&
INCONcc8_a_r&
INCONcs8_a_r&
& is the realization number.

Subdirectories
/*/
* is the percolation flux (mm/yr).

For example, /500/ a subdirectory containing the files for a simulation with a percolation flux of 500 mm/yr.

ITOUGH2 Input files
*

* is the percolation flux.

For example, 500 is a input file for a flux of 500 mm/yr.

Output files

*.out output file for ITOUGH2.
*.sav ITOUGH2 .sav file with output conditions
outq file containing seepage results
t2.msg ITOUGH2 message file providing simulation status

Steps to rerun a example case corresponding to table 12

In Table 12, 3_m rock failure in drift roof and realization 2 with Parameter Set A (the seepage percentage is 11).

Step 1: go to directory drift_geo/drift_cc/drift_cc_r2/, where the correlation length is 0.5 meter, $\sigma = 1.93$, and the realization is 2;

Step 2: go to directory 500, where the percolation flux is 500 mm/yr;

Step 3: type rund and enter to run ITOUGH2v3.2_drift with the input file 500;

Step 4: calculate the seepage percentage from the output file outq.

Table 13

Root Directory
/multi_p/ includes subpaths and data files for episodic percolation simulations

Mesh Filename
MESHGR05 input file mesh for a 5.5 m diameter drift.

Subdirectory
/multi_73+_2-10/

\+ a means Set A, b means Set B.

For example, file multi_73a_2-10 indicates a flux of 73 mm/yr, Parameter Set A, with flux occurring in the first two months of each year.

Initial Conditions Filename INCONl1_1_589 and INCONl1_1_871

Input files
*_^m+?y

*	is the percolation flux during the wet (439) or dry (0) of the year in mm/yr.
^	shows the number of months for the run.
?	is the year number of the run. The sequence starts with 0 .

For example, 439_2m+1y is a input file for a simulation over the two wet months with the percolation flux of 439 mm/yr in the second year. 439_10m+1y is the file for the simulation of the following 10 months.

Output files

*_^m+?y.out	ITOUGH2 output
*_^m+?y.sav	ITOUGH2 .sav file with final simulation conditions
*_^m+?y.tec	ITTOUGH2 .tec file for plotting
outq_^m+?y	output file from ITOUGH2 for seepage rates.

For example, outq_2m+1y is a output file for the percolation flux of 439 mm/yr over the second wet period (second year).

Steps to rerun an example case corresponding to table 13

In Table 13, use Parameter Set A at the end of wet period (the seepage percentage is 5.1).

Step 1: go to directory /multi_p/multi_73a_2-10/;

Step 2: copy 0_10m+2y.sav to INCON as initial condition of the forth wet period. After three years episodic percolation the seepage is near steady state;

Step 3: type rund and enter to run ITOUGH2v3.2_drift with the input file 439_2m+3y;

Step 4: calculate the seepage percentage from the output file outq.

ATTACHMENT II—SOFTWARE ROUTINE CODE LISTING

(Documentation per AP-SI.1Q is included in the records packages submitted for each routine as listed in Table 1 in Section 3.)

Source code for Software Routine frac calc, Version 1.1

```
      program Frac_Calc

c     Version 1.1
c     All changes for Version 1.1 are indicated by MAC V1.1
c     See Scientific Notebook YMP-LBNL-GSB-MC-1.2 pages 14-16

c     Discussion for Version 1.0
c
c     The purpose of this program is to calculate means and variances
c     for fracture properties for UZ model layers     based on detailed
c     line survey (DLS) data for the Exploratory Studies Facility (ESF)
c     that has been downloaded from the Technical Database (TDB).

c     This program was originally written by Eric Sonnenthal with
c     revisions and additions by Mark Cushey (4/98 to 7/98) which are
c     labeled MAC and dated.  Major additions include using data
c     statements and coding to combine subunits for model    layers
c     internally in the program; calculating additional parameters;
c     program     recalculates all numbers for each model layer each time
c     it is executed; calculate apertures; calculate alpha & log alpha
c     and its statistics; calculates spacing, frequencies    and intensity
c     for selected interval lengths; new input format for direct reading
c     of data from TDB after processing through read_tdb.f; and new
c     output formats.

c       MAC V1.1 - updated pages below for references for Version 1.0
c     See Scientific Notebook YMP-LBNL-GSB-MC-1 pages 60-69, 124-125, 137
c     See Scientific Notebook YMP-LBNL-GSB-MC-1.1 pages 98, 101-108, 114-115
c     See Reference Binder YMP-LBNL-GSB-MC-1.1A pages 88-97, 98-106

c     - Mark Cushey 7/98
c-----------------------------------------------------------------------
c     Below comments by E.Sonnenthal
c...  Program to read USGS ESF data and calculate fracture geometries
c...  and densities for plotting (11/4/96: E. Sonnenthal)
c...  Components of hydraulic conductivity tensor (de Marsily, 1986)
c...  11/11/96 E. Sonnenthal
c...  revised 2/6/97 for a fracture size range
c     nf     = Number of fractures
c     blksiz = Block size (m)
c     kfrc   = Hydraulic conductivity of each fracture (m/s)
c     aper   = Aperture of each fracture (m)
c     strike = Strike of each fracture (azimuth in radians)
c     dip    = Dip of each fracture (dip in radians)
c     ktens  = Conductivity tensor (9 component)
c      k(9) = (kxx,kxy,kxz,kyx,kyy,kyz,kzx,kzy,kzz)
c          | kxx  kxy  kxz |
c          | kyx  kyy  kyz |
c          | kzx  kzy  kzz |
```

```
c--------------------------------------------------------------------

c Commented out variables no longer used MAC 7/98
c     integer ni1,ni2
      integer i,k,ni,n,nn,nm1,nfr,nf,ns1,ns2
      parameter (nf = 50000)
      parameter (pi=3.1415926536d0)
      parameter (ni = 199)

c Added MAC 4/13/98
      character*32 fname

c Commented out variables no longer used MAC 7/98
c      character*8 outfile, header2, fstat
c      character*200 header
c      integer dist1
c      double precision height(nf),dist2

      integer nfrint(ni),ns
      double precision blksiz,kf,sdsq,stkrad,diprad,proptf
      double precision fmin,fmax
      double precision kfrc(nf),aper(nf)
      double precision ktens(9)
      double precision kxx,kxy,kxz,kyx,kyy,kyz,kzx,kzy,kzz
      double precision endp1,endp2,totaltr,totalht,adip,bdip
      double precision dist(nf),nfrc(nf)
      double precision strike(nf),dip(nf),alen(nf),blen(nf)
      double precision atrace(nf),btrace(nf),trace(nf)
      double precision trlen,fmesf,frint,fgrp1,fgrp2,fsiz
      double precision trcmax,dipmin,dipmax,aperture
      double precision avgsp,frcint,varsp,sdspac
      double precision freq,sdfreq,frcvol,frcrad,frcpor,blkht,blkdp
      double precision sdlen,varlen,avglen,frarea,frcp2d
      character*1 ans1,ans2

c     MAC V1.1
      double precision intarea, gmlen

c
c-----------------------------------------------------------------------
c     Below added by MAC 4/98 - 5/98
c     Data statements added to identify subunits and later combine
c     subunits for each model layer.
c     Moved to include MAC 6/98 so that various combinations could be
c     used by simply using a different file for include
c     Note that alcove stations are entered with Alcove # in the
c     ten thousandth location.
c     Assignment for model layers based on CRWSM M&O, 1998.
c     For most recent assignment see
c     Scientific Notebook YMP-LBNL-GSB-MC-1.1 pages 36-39.
c
c     Include file 'datablk.f' includes data statements for
c     unitname, modlayer, unitsta, unitend, and logairk

c     MAC V1.1
      include 'datablk11.f'
c
```

```
c     For testing, instead of 'datablk.f', include file 'uzmodel97.f'
c     for comparison with calculations performed for the July 97
c     milestone (Chapter 7, Sonnethal et. al, 1997) or include
c     'sweetkind.f' for comparison with calculations in
c     Sweetkind et. al (1997). Use the data files ericdls.dat and
c     sweetdls.dat, respectively.
c     include 'uzmodel97.f'
c     include 'sweetkind.f'
c     MAC 7/98 For the more detailed PTn model layers use
c     include 'ptnblk.f'


c-----------------------------------------------------------------------------
c Below added MAC 4/98 - 6/98
c     ntotal is the total number of UZ model layers
c     nlayers is the total number of segments along the ESF
c     Both are used for the data statements and are defined in the
c           file 'datablk.f'
c     npar is the number of parameters saved for calculating properties
c     for entire model layer
c     variables with 'int' are for calculating fracture properties for
c           intervals
c     variables for data statements [integer modlayer(ntotal);
c           double precision logairk(nlayers),unitsta(nlayers),
c           unitend(nlayers)] are in file 'datablk.f'

      integer     layer,first,last,npar
c     MAC V1.1 changed npar from 16 to 18
      parameter(npar=18)
      double precision spac,frcp1d,trcmin, combine,kzzkxx,kyykxx,kzzkyy,
      +     alpha,loga,logf,sdalpha
      dimension combine(nlayers,npar)
      character*5 outfile

      integer intn,intmax,intnfr,intlayer
      parameter(intmax=10000)
      double precision intfreq,intspace, intlength, inttrace
      dimension intfreq(intmax),intspace(intmax),intnfr(intmax),
      +     inttrace(intmax)

c...Input file name
2     print *, 'Enter fracture data filename: '
      read (*,*) fname
      open(unit=12,file=fname,status='old',err=5)
      go to 7
5     write(*,*)'File not found'
      go to 2
7     continue

c Removed call to station file -- all in one file MAC 4/13/98

c revised MAC 4/13/98 - starting and end points for model layers
c           now determined internally

c revised MAC 4/17/98   - changed input process
      dipmin = 0.d0
      dipmax = 90.d0
```

```
      ans1 = 'n'
      ans2 = 'y'
      write(*,*)'Enter minimum and maximum fracture length to use'
      read(*,*)fmin,fmax

c Added MAC 7/8/98 - query user for interval length
      write(*,*)'Enter interval length (in meters)'
      read(*,*)intlength
c--------------------
c... Read station file - Removed MAC 4/13/98

c     MAC 4/98 open output files
      open(13,file='all1.par',status='unknown')
      open(14,file='all2.par',status='unknown')
      write(13,441)
      write(14,442)
      open(18,file='interval.par',status='unknown')
      write(18,1999)
      open(20,file='tmp.par')

c
c... Read fracture data file
c Rev MAC 4/13/98
      read (12,*)
      i = 0
10    i = i + 1
c     rev MAC 6/29/98 - Don't read in height
c     read(12,*,end=99)dist(i),strike(i),dip(i),atrace(i),
c     &     btrace(i),height(i)
      read(12,*,end=99)dist(i),strike(i),dip(i),atrace(i),
      &     btrace(i)
      go to 10
99    ns = i - 1
      dist(ns+1)=99999.9
      close(12)
c
c Added MAC 6/25/98
c     initialize combine
      do j=1,npar
            do i=1,nlayers
                  combine(i,j) = 0d0
            end do
      end do

c----------------
c Added MAC 4/17/98
c     Loop through model layers, assiging station ranges
c     Define endp1, endp2, ns1, ns2
c
      DO layer = 1,nlayers
            endp1 = unitsta(layer)
            endp2 = unitend(layer)
            write(*,*)unitname(layer),endp1,endp2
            ns1 = 0
            ns2 = 0
            do i = 1,ns+1
                  if (((dist(i).ge.endp1).and.(dist(i-1).lt.endp1))
```

```
     &          .or.((dist(i).ge.endp1).and.(i.eq.1)))
     &                ns1 = i
                if ((dist(i).gt.endp2).and.(dist(i-1).le.endp2))
     &                ns2 = i     - 1
          end do
c         MAC V1.1 - changed 0.0 to 0
          if ((ns2-ns1).le.0) go to 999
          write(*,*)'     ',dist(ns1),dist(ns2)

c         outfile = unitname(layer)
          outfile = 'dummy'
c         if ((layer.eq.48).or.(layer.eq.27)) then
c               outfile = unitname(layer)
c               write(*,*)'Tecplot file for',unitname(layer),
c    +                unitsta(layer),unitend(layer)
c         end if
c... Find size distribution for all fractures
      if(ans2.eq.'y')then
          fmesf = 0.3d0
          frint = 0.2d0
      do i = ns1,ns2
          trlen = atrace(i) + btrace(i)
        do k = 1, ni
          fgrp1 = fmesf + dble(k-1)*frint
          fgrp2 = fmesf + dble(k)*frint
          if(trlen.ge.fgrp1.and.trlen.lt.fgrp2)
     &            nfrint(k)=nfrint(k)+1
        enddo
      enddo
      endif
c

c Added MAC 4/98 find minimum trace length before excluding
      trcmin = fmax
      do i = ns1,ns2
        trcmin = min((atrace(i)+btrace(i)),trcmin)
      enddo

c... Find fractures that are within range if given
      n = 0
      nfr = 0
      do i = ns1,ns2
        if(dip(i).ge.dipmin.and.dip(i).le.dipmax.and.atrace(i)+
     +    btrace(i).ge.fmin.and.atrace(i)+btrace(i).le.fmax)
     +      then
            n = n + 1
            nfrc(n) = i
            nfr = n
        endif
      enddo
      if (nfr.le.1) go to 999

c
c... Calculate proportion of total fractures
      proptf = dble(nfr)/(dble(ns2-ns1+1))

c
```

```
c... Find total trace length
        do n = 1, nfr
          nn = nfrc(n)
          trace(n) = atrace(nn) + btrace(nn)
        enddo
c
c... Find maximum trace length
      trcmax = -1.d5
      do n = 1, nfr
        trcmax = max(trace(n),trcmax)
      enddo

c
c... Length of fracture segment for plotting is 0.15 inch/meter
      do n = 1, nfr
        nn = nfrc(n)
        alen(n) = atrace(nn)*0.15d0
        blen(n) = btrace(nn)*0.15d0
      enddo
c
c... Calculate blocksize (interval length)
      blksiz = endp2 - endp1
      blkht = 6.d0
      blkdp = 6.d0
c
c Rev MAC 4/17/98 - moved perm, frac volume, porisity to after
c parameters

c Rev MAC 4/98 - zero sum parameters
      totalht = 0d0
      totaltr = 0d0
      ssqht = 0d0
      ssqtr = 0d0
      sspac = 0d0
      ssqsp = 0d0
      ssqlsp =0d0
      slgsp = 0d0
c     MAC V1.1
      gmlen = 0d0
      intarea = 0d0

c Added MAC 5/98
      do n = 1, intmax
            intspace(n) = 0d0
            intfreq(n) = 0d0
            intnfr(n) = 0
            inttrace(n) = 0d0
      end do
      intn = 0
      intlayer = 0
c
c... Calculate fracture parameters - loop through fractures
        do n = 1, nfr
          nn = nfrc(n)
          totaltr = trace(n) + totaltr
          ssqtr = trace(n)**2 + ssqtr
```

```
c           MAC V1.1
            gmlen = gmlen + dlog10(trace(n))

          if(n.gt.1)then
            nm1 = nfrc(n-1)
c rev MAC 4/13/98 - put in if
            spac = dabs(dist(nn)-dist(nm1))
              if (spac.eq.0.0) then
                  write(*,*)'station overlap',dist(nn),nn,nm1
              end if
2099   format(1x,a5,3(1x,f9.2))


            sspac = spac + sspac
c correction MAC 4/13/98
c                 put in '+ slgsp' in place of '+ sspac'
c                 put in dlog10 and if-then
            if (spac.ne.0.0) then
                  slgsp = dlog10(spac) + slgsp
c correction MAC 4/98
c                 put in '+ ssqlsp' in place of '+ ssqsp'
c                 put in dlog10
               ssqlsp = (dlog10(spac))**2 + ssqlsp
            else
c rev MAC 4/98 for zero spacing use 0.005 m which is 1/2
c                 of the measurement precision
               slgsp = dlog10(5d-3) + slgsp
                  ssqlsp = (dlog10(5d-3))**2 + ssqlsp
             end if

            ssqsp = spac**2 + ssqsp


c added MAC 5/98 - for determining frequency and intensity over interval
c                 added MAC 7/98 - if-then statment to prevent from
c                 overextending interval boundary
                  intn = INT((dist(nn)-endp1)/intlength)+1
                  if ( (endp1+(intn*intlength)).le.endp2 ) then
                        if (intn.gt.intmax) then
                              write(*,*)'Max number of intervals exceeded -',
     +                                       ' program stopped'
                              write(*,*)'Resize intmax -
intmax,intn',intmax,intn
                              stop
                        end if
                        intspace(intn) = intspace(intn) + spac
                        intnfr(intn) = intnfr(intn) + 1
                        inttrace(intn) = inttrace(intn) + trace(n)
                        intlayer = intn
                  end if
          endif
300         continue
        enddo

            avgsp = sspac/dble(nfr-1)
            freq = 1.d0/avgsp
```

```
c added MAC 5/98 - for determining frequency and intensity over interval
            do intn = 1,intlayer
                  if (intnfr(intn).gt.1) then
                        intspace(intn) = intspace(intn)/dble(intnfr(intn)-1)
                        intfreq(intn) = 1d0/intspace(intn)
                  else
                        intfreq(intn) = 1d0/intlength
                  end if
                  inttrace(intn) = inttrace(intn)/intlength/blkht
            end do

c           MAC 5/98 added if-then for small # of fractures
            if (nfr.gt.2) then
c                 nfr-1 is the number of pairs used to calculate spacing
                  varsp = (ssqsp - ((sspac**2)/dble(nfr-1)))/(dble(nfr-2))
                  if (varsp.gt.0.0) then
                        sdspac = sqrt(varsp)
c added comment and put in varsp rather than sdspac**2 by MAC 5/98
c V[f]= V[s]*(-E[s]**-2)**2
                        sdfreq = sqrt((((-avgsp)**(-2))**2)*varsp)
                  else
                        sdspac = 0d0
                        sdfreq = 0d0
                  end if
            else
                  varsp = 0d0
                  sdspac = 0d0
                  sdfreq = 0d0
            end if

          frcint = totaltr/blksiz/blkht
          avglen = totaltr/dble(nfr)
            varlen = (ssqtr - ((totaltr**2)/dble(nfr)))/dble(nfr-1)
          if (varlen.gt.0.0) then
                  sdlen = sqrt(varlen)
            else
                  sdlen = 0d0
            end if

c Rev MAC 4/17/98 - calculate b (in um) from airk
            aperture = 1d6*(12d0*(10**logairk(layer))/freq)**(1.0/3.0)

c... Calculate permeability of each fracture and pass to ktensor
      do n = 1, nfr
        aper(n) = aperture*1.d-6
        kfrc(n) = (aper(n)**3)/12.d0
      enddo

c Rev MAC 4/98 - zero sum parameters
      frcvol = 0d0
      frarea = 0d0
      do i = 1,9
            ktens(i) = 0d0
      end do

c... Calculate fracture volume based on penny-shaped fractures
      do n = 1, nfr
```

```
        frcrad = trace(n)*0.5d0
        frcvol = pi*aper(n)*frcrad**2 + frcvol
        frarea = aper(n)*frcrad*2.d0 + frarea
c            MAC V1.1 - will divide by block volume after combining
        intarea = pi*frcrad**2 + intarea

      enddo
c... Calculate fracture porosity
      frcpor = frcvol/(blksiz*blkht*blkdp)
      frcp2d = frarea/(blksiz*blkht)

c Added MAC 4/22/98 - include 1-D porosity
      frcp1d = freq*aperture*1d-6
c
c... Calculate components associated with each fracture, then sum
        radian = pi/180.d0
      do n = 1, nfr
        nn = nfrc(n)
        if(strike(nn).le.90.d0)then
          stkrad = strike(nn)*radian
          diprad = dip(nn)*radian
        elseif(strike(nn).gt.90.d0.and.strike(nn).le.180.d0)then
          stkrad = strike(nn)*radian
          diprad = (180.d0-dip(nn))*radian
        elseif(strike(nn).gt.180.d0.and.strike(nn).le.270.d0)then
          stkrad = strike(nn)*radian
          diprad = (180.d0-dip(nn))*radian
        else
          stkrad = strike(nn)*radian
          diprad = dip(nn)*radian
        endif
        sdsq = (dsin(diprad))**2
        kxx = 1.d0 - ((dcos(stkrad))**2)*sdsq
        kxy = 0.5d0*dsin(2.d0*stkrad)*sdsq
        kxz = -0.5d0*dsin(2.d0*diprad)*dcos(stkrad)
        kyx = kxy
        kyy = 1.d0 - ((dsin(stkrad))**2)*sdsq
        kyz = 0.5d0*dsin(2.d0*diprad)*dsin(stkrad)
        kzx = kxz
        kzy = kyz
        kzz = sdsq
        kf = kfrc(n)*freq
        ktens(1) = kxx*kf + ktens(1)
        ktens(2) = kxy*kf + ktens(2)
        ktens(3) = kxz*kf + ktens(3)
        ktens(4) = kyx*kf + ktens(4)
        ktens(5) = kyy*kf + ktens(5)
        ktens(6) = kyz*kf + ktens(6)
        ktens(7) = kzx*kf + ktens(7)
        ktens(8) = kzy*kf + ktens(8)
        ktens(9) = kzz*kf + ktens(9)
      enddo

c Added MAC 4/21/98
      kzzkxx = ktens(9)/ktens(1)
      kyykxx = ktens(5)/ktens(1)
      kzzkyy = ktens(9)/ktens(5)
```

```
c Added MAC 4/21/98
c     Calculate alpha (see equation 7)
      alpha = aperture*1d-6/2d0/72d-3
c
c Commented out MAC 7/98
c... Open and write permeability components of fracture networks
c      open(11,file=outfile//'.prm',status='unknown')
c        write(11,*)'Permeability Tensor for: ',outfile
c        write(11,450)'kxx','kxy','kxz','kyx','kyy','kyz','kzx',
c     +   'kzy','kzz'
c        write(11,460)ktens(1),ktens(2),ktens(3),ktens(4),
c     +    ktens(5),ktens(6),ktens(7),ktens(8),ktens(9)
c        write(11,*)'kzz/kxx= ',ktens(9)/ktens(1)
c        write(11,*)'kyy/kxx= ',ktens(5)/ktens(1)
c      close(11)

c... Calculate orientations and open and write GMT plot file
             open(11,file=outfile//'.plt',status='unknown')
      do n = 1, nfr
          nn = nfrc(n)
          if(strike(nn).le.90.d0)then
            adip = dip(nn)
            bdip = dip(nn) + 180.d0
          elseif(strike(nn).gt.90.d0.and.strike(nn).le.270.d0)then
            adip = 180.d0 - dip(nn)
            bdip = 360.d0 - dip(nn)
          else
            adip = dip(nn)
            bdip = dip(nn) + 180.d0
          endif
          write(11,404)dist(nn),adip,alen(n),unitname(layer)
          write(11,404)dist(nn),bdip,blen(n),unitname(layer)
        enddo
      close(11)
c-------------------------------------------------------------------
c     Below by MAC 4/98
c     Completely changed output file formatting
c     now 'all1.par' and 'all2.par' which list data for each subunit
c     Deleted E.S. output file writing

      if (endp2.lt.9999.0) then
            write(13,443)unitname(layer),endp1,endp2,trcmin,fmin,
     +      trcmax,nfr,avgsp,sdspac,freq,sdfreq,avglen,sdlen,frcint
            write(14,444)unitname(layer),fmin,nfr,freq,
     +      aperture,frcpor,frcp2d,frcp1d,alpha,kzzkxx,kyykxx,kzzkyy
            write(13,443)'     ',dist(ns1),dist(ns2)
      else
c           alcove data & ECRB data
c           ECRB is read in as if it is alcove 9 MAC 3-23-99
            if (endp1.lt.90000.0) then
             write(13,2443)unitname(layer),INT(endp1/10000.0),trcmin,fmin,
     +       trcmax,nfr,avgsp,sdspac,freq,sdfreq,avglen,sdlen,frcint
            else
             write(13,2445)unitname(layer),trcmin,fmin,
     +       trcmax,nfr,avgsp,sdspac,freq,sdfreq,avglen,sdlen,frcint
            end if
```

```
           write(14,444)unitname(layer),fmin,nfr,freq,
     +     aperture,frcpor,frcp2d,frcp1d,alpha,kzzkxx,kyykxx,kzzkyy
           write(13,2444)(dist(ns2)-dist(ns1))

      end if
441   format(1x,' Unit',1x,'<---Station--->',1x,
      +     ' Min-m',1x,'MinUse',1x,' Max-m',1x,' #Frac',1x,
      +     'Spac-m',1x,'SDSpac',1x,'Fq-1/m',
      +     1x,'SDFreq',1x,'Leng-m',1x,'SDLeng',1x,'Intens')
442   format(1x,' Unit',1x,
      +     'MinUse',1x,' #Frac',1x,'Fq-1/m'
     +      ,1x,'Apr-um',1x,'   Por-3D',1x,'   Por-2D',1x,'   Por-1D'
     +      ,1x,'    alpha',1x,'kzz/kxx',1x,'kyy/kxx',1x,'kzz/kyy')
443   format(1x,a5,2(1x,f7.2),3(1x,f6.2),1x,i6,7(1x,f6.2))
444   format(1x,a5,1x,f6.2,1x,i6,1x,f6.2,1x,f6.0,4(1x,es9.2),
      +           3(1x,f7.2))
2443  format(1x,a5,4x,'Alcove',i2,4x,3(1x,f6.2),1x,i6,7(1x,f6.2))
2444  format(7x,f7.2,1x,'meters')
2445  format(1x,a5,4x,'ECRB  ',2x,4x,3(1x,f6.2),1x,i6,7(1x,f6.2))

c     Save results for combined output
c     added MAC 4/98
      combine(layer,1)=endp1
      combine(layer,2)=endp2
      combine(layer,3)=trcmin
      combine(layer,4)=trcmax
      combine(layer,5)=dble(nfr)
      combine(layer,6)=avgsp*dble(nfr-1)
      combine(layer,7)=ssqsp
      combine(layer,8)=avglen*dble(nfr)
      combine(layer,9)=ssqtr
      combine(layer,10)=frcpor*blksiz/(aperture*1d-6)
      combine(layer,11)=frcp2d*blksiz/(aperture*1d-6)
      combine(layer,12)=ktens(1)/freq
      combine(layer,13)=ktens(5)/freq
      combine(layer,14)=ktens(9)/freq
      combine(layer,15)=slgsp
      combine(layer,16)=ssqlsp
c     MAC V1.1
      combine(layer,17)=intarea
      combine(layer,18)=gmlen

c Added MAC 5/98 - Output interval results to 'interval.par'
      do intn=1,intlayer
                  write(18,2000)unitname(layer),
      +           (endp1+(intn-1)*intlength),
     +            (endp1+(intn)*intlength),
     +            intnfr(intn),intspace(intn),intfreq(intn),
     +            (dble(intnfr(intn))/intlength),inttrace(intn)
      end do
1999  format(1x,' Unit',2(1x,'  Station'),1x,'   #Frac',4x,
      +     'Spacing',2x,'Frequency',3x,'#/Length',2x,'Intensity')
2000  format(1x,a5,2(1x,f9.1),1x,i8,4(1x,f10.2))
c-----------------------------------------------------------------------

c... Write fracture size distributions
      if(ans2.eq.'y')then
```

```
      open(12,file=outfile//'.szd',status='unknown')
      do k = 1, ni
          fgrp1 = fmesf + dble(k-1)*frint
          fsiz = fgrp1 + frint*0.5d0
c rev MAC 5/12/97  write(12,470)fsiz,dble(nfrint(k))/dble(ns)
        write(12,475)fsiz,nfrint(k)
      enddo
      close(12)
        fsum = 0.d0
c             write cumulative size distributions
      open(12,file=outfile//'.csd',status='unknown')
        ftot = 1.d0
        write(12,470)fmesf,ftot
      do k = 1, ni
        fgrp1 = fmesf + dble(k)*frint
        fsum = dble(nfrint(k))/dble(ns) + fsum
        write(12,470)fgrp1,1.d0 - fsum
      enddo
      close(12)
      endif
c

c Added MAC 4/17/98
999   continue
      END DO
      close(13)
      close(14)

c-----------------------------------------------------------------------------
----------
c     Below is all new code added by MAC 4/98

c     Combine results for single values for each model layer
c
c     Output to files 'comb1.par' & 'comb2.par' - combined results of
c     all1.par & all2.par
c     Output to file 'calibrate.par' - data to be used for inversion
c
      open(13,file='comb1.par',status='unknown')
      open(14,file='comb2.par',status='unknown')
      open(15,file='calibrate.par',status='unknown')
      write(13,1441)
      write(14,442)
      write(15,2501)
      DO i = 1,ntotal
            trcmin = 1d6
            trcmax = 0d0
            nfr = 0
            avgsp = 0d0
            sspac = 0d0
            sdspace = 0d0
            ssqsp = 0d0
            avglen = 0d0
            sdlen = 0d0
            ssqtr = 0d0
            frcpor = 0d0
            frcp2d = 0d0
```

```
            blksiz = 0d0
            kxx = 0d0
            kyy = 0d0
            kzz = 0d0
            slgsp = 0d0
            sslgsp = 0d0
c           MAC V1.1
            intarea = 0d0
            gmlen = 0d0

            first = modlayer(i)
            if (i.ne.ntotal) then
                  last = modlayer(i+1) - 1
            else
                  last = nlayers
            end if
            n = last - first + 1
      DO layer = first,last
            trcmin = min(trcmin,combine(layer,3))
            trcmax = max(trcmax,combine(layer,4))
            nfr = nfr + NINT(combine(layer,5))
            sspac = sspac + combine(layer,6)
            ssqsp = ssqsp + combine(layer,7)
            avglen = avglen + combine(layer,8)
            ssqtr = ssqtr + combine(layer,9)
            frcpor = frcpor + combine(layer,10)
            frcp2d = frcp2d + combine(layer,11)
            blksiz = blksiz + combine(layer,2) - combine(layer,1)
            kxx = kxx + combine(layer,12)
            kyy = kyy + combine(layer,13)
            kzz = kzz + combine(layer,14)
c
            slgsp = slgsp + combine(layer,15)
            ssqlsp = ssqlsp + combine(layer,16)

c           MAC V1.1
            intarea = intarea + combine(layer,17)
            gmlen = gmlen + combine(layer,18)
            if ((layer.eq.last).and.(nfr.gt.(n+1))) then
                  avgsp = sspac/dble(nfr-n)
                  freq = 1.d0/avgsp
c                 nfr-n is the number of pairs used to calculate spacing
                  varsp = (ssqsp - ((sspac**2)/dble(nfr-n)))/(dble(nfr-n-1))
                  if (varsp.gt.0.0) then
                        sdspac = dsqrt(varsp)
                  else
                        sdspac = 0d0
                  end if
                  varlen = (ssqtr - ((avglen**2)/dble(nfr-n))) /
     >                                  (dble(nfr-n-1))
                  avglen = avglen/dble(nfr)
                  if (varlen.gt.0.0) then
                        sdlen = dsqrt(varlen)
                  else
                        sdlen = 0d0
                  end if
                  if (sdspac .gt. 0.0) then
```

```
                    sdfreq = dsqrt(varsp/(avgsp**4))
                else
                    sdfreq = 0d0
                end if
                aperture = 1d6*(12d0*(10**logairk(layer))/freq)
     &                           **(1.0/3.0)
                alpha = aperture*1d-6/2d0/72d-3
                frcpor = frcpor*(aperture*1d-6)/blksiz
                frcp2d = frcp2d*(aperture*1d-6)/blksiz
                frcp1d = freq*aperture*1d-6
c               calculate k ratios (note freq cancels)
                kzzkxx = kzz/kxx
                kyykxx = kyy/kxx
                kzzkyy = kzz/kyy
c               calulate fracture intensity
                frcint = avglen*dble(nfr)/blksiz/6e0
c               MAC V1.1
                gmlen = 10**(gmlen/dble(nfr))
                intarea = intarea/blksiz/(gmlen**2)

                write(13,1443)unitname(layer),trcmin,fmin,
     +           trcmax,nfr,avgsp,sdspac,freq,sdfreq,avglen,sdlen,frcint
                write(14,444)unitname(layer),fmin,nfr,freq,
     +          aperture,frcpor,frcp2d,frcp1d,alpha,kzzkxx,kyykxx,kzzkyy

c
                ssqlsp = (ssqlsp - slgsp**2/dble(nfr-n) )/ dble(nfr-n-1)
                slgsp = slgsp / dble(nfr-n)
                logf = - slgsp
                loga = (1d0/3d0)*(dlog10(12d0)+logairk(layer)-logf)
     >                       - dlog10(2d0*72d-3)
                sdalpha = sdfreq*dsqrt(1d0/72d-3) *
     >          ( (10**logairk(layer)) /18d0/(freq**4) )**(1.0/3.0)
                if (ssqlsp.le.0.0) then
                      write(*,2500)unitname(layer),slgsp,ssqlsp
                      ssqlsp = 0.0
                end if

c           MAC V1.1 add new parameters gmlen (gemetric mean length) and
c           intarea (fracture area/block volume where block volume is
c           block length * gmlen^2).  Also changed output for calibrate.par
      write(15,2500)unitname(layer),fmin,frcp2d,(aperture*1d-6),freq,
      +     intarea,gmlen,alpha,sdalpha,loga,dsqrt(ssqlsp/9d0)
2500  format(1x,a5,5x,f9.2,2(3x,es9.2),3x,f9.2,2(3x,f9.3),
      +     2(3x,es9.2),2(3x,f9.2))
2501  format(1x,' Unit',1x,'Min-Fr-Length',1x,'Fr-Porosity',4x,
      +     'Aperture',3x,'Frequency',2x,'Inter-Area',3x,'Gm-length',
     +      4x,'Fr-Alpha',4x,'SD-Alpha',4x,'LogAlpha',1x,'SD-LogAlpha')
c2500 format(1x,a5,2(1x,f7.2),2(1x,es9.2),3(1x,f7.2),1x,f7.3,1x,f7.2,
c     +     1x,i5,2(1x,f7.2))
c2501 format(1x,' Unit',4x,'Freq',2x,'SDFreq',5x,'alpha',3x,'sdalpha',
c     +     4x,'loga',2x,'logsda',2x,'<loga>',
c     +     1x,'s<loga>',2x,'gmFreq',1x,'#Frac',3x,'Block',3x,'#Freq')


c     added else statement - MAC 6/25/98
            else
```

```
                if (layer.eq.last) then
                     write(13,2500)unitname(layer)
                     write(14,2500)unitname(layer)
                     write(15,2500)unitname(layer)
                end if

           end if
      END DO
      END DO
1441  format(1x,' Unit',1x,
      +     ' Min-m',1x,'MinUse',1x,' Max-m',1x,' #Frac',1x,
      +     'Spac-m',1x,'SDSpac',1x,'Fq-1/m',
      +     1x,'SDFreq',1x,'Leng-m',1x,'SDLeng',1x,'Intense')
1443  format(1x,a5,3(1x,f6.2),1x,i6,7(1x,f6.2))
      close(13)
      close(14)


      stop


  400 format(a200)
  404 format(f13.2,1x,f8.4,1x,f9.5,1x,a5)
  408 format(a10)
  410 format(i2,1x,f5.2)
  415 format(a21,2(1x,f7.2))
  420 format(a48,2(1x,f7.3),1x,i5,1x,f5.3)
  425 format(a78)
  430 format(f8.4,5(2x,f8.4),2(2x,e10.4))
  440 format(a40)
  450 format(9(4x,a4,3x))
  460 format(9(1x,e10.3))
  470 format(f10.3,1x,f8.4)
  475 format(f10.3,1x,i8)
c
      stop
      end
```

Source code for Software Routine Read TDB, Version 1.0

```
      program Read_TDB

c     This program reads the data files from the
c     Technical Database.  Output are written
c     unformatted to selected output file.  All messages are
c     recorded to the screen and file 'index.txt'
c     Mark Cushey 4/98

c     Output is limited to 10 numerical datatypes
c     It is assumed that the maximum line length is less than 250

      real anum,bnum,value(10),limvalue(10,2),loctype
      character*4 first
      character*25 filename
      character*250 all
      character*250 datastring
      character*8 astat,bstat,avalue,limtext(10)
      character*1 onestring(250),onedata(8),plus(8),ans
      character*8 dataname(10),limitname(10)
      integer row,iname,istring,idata,icolumn(10),i,loc,rowused,
      +     im,limnum,limtxt

c     ----------------------------------------

c     open output files
      write(*,*)'Enter name of output file:'
      read(*,1000)filename
      open(unit=20,file=filename)
      open(unit=21,file='index.txt')
      write(*,*)'Details on data retrieval are in index.txt'

c     ----------------------------------------
c     query for different data types to be stored
c
      write(*,*)'List names of data types to be retrieved - up to 10'
      write(*,*)'   Enter only the first 8 letters for each'
      write(*,*)'   Enter the word end for last entry'
      i = 0
40    i = i + 1
      read(*,1010)dataname(i)
      if ((dataname(i).ne.'end').and.
      &     (dataname(i).ne.'END')) go to 40
      iname = i - 1
      write(*,1040)iname
      write(21,1040)iname
      write(20,1041)(dataname(i),i=1,iname)
      write(*,*)'Should header be printed in output file - Y or N'
      read(*,1011)ans
      if ((ans.eq.'Y').or.(ans.eq.'y'))
      &     write(21,1041)(dataname(i),i=1,iname)
1010  format(a8)
1011  format(a1)
1040  format(1x,i7,' datatypes selected')
1041  format(10(2x,a8))
c     ----------------------------------------
```

```
c     query for limits on outputting data
      limnum = iname
      limtxt = iname
      write(*,*)'Are there limits for the output - Y or N ?'
      read(*,1011)ans
      if ((ans.eq.'Y').or.(ans.eq.'y')) then
            i = iname
c           write(*,*)'Enter the parameter names for numerical limits'
c           write(*,*)'   Enter only the first 8 letters for each'
c           write(*,*)'   Enter the word end for last entry'
c45         i = i + 1
c           read(*,1010)dataname(i)
c           if ((dataname(i).eq.'end').or.
c     &     (dataname(i).eq.'END')) go to 46
c           write(*,*)'Enter upper and lower value for limit'
c           read(*,*)limvalue(i,1),limvalue(i,2)
c           write(*,*)'Enter next limit or end'
c           go to 45
c46         i = i - 1
c           limnum = i
            write(*,*)'Enter the parameter names for text-defined limits'
            write(*,*)'   Enter only the first 8 letters for each'
            write(*,*)'   Enter the word end for last entry'
47          i = i + 1
            read(*,1010)dataname(i)
            if ((dataname(i).eq.'end').or.
      &     (dataname(i).eq.'END')) go to 49
            write(*,*)'Enter text to exclude - up to 8 characters'
            read(*,1010)limtext(i)
            write(*,*)'Enter next limit or end'
            go to 47
49          limtxt = i - 1
            do i=(iname+1),limtxt
                  if (i.le.limnum) then
                        write(*,1045)dataname(i),limvalue(i,1),limvalue(i,2)
                        write(21,1045)dataname(i),limvalue(i,1),limvalue(i,2)
                  else
                        write(*,1046)dataname(i),limtext(i)
                        write(21,1046)dataname(i),limtext(i)
                  end if
            end do
      end if
1045  format(1x,'Limits on',a8,1x,f9.3,1x,f9.3)
1046  format(1x,'Limits on',a8,1x,'exclude',1x,a8)

c     ------------------------------------------
c     query for input filename and open

50    write(*,*)'Enter next data filename (use MS-DOS filename) or quit'
      read(*,1000)filename
      if ((filename.eq.'quit').or.(filename.eq.'QUIT'))go to 990
      open(unit=10,file=filename,action='READ',
      &     form='FORMATTED',status='old',err=75)
      write(*,*)filename
      write(21,*)'------------------'
      write(21,*)filename
```

```
      write(21,*)'------------------'
1000  format(a25)
      go to 80
75    write(*,*)'File does not exist'
      go to 50

c     ----------------------------------------
c     If one of the parameters is LOCATION, determine type.
c     If LOCATION is station number along DLS, loctype =0
C     If LOCATION is along alcove, loctype = alcove # (can be #.1, #.2)
c     If other, then loctype = -1.
80    loctype = -1.0
      Do i = 1,iname
            if (dataname(i).eq.'LOCATION') then
                  write(*,*)'Is LOCATION a station number along the',
     +' DLS, alcove, or other - d, a, or o'
                  read(*,*)ans
                  if ((ans.eq.'d').or.(ans.eq.'D')) then
                        loctype = 0.0
                  else
                        if ((ans.eq.'a').or.(ans.eq.'A')) then
                              write(*,*)'Which alcove #'
                              read(*,*)loctype
                        else
                              loctype = -1.0
                        end if
                  end if
            end if
      End Do
c     ----------------------------------------

c     find header line (between rows of asteriks)
82    read(10,1001)first
      if (first.ne.'****') go to 82
1001  format(a4)

c     ----------------------------------------

c     find location where different data starts (use header)

      do i=1,limtxt
            icolumn(i)=0
      end do

      read(10,1020)datastring
      read(datastring,1021)(onestring(istring),istring=1,250)
      do i = 1,limtxt
            read(dataname(i),1022)(onedata(idata),idata=1,8)
            do istring = 1,250
             do idata = 1,8
              if( (onestring(istring+idata-1).ne.onedata(idata)) )
     &            go to 98
             end do
98           if (idata.eq.9) go to 99
            end do
99          if (istring.ne.251) then
                  icolumn(i)=istring
```

```
            else
                  write(*,1023)dataname(i)
                  pause
                  stop
            end if
      end do

      write(*,1003)(icolumn(i),i=1,iname)
      write(21,1003)(icolumn(i),i=1,iname)
1003  format(1x,'Column headers at',10(1x,i5))
1020  format(a250)
1021  format(250(a1))
1022  format(8(a1))
1023  format(1x,a8,' not found in file -- stopped')


c     --------------------------------------
c     move forward to first data row

105   read(10,1001)first
      if (first.ne.'****') go to 105
c     skip blank line
      read(10,1002)all
1002  format(a72)

c     ----------------------------------------

c     read data lines from file and get values
      rowused = 0
      row = 0
200   read(10,2001,err=900,end=900)datastring
      if (datastring.eq.'End of Report') go to 900
      if (datastring.eq.'             ') go to 200
      row = row + 1
      write(*,*)row

c     first see if data is within text-defined limits
      do ii=(limnum+1),limtxt
            loc = icolumn(ii)
            read(datastring,1999)all
            if (all.eq.limtext(ii)) then
                  write(*,2025)row,dataname(ii),limtext(ii)
                  write(*,2026)datastring
                  write(21,2025)row,dataname(ii),limtext(ii)
                  write(21,2026)datastring
                  go to 200
            end if
      end do

      do i=1,iname
            loc = icolumn(i)
            read(datastring,1999)avalue

c           first check to see if any are not recorded (NR) or
c           special (*) -- exclude NR and use *
            read(avalue,2002)(onedata(idata),idata=1,8)
            do idata=1,8
```

```
                        if ((onedata(idata)).eq.'N') then
c                       the entire line is excluded
                         write(*,2020)row,onedata(idata),onedata(idata+1),
      &                       dataname(i)
                         write(21,2020)row,onedata(idata),onedata(idata+1),
      &                       dataname(i)
                         go to 200
                        end if
                  if (onedata(idata).eq.'*') then
                        write(*,2021)row
                        write(21,2021)row
                        read(avalue,2024)avalue
                  end if
                  end do

c                 check if entry is a station number -- if loctype = 0
c                 LOCATION is station number along DLS, if loctype = +#
c                 LOCATION is along alcove (number loctype)

                  If ((loctype.ge.0.0).and.(dataname(i).eq.'LOCATION')) then
c                       get station number
                        read(avalue,2005)(plus(ip),ip=1,8)
                        do ip=1,8
                              if (plus(ip).eq.'+') go to 215
                        end do
215                     read(avalue,2010)astat,all,bstat
                        read(astat,*)anum
                        read(bstat,2005)(plus(im),im=1,(8-ip))
                        do im = 1, (8-ip)
                              if (plus(im).eq.'-') go to 216
                        end do
216                     read(bstat,2011)astat
                        read(astat,*)bnum

                        if (loctype.eq.0.0) then
                              value(i) = anum*100 + bnum
                        else
                              value(i) = loctype*10000 + anum*100 + bnum
                        end if
                  else
                        read(avalue,*)value(i)
                  end if

            end do

2001        format(a250)
c           change a8 to larger value if number is more than 8 digits
1999        format(<loc-1>x,a8)
2002        format(8(a1))
2005        format(8(a1))
2010        format(a<ip-1>,a1,a8)
2011        format(a<im-1>)
2020        format(1x,'Row',i5,' has a ',a1,a1,' for ',a8,
            &           ' - this data row is not used')
2021        format(1x,'Row',i5,' has a * - printed value will be used')
2024        format(a<idata-1>)
```

```
2025  format(1x,'Row',i5,' excluded ',a8,' is ',a8)
2026  format(5x,a40)


c     write data to output file and read next line

      write(20,3000)(value(i),i=1,iname)

3000  format(10(f10.3))
      rowused = rowused + 1
      go to 200

900   close(10)
      write(*,*)row,' rows read and',rowused,' used'
      write(21,*)row,' rows read and',rowused,' used'
c     ask for next file
      go to 50

990   close(20)
      close(21)
      pause
      stop
999   write(*,*)'Error in file formatting -- stopped'
      write(*,*)'Error in file formatting -- stopped'
      close(20)
      close(21)
      close(10)
      pause
      stop
      end
```

Source code for Software Routine Meshbd.f, Version 1.0

```
      program Meshbd
c
c change mesh order
c change z direction from "-" to "+"
c change interface at top boundary
c
      implicit double precision (a-h,o-z)
      integer nc,ne
      integer me,mc,nh
      parameter (me  = 88500)
      parameter (mc  =310000)
      parameter (nh  = 1000)
      double precision voll(mc),aa(mc)
      character*5 dddd,ccc,cccc
      character*5 texte
      character*1 text
      character*5 wrd,wrd2
      nx=12
      ny=30
      nz=42
c
      open(unit=2,file='MESH',status='unknown')
      rewind(2)
      texte='ELEME'
      write(2,'(a)')texte
c
      open(unit=1,file='meshm.mes',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
c
      ne = 0
      nesum = 0
      locat = 1
      do i=1,nx
        do j=1,ny
          do k=1,nz
            ne=ne+1
            read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &      dddd,texte,voll(ne),v1,x1,y1,z1
          nesum = nesum + 1
            if(k.eq.nz)then
              texte='BUNOF'
            elseif(k.eq.1)then
              texte='DRAIN'
            voll(ne)=1.0e+50
            else
              texte='SOILF'
            endif
            write(2,'(a,10x,a,2e10.4,10x,3e10.4)')
     &      dddd,texte,voll(ne),v1,x1,y1,-z1

          enddo
```

```
          enddo
        enddo

c
        read(1,*)
        read(1,'(a)')cccc
        write(2,*)
        cccc='CONNE'
        write(2,'(a)')cccc

        nc=0
        locat =1
30      read(1,'(2a,19x,a,4e10.4)',end=40)wrd,wrd2,text,v1,v2,aa(nc+1),v3
        if(wrd.ne. '     ' .and.wrd.ne.'+++  ')then
         if(wrd(1:2).eq.'B7'.and.wrd2(1:2).eq.'B7')aa(nc+1)=100.0
        write(2,'(2a,19x,a,4e10.4)')wrd,wrd2,text,v1,v2,aa(nc+1),v3
           nc=nc+1
           goto 30
        endif

c
        texte='     '
        write(2,'(a)')texte
        close(1)
        close(2)
        stop
   40   stop'Premature End of File'
        end
```

Source code for Software Routine mininipresf.f, Version 1.0

```
      program mininipresf
c for 12x30x42 mesh (5.23x15x20 m)
c make incon block from
c MESH
c
      implicit double precision(a-h,o-z)
      character name*5,head*80
      dimension xfield(100,100,100,20),class(100)
c read mod.in
      nz=42
      ny=30
      nx=12
      ndual=1
      do i=1,nx
      do j=1,ny
         do k=1,nz
        do kk=1,ndual
           xfield(i,j,k,kk)=4.e-18
        enddo
       enddo
       enddo
      enddo

c read kfield
      open(unit=1,file='permcut.dat',status='old')
      rewind(1)
      read(1,*)
      do k=1,nz
      do j=1,ny
      do i=1,nx
      read(1,*)xfield(i,j,k,1)
      enddo
      enddo
      enddo
      close(1)
c check input field
      do k=1,100
      class(k)=0.0d0
      enddo
      write(*,*)'   number of classes'
      read(*,*)inums
      xmins=1.0e+30
      xmaxs=-1.0e+30
         do k=2,nz-1
         do j=1,ny
         do i=1,nx
         if(xfield(i,j,k,1).lt.xmins)xmins=xfield(i,j,k,1)
         if(xfield(i,j,k,1).gt.xmaxs)xmaxs=xfield(i,j,k,1)
         enddo
         enddo
         enddo
         write(*,*)'min= ',xmins
         write(*,*)'max= ',xmaxs
      xmeans=0.0d0
      sss=0.0d0
```

```
      dxs=(xmaxs-xmins)/dble(inums)
      iouts=0
      do kk=2,nz-1
      do j=1,ny
      do i=1,nx
         do k=1,inums
         x1=xmins+(k-1)*dxs
         x2=xmins+k*dxs
         if(xfield(i,j,kk,1).ge.x1.and.xfield(i,j,kk,1).le.x2)then
         class(k)=class(k)+1.0d0
         goto 12
         endif
         enddo
         enddo
      iouts=iouts+1
   12 enddo
      enddo

      do k=2,nz-1
      do j=1,ny
      do i=1,nx
      xmeans=xmeans + xfield(i,j,k,1)
      enddo
      enddo
      enddo

      xmeans=xmeans/dble(12*30*40)

      do k=2,nz-1
      do j=1,ny
      do i=1,nx
      sss=sss+(xfield(i,j,k,1)-xmeans)*(xfield(i,j,k,1)-xmeans)
      enddo
      enddo
      enddo

      sss=sss/dble(12*30*40)
      sssd=sqrt(sss)

      do i=1,inums
      class(i)=class(i)/dble(12*30*40)
      enddo
      open(unit=3,file='perm.tec',status='unknown')
      rewind(3)
      write(3,*)'MEAN IN Log10 ',xmeans
      write(3,*)'STANTARD DIVIATION IN Log10 and Ln ',sssd,2.3026*sssd
      write(3,*)'TITLE="FREQUENCY OF PERMEABILITY"'
      write(3,*)'VARIABLES = "LOG10 PERM", "FREQUENCY"'
      write(3,*)'ZONE, I = ',2*inums
         do k=1,inums
         write(3,'(2e15.6)')xmins+(k-1)*dxs,class(k)/dxs
         write(3,'(2e15.6)')xmins+k*dxs,class(k)/dxs
         enddo
         close(3)

c read and write incon
      open(unit=1,file='MESH',status='old')
```

```
      rewind(1)
      open(unit=2,file='inconsf.out',status='unknown')
      rewind(2)
c
      read(1,'(a)')dddd
      write(2,*)'INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY '
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a,14x,a,2e10.4,10x,3e12.6)')name
c      sat=sini

      if(k.eq.1)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,2,kk))
      porm=0.000124
      sat=0.011
      alfa0=0.
      else
      xkf=xfield(i,j,1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
      goto 99
      endif

      if(k.eq.nz)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,nz-1,kk))
      porm=0.000124
      sat=0.011
      alfa0=0.
      else
      xkf=xfield(i,j,nz,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500
      endif
      goto 99
      endif


      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,k,kk))
      porm=0.000124
      sat=0.011
      alfa0=0.
      else
      xkf=xfield(i,j,k-1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
```

```
   99 continue
c
      por=porm
      write(2,'(a5,2i5,e15.9,5e10.4)')name,idum,idum,porm,xkf,alfa0
      write(2,'(2e20.14)')sat
      enddo
      enddo
      enddo
      enddo
      texte='     '
      write(2,'(a)')texte
      write(2,*)
      close(1)
      close(2)
      stop
      end
```

Source code for Software Routine mddf.f, Version 1.0

```
      program mddf
c cut round tunnel with radius R in 3D FD mesh
c truncate elements and connections within R
c cut for refined mesh
c write connectivity list for tunnel bound elements to tunnel element
c file: 'drift3d.con'
c write list with coordinates of tunnel bound elements in
c file: 'drift3d.coor'
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 128)
      character*5 ,id(me)
      double precision x(3,me)
      double precision a(mc),rdrift,dx,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc
      integer nel
      integer nel
      integer ne2
      integer nu1
      integer nu2
      write(*,*)'radius tunnel'
      read(*,*)rdrift
      call rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      stop
      end
c
      subroutine rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      character*5 id(me)
      character*5 irock
      character*1 text
      double precision x(3,me)
      double precision a(mc),rdrift,rr,v1,v2,v3,dy,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
```

```
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc,neall,nz
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      open(unit=1,file='MESH',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      open(unit=10,file='MESHsf.new',status='unknown')
      rewind(10)
      write(10,'(a)') wrd
      open(unit=3,file='driftff.con',status='unknown')
      rewind(3)
      open(unit=9,file='driftff.coor',status='unknown')
      rewind(9)
      open(unit=7,file='driftff.tec',status='unknown')
      rewind(7)
      write(3,*)'CONNE'
      write(9,*)'COOR'
      ne = 0
      neall=0
      nz=42
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),irock,vol,v1,x1,y1,z1

      neall=neall+1
      x(1,ne+1) = x1
      x(2,ne+1) = y1
      x(3,ne+1) = z1
      if(id(ne+1) .ne. '     ') then
         if(vol .eq. 0.) goto 10
c
      dy=dabs(y1-7.5)
c      dy=idint(dy/0.5)*0.5+0.25
      dz=dabs(z1- 7.75)
c      dz=idint(dz/0.5)*0.5+0.25
c
c check radius
         rr=sqrt(dy*dy+dz*dz)
         if(rr.lt.rdrift) goto 10
         write(10,'(a,10x,a,2e10.4,10x,3e10.4)')
     &         id(ne + 1),irock,vol,v1,x1,y1,z1
         ne = ne + 1
         ind(ne) = ne
```

```
            if(x1 .ne. 0.0 .or. y1 .ne. 0.0 .or. z1 .ne. 0.0) locat = 0
            goto 10
         endif
         call hash(id,ind,hsh,ne,nh,ec)
         if(locat .ne. 0) then
            do i = 1, ne
               x(2,i) = -999.d0
               x(3,i) = -999.d0
            enddo
            open(unit=2,file='locat',status='old')
            read(2,'(a)',end=50) wrd
            if(wrd .ne. 'locat' .and. wrd .ne. 'LOCAT') then
               stop 'no locat in locat'
            endif
 20         read(2,'(a5,5x,2f20.0)',end=50) wrd, y1, z1
            if(wrd .ne. '     ') then
               nu1 = ihash(wrd, id,ind,hsh,ne,nh)
               if(nu1 .eq. 0) then
                  goto 20
               endif
               x(2,nu1) = y1
               x(3,nu1) = z1
               goto 20
            endif
            write(10,*)
         endif
         if(ne .ge. me) then
            stop 'Exceeded maximum number of elements'
         endif
         ixyz=3
         ne1 = 0
         ne2 = ne
         do while(ne1 .lt. ne2)
            x1 = x(1,ne1+1)
            y1 = x(2,ne1+1)
            z1 = x(3,ne1+1)
            if(y1 .ne. -999.d0 .or. z1 .ne. -999.d0) then
               if(ne1 .eq. 0) then
                 xhi = x1
                 xlo = x1
                 yhi = y1
                 ylo = y1
                 zhi = z1
                 zlo = z1
             else
                 xhi = max(xhi,x1)
                 xlo = min(xlo,x1)
                 yhi = max(yhi,y1)
                 ylo = min(ylo,y1)
                 zhi = max(zhi,z1)
                 zlo = min(zlo,z1)
             endif
               ne1 = ne1 + 1
            else if(x(2,ne2) .eq. -999.d0 .and. x(3,ne2) .eq. -999.d0) then
               ne2 = ne2 - 1
            else
               wrd = id(ne1+1)
```

```
            x(1,ne1+1) = x(1,ne2)
            x(2,ne1+1) = x(2,ne2)
            x(3,ne1+1) = x(3,ne2)
            id(ne1+1) = id(ne2)
            x(1,ne2) = x1
            x(2,ne2) = y1
            x(3,ne2) = z1
            id(ne2) = wrd
         endif
      enddo
      if(ixyz .eq. 0) then
         xhi = xhi - xlo
         yhi = yhi - ylo
         zhi = zhi - zlo
         if(zhi .le. min(xhi,yhi)) then
            ixyz = 3
         else if (yhi .le. min(xhi,zhi)) then
            ixyz = 2
         else
            ixyz = 1
         endif
      endif
      if(ixyz .eq. 2) then
         do i = 1, ne1
            x(2,i) = x(3,i)
         enddo
      elseif(ixyz .eq. 1) then
         do i = 1, ne1
            x(1,i) = x(2,i)
            x(2,i) = x(3,i)
         enddo
      endif
      call hash(id,ind,hsh,ne,nh,ec)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'conne' .and. wrd .ne. 'CONNE') then
         stop 'no conne in MESH'
      endif
      write(10,*)
      write(10,'(a)')wrd
      nc = 0
      do i = 1, ne
         ec(i) = 0
      enddo
 30   read(1,'(2a,19x,a,4e10.4)',end=40) wrd,wrd2,text,v1,v2,a(nc+1),v3
      if(wrd .ne. '     ' .and. wrd .ne. '+++  ') then
         nu1 = ihash(wrd, id,ind,hsh,ne,nh)
         nu2 = ihash(wrd2,id,ind,hsh,ne,nh)
         if(nu1 .eq. 0) then
c              write(6,60) wrd,nc+1
            if(nu2 .ne. 0)then
            wrd='DRI 1'
            text='3'
c  no gravity
          write(3,'(2a,19x,a,4e10.4)')
     &      wrd2,wrd,text,v2,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd2,x(1,nu2),x(2,nu2),
     &      x(3,nu2),v3
```

```
            endif
            goto 30
         else if(nu2 .eq. 0) then
c                write(6,60) wrd2,nc+1
            if(nu1 .ne. 0)then
            wrd2='DRI 1'
            text='3'
            write(3,'(2a,19x,a,4e10.4)')
     &      wrd,wrd2,text,v1,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd,x(1,nu1),x(2,nu1),
     &      x(3,nu1),v3
            endif
            goto 30
         endif
      write(10,'(2a,19x,a,4e10.4)') wrd,wrd2,text,v1,v2,a(nc+1),v3
      nc=nc+1
         e(1,nc) = nu1
         e(2,nc) = nu2
         if(nu1 .gt. ne1 .or. nu2 .gt. ne1) goto 30
         cc(1,nc) = ec(nu1)
         cc(2,nc) = ec(nu2)
         ec(nu1) = nc
         ec(nu2) = nc
         goto 30
      endif
      if(nc .ge. mc) then
         stop 'Exceeded maximum number of connections'
      endif
      close(unit=1)
      close(unit=10)
      close(unit=3)
      close(unit=9)
      ne = ne1
      return
 40   stop 'Premature EOF on MESH'
 50   stop 'Premature EOF on locat'
 60   format(' Unknown element "',a,'" at connection',i8)
      end
      subroutine hash(id,ind,hsh,ne,nh,h)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer h(ne)
      integer hsh(nh)
      character*5 w1
      integer i,i1,i2,j,k,n
      do j = 1, ne
         w1 = id(j)
         if(w1(4:4) .eq. '0') w1(4:4) = ' '
         n = 0
         do i = 1, 5
            n = n + i * ichar(w1(i:i))
         enddo
         h(j) = mod(n,nh) + 1
      enddo
      i1 = 1
```

```
do i = 1, nh
   i2 = i1
   do j = i2, ne
      k = ind(j)
      if(h(k) .eq. i) then
         h(k) = 0
         ind(j) = ind(i1)
         ind(i1) = k
         i1 = i1 + 1
      endif
   enddo
   hsh(i) = i1
enddo
return
end
integer function ihash(wrd,id,ind,hsh,ne,nh)
implicit none
integer ne, nh
character*5 id(ne)
integer ind(ne)
integer hsh(nh)
character*5 wrd, w1, w2
integer i,i1,i2,n
w1 = wrd
if(w1(4:4) .eq. '0') w1(4:4) = ' '
n = 0
do i = 1, 5
   n = n + i * ichar(w1(i:i))
enddo
n = mod(n,nh) + 1
i1 = 1
if(n .gt. 1) i1 = hsh(n - 1)
i2 = hsh(n) - 1
do i = i1, i2
   ihash = ind(i)
   w2 = id(ihash)
   if(w2(4:4) .eq. '0') w2(4:4) = ' '
   if(w1 .eq. w2) then
      if(ihash .gt. ne) ihash = 0
      return
   endif
enddo
ihash = 0
return
end
```

Source code for Software Routine mk gener.f, Version 1.0

```
      program mk_gener
c makes gener block for heater in drift and wing heaters
      implicit double precision (a-h,o-z)
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 2500)
      character*5 id(me)
      character*5 tfeld(me)
      double precision x(3,me)
      double precision a(mc),voll(me)
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      call rmesh
     &(rdrift,ne,id,tfeld,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz,voll)
      stop
      end
c
      subroutine rmesh
     &(rdrift,ne,id,tfeld,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz,voll)
      implicit double precision (a-h,o-z)
      character*5 id(me)
      character*5 texte
      character*5 tfeld(me)
      double precision x(3,me)
      double precision a(mc)
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision voll(me)
      character*5 wrd
c
      write(*,*)'Infiltration Rate in mm/a'
      read(*,*)rinf
c
      open(unit=2,file='GENERsf',status='unknown')
      rewind(2)
      texte='GENER'
      write(2,'(a)')texte
      iw1=0
      iw2=0
c
      open(unit=1,file='MESHSF',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
c
```

```
      ne = 0
      nesum = 0
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),texte,voll(ne+1),v1,x1,y1,z1
      nesum = nesum + 1
      if(id(ne+1) .ne. '     ') then
c        if(vol .eq. 0.) goto 10
         if(texte.eq.'BUNOF')ne = ne + 1
       goto 10
      endif
c
      volsum=0.0
      do i=1,ne
      volsum=volsum+voll(i)
      enddo
c
      do i=1,ne
      fakt=voll(i)/volsum
      write(2,'(2a,i4,25x,a,e10.4)')
     &id(i),'I',i,'WATE ',fakt*rinf*78.45*3.171e-08
      enddo
c
      close(1)
      close(2)
      stop
   40 stop'Premature End of File'
      end
```

Source code for Software Routine mk scale k.f, Version 1.0

```
      program mk_scale_k
c for 12x30x42 mesh (5.23x15x20 m)
c
      implicit double precision(a-h,o-z)
      character name*5,head*80
      dimension xfield(100,100,100,20),class(100)
c read mod.in
      nz=42
      ny=30
      nx=12
      ndual=1

c read kfield
      open(unit=1,file='permd5_r3.dat',status='old')
      rewind(1)
      read(1,*)
      do k=1,nz
      do j=1,ny
      do i=1,nx
      read(1,*)xfield(i,j,k,1)
      enddo
      enddo
      enddo
      close(1)

      do k=1,nz
      do j=1,ny
      do i=1,nx
      xmeans=xmeans + xfield(i,j,k,1)
      enddo
      enddo
      enddo

      xmeans=xmeans/dble(12*30*42)

      do k=1,nz
      do j=1,ny
      do i=1,nx
      sss=sss+(xfield(i,j,k,1)-xmeans)*(xfield(i,j,k,1)-xmeans)
      enddo
      enddo
      enddo

      sss=sss/dble(12*30*42)
      sssd=sqrt(sss)

      open(unit=3,file='perm.new',status='unknown')
      rewind(3)
      write(3,*)'MEAN IN Log10 ',xmeans

      do k=1,nz
      do j=1,ny
      do i=1,nx
      scalek=(xfield(i,j,k,1)-xmeans)*0.860+xmeans
      write(3,*)scalek
```

```
enddo
enddo
enddo

close(1)
close(3)
stop
end
```

Source code for Software Routine mininipresf ir.f, Version 1.0

```
      program mininipresf_ir
c for 12x30x42 mesh (5.23x15x20 m, with rock fall)
c make incon block from
c MESH
c
      implicit double precision(a-h,o-z)
      character name*5,head*80
      dimension xfield(100,100,100,20),class(100)
c read mod.in
      nz=42
      ny=30
      nx=12
      ndual=1
      do i=1,nx
      do j=1,ny
         do k=1,nz
        do kk=1,ndual
          xfield(i,j,k,kk)=4.e-18
        enddo
       enddo
       enddo
      enddo

c read kfield
      open(unit=1,file='permcut.dat',status='old')
      rewind(1)
      read(1,*)
      do k=1,nz
      do j=1,ny
      do i=1,nx
      read(1,*)xfield(i,j,k,1)
      enddo
      enddo
      enddo
      close(1)
c check input field
      do k=1,100
      class(k)=0.0d0
      enddo
      write(*,*)'   number of classes'
      read(*,*)inums
      xmins=1.0e+30
      xmaxs=-1.0e+30
         do k=2,nz-1
         do j=1,ny
         do i=1,nx
         if(xfield(i,j,k,1).lt.xmins)xmins=xfield(i,j,k,1)
         if(xfield(i,j,k,1).gt.xmaxs)xmaxs=xfield(i,j,k,1)
         enddo
         enddo
         enddo
         write(*,*)'min= ',xmins
         write(*,*)'max= ',xmaxs
      xmeans=0.0d0
      sss=0.0d0
```

```
      dxs=(xmaxs-xmins)/dble(inums)
      iouts=0
      do kk=2,nz-1
      do j=1,ny
      do i=1,nx
         do k=1,inums
         x1=xmins+(k-1)*dxs
         x2=xmins+k*dxs
         if(xfield(i,j,kk,1).ge.x1.and.xfield(i,j,kk,1).le.x2)then
         class(k)=class(k)+1.0d0
         goto 12
         endif
         enddo
         enddo
      iouts=iouts+1
   12 enddo
      enddo

      do k=2,nz-1
      do j=1,ny
      do i=1,nx
      xmeans=xmeans + xfield(i,j,k,1)
      enddo
      enddo
      enddo

      xmeans=xmeans/dble(12*30*40)

      do k=2,nz-1
      do j=1,ny
      do i=1,nx
      sss=sss+(xfield(i,j,k,1)-xmeans)*(xfield(i,j,k,1)-xmeans)
      enddo
      enddo
      enddo

      sss=sss/dble(12*30*40)
      sssd=sqrt(sss)

      do i=1,inums
      class(i)=class(i)/dble(12*30*40)
      enddo
      open(unit=3,file='perm.tec',status='unknown')
      rewind(3)
      write(3,*)'MEAN IN Log10 ',xmeans
      write(3,*)'STANTARD DIVIATION IN Log10 and Ln ',sssd,2.3026*sssd
      write(3,*)'TITLE="FREQUENCY OF PERMEABILITY"'
      write(3,*)'VARIABLES = "LOG10 PERM", "FREQUENCY"'
      write(3,*)'ZONE, I = ',2*inums
         do k=1,inums
         write(3,'(2e15.6)')xmins+(k-1)*dxs,class(k)/dxs
         write(3,'(2e15.6)')xmins+k*dxs,class(k)/dxs
         enddo
         close(3)

c read and write incon
      open(unit=1,file='MESH',status='old')
```

```
      rewind(1)
      open(unit=2,file='inconsf.out',status='unknown')
      rewind(2)
c
      read(1,'(a)')dddd
      write(2,*)'INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY '
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a,14x,a,2e10.4,10x,3e12.6)')name
c      sat=sini

      if(k.eq.1)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,2,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
      goto 99
      endif

      if(k.eq.nz)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,nz-1,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,nz,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500
      endif
      goto 99
      endif

      yyy=(j-1)*0.5+0.25
      zzz=(k-2)*0.5+0.25

      if(kk.eq.1)then
      if((yyy.gt.3.0.and.yyy.lt.11.5).and.
     j   (zzz.gt.3.5.and.zzz.lt.12.0))then
      xkf=10.0*(10.0**((xfield(i,j,k,kk)+13.05)*0.860-13.05))
        alfa0=100.
      else
      xkf=(10.0**xfield(i,j,k,kk))
        alfa0=1000.
      end if
```

```
      porm=0.000124
      sat=0.011
      else
      xkf=xfield(i,j,k-1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif

   99 continue
c
      por=porm
      write(2,'(a5,2i5,e15.9,5e10.4)')name,idum,idum,porm,xkf,alfa0
      write(2,'(2e20.14)')sat
      enddo
      enddo
      enddo
      enddo
      texte='     '
      write(2,'(a)')texte
      write(2,*)
      close(1)
      close(2)
      stop
      end
```

Source code for Software Routine mddf CC8.f, Version 1.0

```
      program mddf_cc8
c cut round tunnel with radius R in 3D FD mesh and rock fall from the crown
c truncate elements and connections within R
c cut for refined mesh
c write connectivity list for tunnel bound elements to tunnel element
c file: 'drift3d.con'
c write list with coordinates of tunnel bound elements in
c file: 'drift3d.coor'
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 128)
      character*5 ,id(me)
      double precision x(3,me)
      double precision a(mc),rdrift,dx,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc
      integer ne1
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      write(*,*)'radius tunnel'
      read(*,*)rdrift
      call rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      stop
      end
c
      subroutine rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      character*5 id(me)
      character*5 irock
      character*1 text
      double precision x(3,me)
      double precision a(mc),rdrift,rr,v1,v2,v3,dy,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
```

```
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc,neall,nz
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      open(unit=1,file='MESH',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      open(unit=10,file='MESHsf.new',status='unknown')
      rewind(10)
      write(10,'(a)') wrd
      open(unit=3,file='driftff.con',status='unknown')
      rewind(3)
      open(unit=9,file='driftff.coor',status='unknown')
      rewind(9)
      open(unit=7,file='driftff.tec',status='unknown')
      rewind(7)
      write(3,*)'CONNE'
      write(9,*)'COOR'
      ne = 0
      neall=0
      nz=42
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),irock,vol,v1,x1,y1,z1

      neall=neall+1
      x(1,ne+1) = x1
      x(2,ne+1) = y1
      x(3,ne+1) = z1
      if(id(ne+1) .ne. '     ') then
         if(vol .eq. 0.) goto 10
c
      dy=dabs(y1-7.5)
c      dy=idint(dy/0.5)*0.5+0.25
      dz=dabs(z1- 7.75)
c      dz=idint(dz/0.5)*0.5+0.25
c
c check radius
         rr=sqrt(dy*dy+dz*dz)
         if(rr.lt.rdrift) goto 10

      if(x1.gt.2.2.and.x1.lt.3.0)then
      if(y1.gt.7.1.and.y1.lt.7.9)then
      if(z1.gt.10.20.and.z1.lt.11.30)then
```

```
               go to 10

            end if
            end if
            end if


               write(10,'(a,10x,a,2e10.4,10x,3e10.4)')
     &               id(ne + 1),irock,vol,v1,x1,y1,z1
               ne = ne + 1
               ind(ne) = ne
               if(x1 .ne. 0.0 .or. y1 .ne. 0.0 .or. z1 .ne. 0.0) locat = 0
               goto 10
            endif
            call hash(id,ind,hsh,ne,nh,ec)
            if(locat .ne. 0) then
               do i = 1, ne
                  x(2,i) = -999.d0
                  x(3,i) = -999.d0
               enddo
               open(unit=2,file='locat',status='old')
               read(2,'(a)',end=50) wrd
               if(wrd .ne. 'locat' .and. wrd .ne. 'LOCAT') then
                  stop 'no locat in locat'
               endif
 20            read(2,'(a5,5x,2f20.0)',end=50) wrd, y1, z1
               if(wrd .ne. '     ') then
                  nu1 = ihash(wrd, id,ind,hsh,ne,nh)
                  if(nu1 .eq. 0) then
                     goto 20
                  endif
                  x(2,nu1) = y1
                  x(3,nu1) = z1
                  goto 20
               endif
               write(10,*)
            endif
            if(ne .ge. me) then
               stop 'Exceeded maximum number of elements'
            endif
            ixyz=3
            ne1 = 0
            ne2 = ne
            do while(ne1 .lt. ne2)
               x1 = x(1,ne1+1)
               y1 = x(2,ne1+1)
               z1 = x(3,ne1+1)
               if(y1 .ne. -999.d0 .or. z1 .ne. -999.d0) then
                  if(ne1 .eq. 0) then
                    xhi = x1
                    xlo = x1
                    yhi = y1
                    ylo = y1
                    zhi = z1
                    zlo = z1
                else
```

```
            xhi = max(xhi,x1)
            xlo = min(xlo,x1)
            yhi = max(yhi,y1)
            ylo = min(ylo,y1)
            zhi = max(zhi,z1)
            zlo = min(zlo,z1)
        endif
          ne1 = ne1 + 1
       else if(x(2,ne2) .eq. -999.d0 .and. x(3,ne2) .eq. -999.d0) then
          ne2 = ne2 - 1
       else
          wrd = id(ne1+1)
          x(1,ne1+1) = x(1,ne2)
          x(2,ne1+1) = x(2,ne2)
          x(3,ne1+1) = x(3,ne2)
          id(ne1+1) = id(ne2)
          x(1,ne2) = x1
          x(2,ne2) = y1
          x(3,ne2) = z1
          id(ne2) = wrd
       endif
    enddo
    if(ixyz .eq. 0) then
       xhi = xhi - xlo
       yhi = yhi - ylo
       zhi = zhi - zlo
       if(zhi .le. min(xhi,yhi)) then
          ixyz = 3
       else if (yhi .le. min(xhi,zhi)) then
          ixyz = 2
       else
          ixyz = 1
       endif
    endif
    if(ixyz .eq. 2) then
       do i = 1, ne1
          x(2,i) = x(3,i)
       enddo
    elseif(ixyz .eq. 1) then
       do i = 1, ne1
          x(1,i) = x(2,i)
          x(2,i) = x(3,i)
       enddo
    endif
    call hash(id,ind,hsh,ne,nh,ec)
    read(1,'(a)',end=40) wrd
    if(wrd .ne. 'conne' .and. wrd .ne. 'CONNE') then
       stop 'no conne in MESH'
    endif
    write(10,*)
    write(10,'(a)')wrd
    nc = 0
    do i = 1, ne
       ec(i) = 0
    enddo
30  read(1,'(2a,19x,a,4e10.4)',end=40) wrd,wrd2,text,v1,v2,a(nc+1),v3
    if(wrd .ne. '     ' .and. wrd .ne. '+++  ') then
```

```
         nu1 = ihash(wrd, id,ind,hsh,ne,nh)
         nu2 = ihash(wrd2,id,ind,hsh,ne,nh)
         if(nu1 .eq. 0) then
c             write(6,60) wrd,nc+1
            if(nu2 .ne. 0)then
            wrd='DRI 1'
            text='3'
c  no gravity
          write(3,'(2a,19x,a,4e10.4)')
     &      wrd2,wrd,text,v2,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd2,x(1,nu2),x(2,nu2),
     &      x(3,nu2),v3
            endif
            goto 30
         else if(nu2 .eq. 0) then
c             write(6,60) wrd2,nc+1
            if(nu1 .ne. 0)then
            wrd2='DRI 1'
            text='3'
            write(3,'(2a,19x,a,4e10.4)')
     &      wrd,wrd2,text,v1,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd,x(1,nu1),x(2,nu1),
     &      x(3,nu1),v3
            endif
            goto 30
         endif
      write(10,'(2a,19x,a,4e10.4)') wrd,wrd2,text,v1,v2,a(nc+1),v3
      nc=nc+1
         e(1,nc) = nu1
         e(2,nc) = nu2
         if(nu1 .gt. ne1 .or. nu2 .gt. ne1) goto 30
         cc(1,nc) = ec(nu1)
         cc(2,nc) = ec(nu2)
         ec(nu1) = nc
         ec(nu2) = nc
         goto 30
      endif
      if(nc .ge. mc) then
         stop 'Exceeded maximum number of connections'
      endif
      close(unit=1)
      close(unit=10)
      close(unit=3)
      close(unit=9)
      ne = ne1
      return
 40   stop 'Premature EOF on MESH'
 50   stop 'Premature EOF on locat'
 60   format(' Unknown element "',a,'" at connection',i8)
      end
      subroutine hash(id,ind,hsh,ne,nh,h)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer h(ne)
      integer hsh(nh)
```

```
      character*5 w1
      integer i,i1,i2,j,k,n
      do j = 1, ne
         w1 = id(j)
         if(w1(4:4) .eq. '0') w1(4:4) = ' '
         n = 0
         do i = 1, 5
            n = n + i * ichar(w1(i:i))
         enddo
         h(j) = mod(n,nh) + 1
      enddo
      i1 = 1
      do i = 1, nh
         i2 = i1
         do j = i2, ne
            k = ind(j)
            if(h(k) .eq. i) then
               h(k) = 0
               ind(j) = ind(i1)
               ind(i1) = k
               i1 = i1 + 1
            endif
         enddo
         hsh(i) = i1
      enddo
      return
      end
      integer function ihash(wrd,id,ind,hsh,ne,nh)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer hsh(nh)
      character*5 wrd, w1, w2
      integer i,i1,i2,n
      w1 = wrd
      if(w1(4:4) .eq. '0') w1(4:4) = ' '
      n = 0
      do i = 1, 5
         n = n + i * ichar(w1(i:i))
      enddo
      n = mod(n,nh) + 1
      i1 = 1
      if(n .gt. 1) i1 = hsh(n - 1)
      i2 = hsh(n) - 1
      do i = i1, i2
         ihash = ind(i)
         w2 = id(ihash)
         if(w2(4:4) .eq. '0') w2(4:4) = ' '
         if(w1 .eq. w2) then
            if(ihash .gt. ne) ihash = 0
            return
         endif
      enddo
      ihash = 0
      return
      end
```

Source code for Software Routine mddf CS8.f, Version 1.0

```
      program mddf_cs8
c cut round tunnel with radius R in 3D FD mesh with rock fall around the spring
line
c truncate elements and connections within R
c cut for refined mesh
c write connectivity list for tunnel bound elements to tunnel element
c file: 'drift3d.con'
c write list with coordinates of tunnel bound elements in
c file: 'drift3d.coor'
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 128)
      character*5 ,id(me)
      double precision x(3,me)
      double precision a(mc),rdrift,dx,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc
      integer ne1
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      write(*,*)'radius tunnel'
      read(*,*)rdrift
      call rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      stop
      end
c
      subroutine rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      character*5 id(me)
      character*5 irock
      character*1 text
      double precision x(3,me)
      double precision a(mc),rdrift,rr,v1,v2,v3,dy,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
```

```
      integer hsh(nh)
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc,neall,nz
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      open(unit=1,file='MESH',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      open(unit=10,file='MESHsf.new',status='unknown')
      rewind(10)
      write(10,'(a)') wrd
      open(unit=3,file='driftff.con',status='unknown')
      rewind(3)
      open(unit=9,file='driftff.coor',status='unknown')
      rewind(9)
      open(unit=7,file='driftff.tec',status='unknown')
      rewind(7)
      write(3,*)'CONNE'
      write(9,*)'COOR'
      ne = 0
      neall=0
      nz=42
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),irock,vol,v1,x1,y1,z1

      neall=neall+1
      x(1,ne+1) = x1
      x(2,ne+1) = y1
      x(3,ne+1) = z1
      if(id(ne+1) .ne. '     ') then
         if(vol .eq. 0.) goto 10
c
      dy=dabs(y1-7.5)
c       dy=idint(dy/0.5)*0.5+0.25
      dz=dabs(z1- 7.75)
c       dz=idint(dz/0.5)*0.5+0.25
c
c check radius
         rr=sqrt(dy*dy+dz*dz)
         if(rr.lt.rdrift) goto 10

      if(x1.gt.2.2.and.x1.lt.3.0)then
      if(y1.gt.3.9.and.y1.lt.4.9)then
```

```
      if(z1.gt.7.5.and.z1.lt.8.5)then

         go to 10

      end if
      end if
      end if


         write(10,'(a,10x,a,2e10.4,10x,3e10.4)')
     &         id(ne + 1),irock,vol,v1,x1,y1,z1
         ne = ne + 1
         ind(ne) = ne
         if(x1 .ne. 0.0 .or. y1 .ne. 0.0 .or. z1 .ne. 0.0) locat = 0
         goto 10
      endif
      call hash(id,ind,hsh,ne,nh,ec)
      if(locat .ne. 0) then
         do i = 1, ne
            x(2,i) = -999.d0
            x(3,i) = -999.d0
         enddo
         open(unit=2,file='locat',status='old')
         read(2,'(a)',end=50) wrd
         if(wrd .ne. 'locat' .and. wrd .ne. 'LOCAT') then
            stop 'no locat in locat'
         endif
20       read(2,'(a5,5x,2f20.0)',end=50) wrd, y1, z1
         if(wrd .ne. '     ') then
            nu1 = ihash(wrd, id,ind,hsh,ne,nh)
            if(nu1 .eq. 0) then
               goto 20
            endif
            x(2,nu1) = y1
            x(3,nu1) = z1
            goto 20
         endif
         write(10,*)
      endif
      if(ne .ge. me) then
         stop 'Exceeded maximum number of elements'
      endif
      ixyz=3
      ne1 = 0
      ne2 = ne
      do while(ne1 .lt. ne2)
         x1 = x(1,ne1+1)
         y1 = x(2,ne1+1)
         z1 = x(3,ne1+1)
         if(y1 .ne. -999.d0 .or. z1 .ne. -999.d0) then
            if(ne1 .eq. 0) then
              xhi = x1
              xlo = x1
              yhi = y1
              ylo = y1
              zhi = z1
              zlo = z1
```

```
         else
            xhi = max(xhi,x1)
            xlo = min(xlo,x1)
            yhi = max(yhi,y1)
            ylo = min(ylo,y1)
            zhi = max(zhi,z1)
            zlo = min(zlo,z1)
         endif
           ne1 = ne1 + 1
        else if(x(2,ne2) .eq. -999.d0 .and. x(3,ne2) .eq. -999.d0) then
           ne2 = ne2 - 1
        else
           wrd = id(ne1+1)
           x(1,ne1+1) = x(1,ne2)
           x(2,ne1+1) = x(2,ne2)
           x(3,ne1+1) = x(3,ne2)
           id(ne1+1) = id(ne2)
           x(1,ne2) = x1
           x(2,ne2) = y1
           x(3,ne2) = z1
           id(ne2) = wrd
        endif
     enddo
     if(ixyz .eq. 0) then
        xhi = xhi - xlo
        yhi = yhi - ylo
        zhi = zhi - zlo
        if(zhi .le. min(xhi,yhi)) then
           ixyz = 3
        else if (yhi .le. min(xhi,zhi)) then
           ixyz = 2
        else
           ixyz = 1
        endif
     endif
     if(ixyz .eq. 2) then
        do i = 1, ne1
           x(2,i) = x(3,i)
        enddo
     elseif(ixyz .eq. 1) then
        do i = 1, ne1
           x(1,i) = x(2,i)
           x(2,i) = x(3,i)
        enddo
     endif
     call hash(id,ind,hsh,ne,nh,ec)
     read(1,'(a)',end=40) wrd
     if(wrd .ne. 'conne' .and. wrd .ne. 'CONNE') then
        stop 'no conne in MESH'
     endif
     write(10,*)
     write(10,'(a)')wrd
     nc = 0
     do i = 1, ne
        ec(i) = 0
     enddo
30   read(1,'(2a,19x,a,4e10.4)',end=40) wrd,wrd2,text,v1,v2,a(nc+1),v3
```

```
      if(wrd .ne. '     ' .and. wrd .ne. '+++  ') then
         nu1 = ihash(wrd, id,ind,hsh,ne,nh)
         nu2 = ihash(wrd2,id,ind,hsh,ne,nh)
         if(nu1 .eq. 0) then
c             write(6,60) wrd,nc+1
            if(nu2 .ne. 0)then
            wrd='DRI 1'
            text='3'
c  no gravity
           write(3,'(2a,19x,a,4e10.4)')
     &      wrd2,wrd,text,v2,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd2,x(1,nu2),x(2,nu2),
     &      x(3,nu2),v3
            endif
            goto 30
         else if(nu2 .eq. 0) then
c             write(6,60) wrd2,nc+1
            if(nu1 .ne. 0)then
            wrd2='DRI 1'
            text='3'
            write(3,'(2a,19x,a,4e10.4)')
     &      wrd,wrd2,text,v1,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd,x(1,nu1),x(2,nu1),
     &      x(3,nu1),v3
            endif
            goto 30
         endif
      write(10,'(2a,19x,a,4e10.4)') wrd,wrd2,text,v1,v2,a(nc+1),v3
      nc=nc+1
         e(1,nc) = nu1
         e(2,nc) = nu2
         if(nu1 .gt. ne1 .or. nu2 .gt. ne1) goto 30
         cc(1,nc) = ec(nu1)
         cc(2,nc) = ec(nu2)
         ec(nu1) = nc
         ec(nu2) = nc
         goto 30
      endif
      if(nc .ge. mc) then
         stop 'Exceeded maximum number of connections'
      endif
      close(unit=1)
      close(unit=10)
      close(unit=3)
      close(unit=9)
      ne = ne1
      return
 40   stop 'Premature EOF on MESH'
 50   stop 'Premature EOF on locat'
 60   format(' Unknown element "',a,'" at connection',i8)
      end
      subroutine hash(id,ind,hsh,ne,nh,h)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer h(ne)
```

```
      integer hsh(nh)
      character*5 w1
      integer i,i1,i2,j,k,n
      do j = 1, ne
         w1 = id(j)
         if(w1(4:4) .eq. '0') w1(4:4) = ' '
         n = 0
         do i = 1, 5
            n = n + i * ichar(w1(i:i))
         enddo
         h(j) = mod(n,nh) + 1
      enddo
      i1 = 1
      do i = 1, nh
         i2 = i1
         do j = i2, ne
            k = ind(j)
            if(h(k) .eq. i) then
               h(k) = 0
               ind(j) = ind(i1)
               ind(i1) = k
               i1 = i1 + 1
            endif
         enddo
         hsh(i) = i1
      enddo
      return
      end
      integer function ihash(wrd,id,ind,hsh,ne,nh)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer hsh(nh)
      character*5 wrd, w1, w2
      integer i,i1,i2,n
      w1 = wrd
      if(w1(4:4) .eq. '0') w1(4:4) = ' '
      n = 0
      do i = 1, 5
         n = n + i * ichar(w1(i:i))
      enddo
      n = mod(n,nh) + 1
      i1 = 1
      if(n .gt. 1) i1 = hsh(n - 1)
      i2 = hsh(n) - 1
      do i = i1, i2
         ihash = ind(i)
         w2 = id(ihash)
         if(w2(4:4) .eq. '0') w2(4:4) = ' '
         if(w1 .eq. w2) then
            if(ihash .gt. ne) ihash = 0
            return
         endif
      enddo
      ihash = 0
      return
```

```
end
```

Source code for Software Routine mddf cc.f, Version 1.0

```
      program mddf_cc
c cut round tunnel with radius R in 3D FD mesh with 3-m rock failure in the roof
c truncate elements and connections within R
c cut for refined mesh
c write connectivity list for tunnel bound elements to tunnel element
c file: 'drift3d.con'
c write list with coordinates of tunnel bound elements in
c file: 'drift3d.coor'
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 128)
      character*5 ,id(me)
      double precision x(3,me)
      double precision a(mc),rdrift,dx,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc
      integer ne1
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      write(*,*)'radius tunnel'
      read(*,*)rdrift
      call rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      stop
      end
c
      subroutine rmesh(rdrift,ne,id,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz)
      implicit none
      integer ne,ixyz
      integer me,mc,nh
      character*5 id(me)
      character*5 irock
      character*1 text
      double precision x(3,me)
      double precision a(mc),rdrift,rr,v1,v2,v3,dy,dz
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
```

```
      integer ind(me)
      double precision vol
      double precision x1, y1, z1
      double precision xhi, yhi, zhi
      double precision xlo, ylo, zlo
      character*5 wrd, wrd2
      integer i
      integer ihash
      integer locat
      integer nc,neall,nz
      integer ne1
      integer ne2
      integer nu1
      integer nu2
      open(unit=1,file='MESH',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      open(unit=10,file='MESHsf.new',status='unknown')
      rewind(10)
      write(10,'(a)') wrd
      open(unit=3,file='driftff.con',status='unknown')
      rewind(3)
      open(unit=9,file='driftff.coor',status='unknown')
      rewind(9)
      open(unit=7,file='driftff.tec',status='unknown')
      rewind(7)
      write(3,*)'CONNE'
      write(9,*)'COOR'
      ne = 0
      neall=0
      nz=42
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),irock,vol,v1,x1,y1,z1

      neall=neall+1
      x(1,ne+1) = x1
      x(2,ne+1) = y1
      x(3,ne+1) = z1
      if(id(ne+1) .ne. '     ') then
         if(vol .eq. 0.) goto 10
c
      dy=dabs(y1-7.5)
c      dy=idint(dy/0.5)*0.5+0.25
      dz=dabs(z1- 7.75)
c      dz=idint(dz/0.5)*0.5+0.25
c
c check radius
         rr=sqrt(dy*dy+dz*dz)
         if(rr.lt.rdrift) goto 10

      if(x1.gt.2.2.and.x1.lt.3.0)then

      if((y1.gt.7.0.and.y1.lt.7.5).and.(z1.gt.8.0.and.z1.lt.11.0))then
```

```
            go to 10
         elseif((y1.gt.6.5.and.y1.lt.7.0).and.(z1.gt.8.0.and.z1.lt.11.5))then
            go to 10
         elseif((y1.gt.6.0.and.y1.lt.6.5).and.(z1.gt.8.0.and.z1.lt.12.0))then
            go to 10
         elseif((y1.gt.5.5.and.y1.lt.6.0).and.(z1.gt.8.0.and.z1.lt.13.0))then
            go to 10
         end if

         end if


            write(10,'(a,10x,a,2e10.4,10x,3e10.4)')
     &          id(ne + 1),irock,vol,v1,x1,y1,z1
            ne = ne + 1
            ind(ne) = ne
            if(x1 .ne. 0.0 .or. y1 .ne. 0.0 .or. z1 .ne. 0.0) locat = 0
            goto 10
         endif
         call hash(id,ind,hsh,ne,nh,ec)
         if(locat .ne. 0) then
            do i = 1, ne
               x(2,i) = -999.d0
               x(3,i) = -999.d0
            enddo
            open(unit=2,file='locat',status='old')
            read(2,'(a)',end=50) wrd
            if(wrd .ne. 'locat' .and. wrd .ne. 'LOCAT') then
               stop 'no locat in locat'
            endif
 20         read(2,'(a5,5x,2f20.0)',end=50) wrd, y1, z1
            if(wrd .ne. '     ') then
               nu1 = ihash(wrd, id,ind,hsh,ne,nh)
               if(nu1 .eq. 0) then
                  goto 20
               endif
               x(2,nu1) = y1
               x(3,nu1) = z1
               goto 20
            endif
            write(10,*)
         endif
         if(ne .ge. me) then
            stop 'Exceeded maximum number of elements'
         endif
         ixyz=3
         ne1 = 0
         ne2 = ne
         do while(ne1 .lt. ne2)
            x1 = x(1,ne1+1)
            y1 = x(2,ne1+1)
            z1 = x(3,ne1+1)
            if(y1 .ne. -999.d0 .or. z1 .ne. -999.d0) then
               if(ne1 .eq. 0) then
                 xhi = x1
                 xlo = x1
                 yhi = y1
```

```
            ylo = y1
            zhi = z1
            zlo = z1
        else
            xhi = max(xhi,x1)
            xlo = min(xlo,x1)
            yhi = max(yhi,y1)
            ylo = min(ylo,y1)
            zhi = max(zhi,z1)
            zlo = min(zlo,z1)
        endif
          ne1 = ne1 + 1
       else if(x(2,ne2) .eq. -999.d0 .and. x(3,ne2) .eq. -999.d0) then
          ne2 = ne2 - 1
       else
          wrd = id(ne1+1)
          x(1,ne1+1) = x(1,ne2)
          x(2,ne1+1) = x(2,ne2)
          x(3,ne1+1) = x(3,ne2)
          id(ne1+1) = id(ne2)
          x(1,ne2) = x1
          x(2,ne2) = y1
          x(3,ne2) = z1
          id(ne2) = wrd
       endif
    enddo
    if(ixyz .eq. 0) then
       xhi = xhi - xlo
       yhi = yhi - ylo
       zhi = zhi - zlo
       if(zhi .le. min(xhi,yhi)) then
          ixyz = 3
       else if (yhi .le. min(xhi,zhi)) then
          ixyz = 2
       else
          ixyz = 1
       endif
    endif
    if(ixyz .eq. 2) then
       do i = 1, ne1
          x(2,i) = x(3,i)
       enddo
    elseif(ixyz .eq. 1) then
       do i = 1, ne1
          x(1,i) = x(2,i)
          x(2,i) = x(3,i)
       enddo
    endif
    call hash(id,ind,hsh,ne,nh,ec)
    read(1,'(a)',end=40) wrd
    if(wrd .ne. 'conne' .and. wrd .ne. 'CONNE') then
       stop 'no conne in MESH'
    endif
    write(10,*)
    write(10,'(a)')wrd
    nc = 0
    do i = 1, ne
```

```
         ec(i) = 0
      enddo
 30   read(1,'(2a,19x,a,4e10.4)',end=40) wrd,wrd2,text,v1,v2,a(nc+1),v3
      if(wrd .ne. '     ' .and. wrd .ne. '+++  ') then
         nu1 = ihash(wrd, id,ind,hsh,ne,nh)
         nu2 = ihash(wrd2,id,ind,hsh,ne,nh)
         if(nu1 .eq. 0) then
c              write(6,60) wrd,nc+1
            if(nu2 .ne. 0)then
            wrd='DRI 1'
            text='3'
c  no gravity
           write(3,'(2a,19x,a,4e10.4)')
     &      wrd2,wrd,text,v2,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd2,x(1,nu2),x(2,nu2),
     &      x(3,nu2),v3
            endif
            goto 30
         else if(nu2 .eq. 0) then
c              write(6,60) wrd2,nc+1
            if(nu1 .ne. 0)then
            wrd2='DRI 1'
            text='3'
            write(3,'(2a,19x,a,4e10.4)')
     &      wrd,wrd2,text,v1,1.0e-08,a(nc+1),0.0!v3
            write(9,'(a,5x,4e12.6)')wrd,x(1,nu1),x(2,nu1),
     &      x(3,nu1),v3
            endif
            goto 30
         endif
      write(10,'(2a,19x,a,4e10.4)') wrd,wrd2,text,v1,v2,a(nc+1),v3
      nc=nc+1
         e(1,nc) = nu1
         e(2,nc) = nu2
         if(nu1 .gt. ne1 .or. nu2 .gt. ne1) goto 30
         cc(1,nc) = ec(nu1)
         cc(2,nc) = ec(nu2)
         ec(nu1) = nc
         ec(nu2) = nc
         goto 30
      endif
      if(nc .ge. mc) then
         stop 'Exceeded maximum number of connections'
      endif
      close(unit=1)
      close(unit=10)
      close(unit=3)
      close(unit=9)
      ne = ne1
      return
 40   stop 'Premature EOF on MESH'
 50   stop 'Premature EOF on locat'
 60   format(' Unknown element "',a,'" at connection',i8)
      end
      subroutine hash(id,ind,hsh,ne,nh,h)
      implicit none
      integer ne, nh
```

```
      character*5 id(ne)
      integer ind(ne)
      integer h(ne)
      integer hsh(nh)
      character*5 w1
      integer i,i1,i2,j,k,n
      do j = 1, ne
         w1 = id(j)
         if(w1(4:4) .eq. '0') w1(4:4) = ' '
         n = 0
         do i = 1, 5
            n = n + i * ichar(w1(i:i))
         enddo
         h(j) = mod(n,nh) + 1
      enddo
      i1 = 1
      do i = 1, nh
         i2 = i1
         do j = i2, ne
            k = ind(j)
            if(h(k) .eq. i) then
               h(k) = 0
               ind(j) = ind(i1)
               ind(i1) = k
               i1 = i1 + 1
            endif
         enddo
         hsh(i) = i1
      enddo
      return
      end
      integer function ihash(wrd,id,ind,hsh,ne,nh)
      implicit none
      integer ne, nh
      character*5 id(ne)
      integer ind(ne)
      integer hsh(nh)
      character*5 wrd, w1, w2
      integer i,i1,i2,n
      w1 = wrd
      if(w1(4:4) .eq. '0') w1(4:4) = ' '
      n = 0
      do i = 1, 5
         n = n + i * ichar(w1(i:i))
      enddo
      n = mod(n,nh) + 1
      i1 = 1
      if(n .gt. 1) i1 = hsh(n - 1)
      i2 = hsh(n) - 1
      do i = i1, i2
         ihash = ind(i)
         w2 = id(ihash)
         if(w2(4:4) .eq. '0') w2(4:4) = ' '
         if(w1 .eq. w2) then
            if(ihash .gt. ne) ihash = 0
            return
         endif
```

```
      enddo
      ihash = 0
      return
      end
```

Source code for Software Routine minrefine3df.f, Version 1.0

```
      program minrefine3df
c make incon block from inconsf.out
c and MESH (refined new mesh)
c
c
      implicit double precision(a-h,o-z)
      character*5 name,wrd
      character head*60
      character*1 text
      character*5 irock
      dimension x(160000),y(160000),z(160000)
      dimension por(70,45,55,5),xperm(70,45,55,5),
     j     xalfa(70,45,55,5)
      dimension xsat(70,45,55,5)
      character*5 id(160000)
      character*5 iinc(70,45,55,5)
c
c read refined mesh

      ndual=1

      open(unit=1,file='MESHsf.new',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      ne = 0
   10 read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),irock,vol,v1,x1,y1,z1
      if(id(ne+1) .eq. '     ') goto 100
      ne = ne + 1
      x(ne) = x1
      y(ne) = y1
      z(ne) = z1
      goto 10
  100 close(1)
c
c read incon    (not refined)
      nx=12
      ny=30
      nz=42
c
      open(unit=1,file='inconsf.out',status='old')
      rewind(1)
      read(1,'(a60)')head
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a5,2i5,e15.9,2e10.4)')
     &iinc(i,j,k,kk),idum,idum,por(i,j,k,kk),xperm(i,j,k,kk),
     j   xalfa(i,j,k,kk)
      read(1,'(e20.14)')xsat(i,j,k,kk)
      enddo
```

```
      enddo
      enddo
      enddo

c
      open(unit=2,file='INCONsf',status='unknown')
      rewind(2)
      write(2,'(a60)')head
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      do nn=1,ne
      if(id(nn).eq.iinc(i,j,k,kk))then
          write(2,'(a5,2i5,e15.9,2e10.4)')
     &     id(nn),idum,idum,por(i,j,k,kk),10.0*xperm(i,j,k,kk),
     &     xalfa(i,j,k,kk)
          write(2,'(e20.14)')xsat(i,j,k,kk)
        endif
      enddo
      enddo
      enddo
      enddo
      enddo


c
      write(2,*)
      close(1)
      close(2)
      stop
 40   stop 'Premature EOF on MESH'
      end
```

mddf_cc.f 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:
   mddf_cc.f 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 based on the routine mddf.f v1.0 and is used to cut out a 3 x 2 meter rock-fall around the crown of the drift in a ITOUGH2 V3.2_drift MESH file. The new MESH file as saved with a new filename.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 118-123 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     First, the MESH will be cut with a cylinder with radius R through the center of the original 3D MESH. Second, the code will then remove a 3 x 2 x 1meter set of elements representing a "rock-fall" at the crown of the drift. Third, the elements that are within the removed area will be renamed to indicate their position. The connections will then be defined for those elements on the drift/rock-fall wall. The connection information for the drift and rock-fall neighboring elements will be used to form a new MESH file named MESHSF_cc. The test will be checked by successfully running the code without error messages and by visually checking the MESH file as well as a 3D rendering of the output MESH to verify that the changes in formatting are correct. The visual check will consist of verifying that the elements at the XYZ coordinates specified in the input are in fact removed correctly from the output. The 3D visual-check method is also used because the output data is very large and it is most effective to visually check the results in 3D rather than check the output data line by line.

   - Specify the range of input values to be used and why the range is valid
     The input is the original MESH file, a radius value of 2.75 and the rock cut dimensions given on pp. 153-154, S/N YMP-LBNL-CFT-GL-1. This test case input range is deemed valid because the input data set is the data set used to model the drift scale problem.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input)
     The output from the test is the file MESHSF. A graphic display of this MESH is printed on p. 154 , S/N YMP-LBNL-CFT-GL-1 and file MESHSF_cc is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cc/. Any ITOUGH2 V.3.2_drift MESH file of comparable size to this model could possibly be used. Any radius or rock-cut size used for a problem would have to be small enough so that the cylinder or drift would not intersect the outer boundary of the MESH.

- Description of how the testing shows that the results are correct for the specified input.
  Visual inspection of both the input and output data files provided on the accompanying CD, as well as a 3D visualization of the final output (MESHSF_cc) shows that the routine successfully removes the elements represented by the drift/rock fall and that all connections and elements are redefined properly. In addition, the test was successful because the routine successfully ran without error messages and the new MESHSF_cc was successfully imported into ITOUGH2 V3.2_drift without errors. Therefore, the test case and routine are acceptable.

- List limitations or assumptions to this test case and code in general
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift. This routine assumes that the drift is perfectly cylindrical and straight and that the rock fall occurs as a square 3 x 2 x 1 meter block at the crown of the drift.

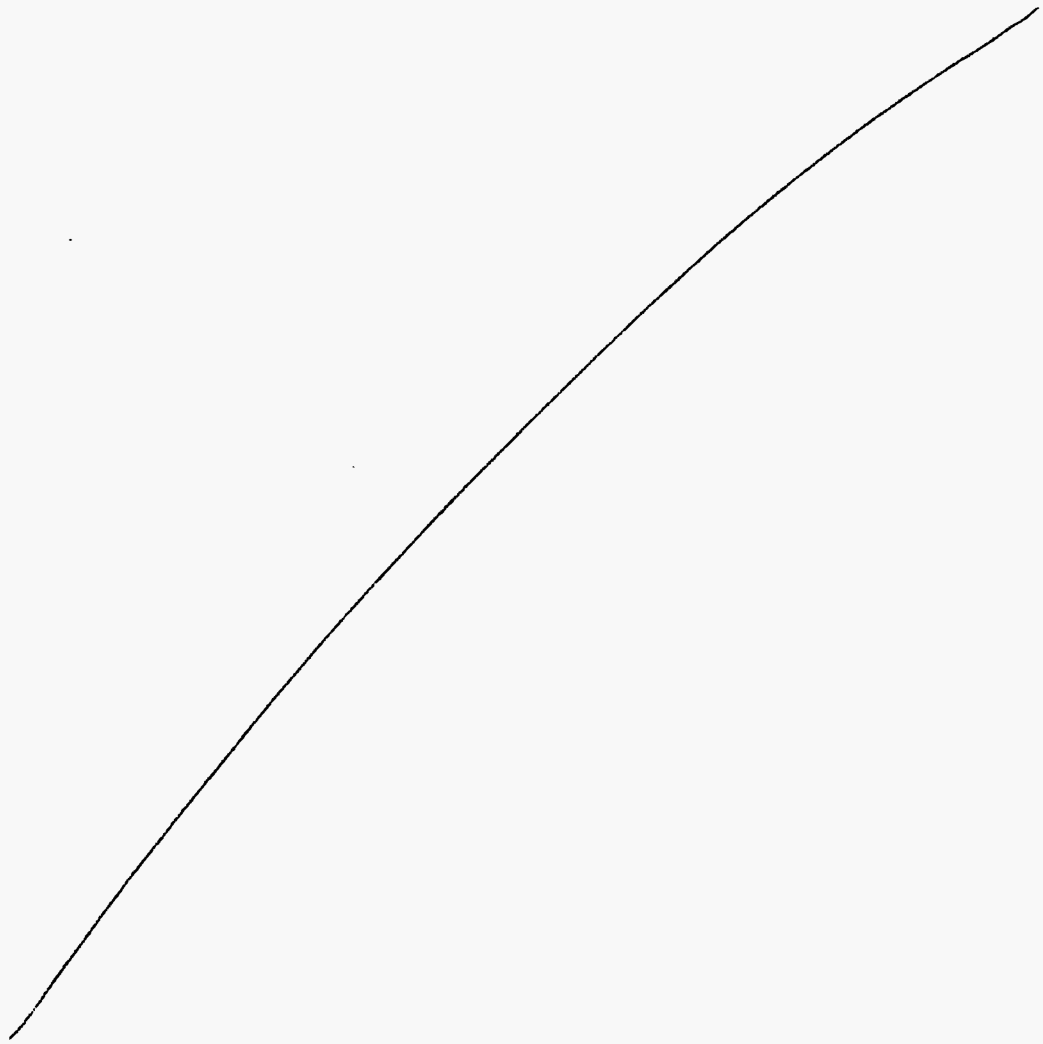
- Electronic files identified by name and location (include disc if necessary)
  The routine, test files and its description can be found on pp. 153-154, from S/N YMP-LBNL-CFT-GL-1 and pp. 118-123 from S/N YMP-LBNL-CFT-GL-1A Reference Binder. The routine (mddf_cc.fV1.0), input file (MESH) and output file (MESHSF_cc) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cc/

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 153-154 for S/N YMP-LBNL-CFT-GL-1; and pp. 118-123 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

p153



(Version 1.0) G.L. 2/18/00

△ Extended Rock failure at the ceiling

Code, mddf_cc.f, modified from mddf.f (See page 33-36, 131, 146), is used to cut 3 m depth and 2 m from the drift crown in mesh file.

JEH 1/16/01

SIGNATURE [signature] DATE 2-18 19 2000

READ AND UNDERSTOOD ____ DATE ____ 19 ____

PROJECT NAME (Version 1.0) G.L. 2/18/00 NOTEBOOK NO.

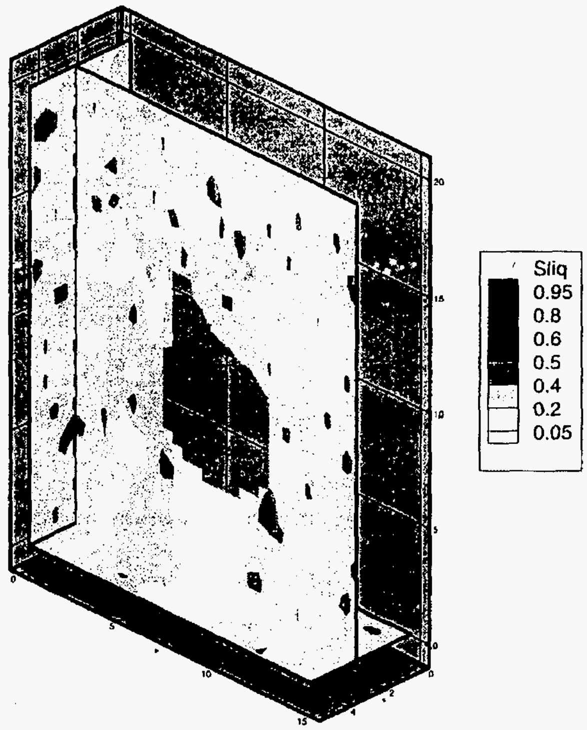
mddf_cc.f (under guomin/0999/prog_ir/)

```
c check radius
      rr=sqrt(dy*dy+dz*dz)
      if(rr.lt.rdrift) goto 10

   if(x1.gt.2.2.and.x1.lt.3.0)then

   if((y1.gt.7.0.and.y1.lt.7.5).and.(z1.gt.8.0.and.z1.lt.11.0))then
      go to 10
   elseif((y1.gt.6.5.and.y1.lt.7.0).and.(z1.gt.8.0.and.z1.lt.11.5))then
      go to 10
   elseif((y1.gt.6.0.and.y1.lt.6.5).and.(z1.gt.8.0.and.z1.lt.12.0))then
      go to 10
   elseif((y1.gt.5.5.and.y1.lt.6.0).and.(z1.gt.8.0.and.z1.lt.13.0))then
      go to 10
   end if

   end if

c        if(neall/nz*nz.eq.neall)then
c        text='2'
```

Cut out a drift

Cut out 0.5-3 m depth and 2 m width from the drift crown.

Following figure shows the cutted rock-fall and drift.



This figure can be produced from the data file named 500_ath_cc.plt under PC's directory:

c:/0999 fig/

Seepage rate:	Case
4.47	Case B
4.52	1 m³ rock-fall from crown
4.47	1 m³ : : spring line
5.82	3 (depth) ~ 2 (width) m : : ceiling G.L. 10/28/99

All input and output files saved under.
guomin/0999/drift_geo/ drift_cc, drift_cc8 and drift_cs8.

SIGNATURE [signature] DATE 10-28 19 99
READ AND UNDERSTOOD DATE 19

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li (mc 12/10/99)
4. Document Title: Scientific Notebook: page 154 for Macro/Routine mddf_cc.f V1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria: Technical (Taken from Attachment 5)

11. ☒ Specific Review Criteria:
- ☐ Source:
- ☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
- ☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL / Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-30-99
Signature Date

19. Mandatory Comments: ☐ Yes ☒ No

CONCURRENCE:

21. Document Draft No: N/A Date: 1-18-01

22. Reviewer: [signature] 12/9/99
Signature Date

23. PM: [signature] ~~12/10/99~~ 1/19/01 GSB
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. [signature] 01/18/01
Print Name/Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (page 154) YMP-LBNL-CFT-GL-1

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
GL. 12-9-11 YMP-LBNL-CFT-GL-1	pages 154

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 154			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually the code and no error is found checked visually the test results and found that they are acceptable.		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin Li
4. Document Title: Documentation for Routine mddf_cc.f 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: N/A (Taken from Attachment 5)
11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:
15. Due Date: 25 FEB 2000
16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:
17. Randall F. Hedegaard
Print Name
18. [signature] 2-28-00
Signature Date
19. Mandatory Comments: ☐ Yes ☑ No

CONCURRENCE:
21. Document Draft No: NA Date:
22. Reviewer: [signature] 2-28-00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

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

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine Documentation for mddf_cc.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mddf_cc.f 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-CFT-GL-1 Scientific Notebook	pp. 153-154
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 118-123
Routine Documentation Sheet	pp. 1&2

mddf_cc8.f 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:
   mddf_cc8.f 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 based on the routine mddf.f v1.0 and is used to cut out a 1 cubic meter rock-fall around the crown of the drift in a ITOUGH2 V3.2_drift MESH file. The new MESH file as saved with a new filename.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 106-111 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     First, the MESH will be cut with a cylinder with radius R through the center of the original 3D MESH. Second, the code will then remove a 1 x 1 x 1meter set of elements representing a "rock-fall" at the crown of the drift. Third, the elements that are within the removed area will be renamed to indicate their position. The connections will then be defined for those elements on the drift/rock-fall wall. The connection information for the drift and rock-fall neighboring elements will be used to form a new MESH file named MESHSF_cc8. The test will be checked by successfully running the code without error messages and by visually checking the MESH file as well as a 3D rendering of the output MESH to verify that the changes in formatting are correct. The visual check will consist of verifying that the elements at the XYZ coordinates specified in the input are in fact removed correctly from the output. The 3D visual-check method is also used because the output data is very large and it is most effective to visually check the results in 3D rather than check the output data line by line.

   - Specify the range of input values to be used and why the range is valid
     The input is the original MESH file, a radius value of 2.75 and the rock cut dimensions given on pp. 153, S/N YMP-LBNL-CFT-GL-1. This test case input range is deemed valid because the input data set is the data set used to model the drift scale problem.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input)
     The output from the test is the file MESHSF_cc8. A graphic display of this MESH is printed on p. 125 , S/N YMP-LBNL-CFT-GL-1 and file MESHSF_cc8 is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cc8/. Any ITOUGH2 V.3.2_drift MESH file of comparable size to this model could possibly be used. Any radius or rock-cut size used for a problem would have to be small enough so that the cylinder or drift would not intersect the outer boundary of the MESH.

- Description of how the testing shows that the results are correct for the specified input.
  Visual inspection of both the input and output data files provided on the accompanying CD, as well as a 3D visualization of the final output (MESHSF_cc) shows that the routine successfully removes the elements represented by the drift/rock fall and that all connections and elements are redefined properly. In addition, the test was successful because the routine successfully ran without error messages and the new MESHSF_cc was successfully imported into ITOUGH2 V3.2_drift without errors. Therefore, the test case and routine are acceptable.

- List limitations or assumptions to this test case and code in general
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift. This routine assumes that the drift is perfectly cylindrical and straight and that the rock fall occurs as a square 1 x 1 x 1 meter block at the crown of the drift.

- Electronic files identified by name and location (include disc if necessary)
  The routine, test files and its description can be found on pp. 153 and 125, from S/N YMP-LBNL-CFT-GL-1 and pp. 106-111 from S/N YMP-LBNL-CFT-GL-1A Reference Binder. The routine (mddf_cc8.fV1.0), input file (MESH) and output file (MESHSF_cc8 are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cc8/

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 153 and 125 for S/N YMP-LBNL-CFT-GL-1; and pp. 106-111 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

10-28-99

Effects of Rock Fall

(Version 1.0) G.L. 2/18/00

6 1 cubic meter [rock]-fall from crown:

Code, mddf_cc8.f, modified from mddf.f (See page 33-36, 131, 146) to cut out 1 m^3 (2×2×2 grids) from the crown in mesh file.

mddf_cc8.f (under gwomin/0999/ ~~drift_geo/drif~~ prog-ir/) g.l. 10/28/99

```
c check radius
        rr=sqrt(dy*dy+dz*dz)
        if(rr.lt.rdrift) goto 10

      if(x1.gt.2.2.and.x1.lt.3.0)then
      if(y1.gt.7.1.and.y1.lt.7.9)then
      if(z1.gt.10.20.and.z1.lt.11.30)then

        go to 10

      end if
      end if
      end if


c          if(neall/nz*nz.eq.neall)then
c          text='2'
```

– cut out a round tunnel

– cut out 2×2×2 grids around the crown.

The figure on page 125 shown this routine successfully cut out a drift and rock-fall from the crown.

8-8-99

Seepage rate affected by drift-collapse.

Model: as that described on page 22-38 of this notebook.

Percolation flux: 1000 mm/yr.
Realization 1.

Figure 1 shows the saturation contours on vertical plates for 1 cubic meter rock-fall from the drift-crown.

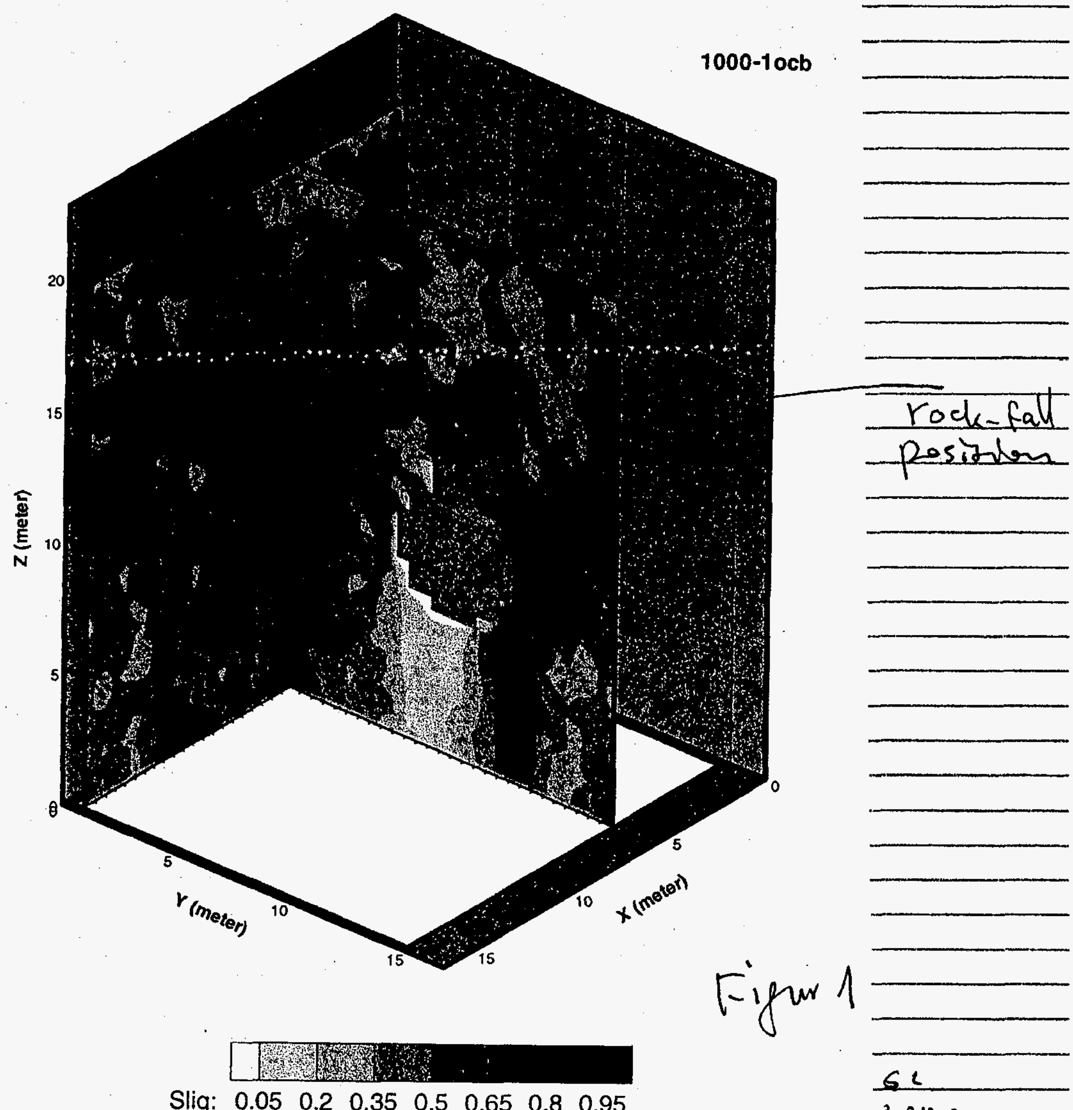


Figure 1

SIGNATURE ______ DATE ~~3-18~~ ~~19~~ ~~2000~~ 3-21-00
READ AND UNDERSTOOD ______ DATE ______ 19 ______

MDL-NBS-HS-000002 REV01 Attachment II-78 December 2000

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li GL 12/9/99 MC 12/10/99
4. Document Title: Scientific Notebook: page ~~445~~, 153, 33-36, 125 for Macro/Routine mddf-cc8.f V1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical (Taken from Attachment 5)
11. ☒ Specific Review Criteria:
☐ Source:
☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL / Hydrol.	Technical			

COMMENTS DUE:
15. Due Date: 11/29/99
16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:
17. Hui Hai Liu
Print Name
18. [signature] 11-30-99
Signature Date
19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:
21. Document Draft No: N/A Date:
22. Reviewer: [signature] 12/9/99
Signature Date
23. PM: [signature] 12/10/99
Signature Date

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

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (page ~~145~~ 33-36, 153, 125) YMP-LBNL-CFT-GL-1

Date of Document (or revision, draft revision number, as applicable): GL 12-9-99

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.

G.L. 12-9-99

Document(s) Title/Data	Relevant Sections/Pages
YMP-LBNL-~~CFT~~-GL-1	~~pages~~ ~~145~~, 153, 33-36, 125 G.L. 12-9-99

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 33-36, 153, 125			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually the code and no error is found. checked visually the test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin Li
4. Document Title: Documentation for Routine mddf_cc8.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:
15. Due Date: 25 FEB 2000
16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:
17. Randall F. Hedegaard
Print Name
18. [signature] 2-28-00
Signature Date
19. Mandatory Comments: ☐ Yes ☑ No

CONCURRENCE:
21. Document Draft No: NA Date:
22. Reviewer: [signature] 2-28-00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

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

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for mddf_cc8.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mddf_cc8.f 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-CFT-GL-1 Scientific Notebook	pp. 153 & 125
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 106-111
Routine Documentation Form	pp 1 & 2

mddf_cs8.f 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:
   mddf_cs8.f 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 based on the routine mddf.f v1.0 and is used to cut out a 1 cubic meter rock-fall around the spring-line of the drift in a ITOUGH2 V3.2_drift MESH file. The new MESH file as saved with a new filename.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 112-117 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     First, the MESH will be cut with a cylinder with radius R through the center of the original 3D MESH. Second, the code will then remove a 1 x 1 x 1meter set of elements representing a "rock-fall" at the spring line of the drift. Third, the elements that are within the removed area will be renamed to indicate their position. The connection information for the drift and rock-fall neighboring elements will be used to form a new MESH file named MESHSF_cs8. The test will be checked by successfully running the code without error messages and by visually checking the MESH file as well as a 3D rendering of the output MESH to verify that the changes in formatting are correct.. The visual check will consist of verifying that the elements at the XYZ coordinates specified in the input are in fact removed correctly from the output. The 3D visual-check method is also used because the output data is very large and it is most effective to visually check the results in 3D rather than check the output data line by line.

   - Specify the range of input values to be used and why the range is valid
     The input is the original MESH file, a radius value of 2.75 and the rock cut dimensions given on pp. 153, S/N YMP-LBNL-CFT-GL-1. This test case input range is deemed valid because the input data set is the data set used to model the drift scale problem.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input)
     The output from the test is the file MESHSF. A graphic display of this MESH is printed on p. 126 , S/N YMP-LBNL-CFT-GL-1 and file MESHSF_cs8 is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cs8/. Any ITOUGH2 V.3.2_drift MESH file of comparable size to this model could possibly be used. Any radius or rock-cut size used for a problem would have to be small enough so that the cylinder or drift would not intersect the outer boundary of the MESH.

- Description of how the testing shows that the results are correct for the specified input.
  Visual inspection of both the input and output data files provided on the accompanying CD, as well as a 3D visualization of the final output (MESHSF_cs8) shows that the routine successfully removes the elements represented by the drift/rock fall and that all connections and elements are redefined properly. In addition, the test was successful because the routine successfully ran without error messages and the new MESHSF_cs8 was successfully imported into ITOUGH2 V3.2_drift without errors. Therefore, the test case and routine are acceptable.

- List limitations or assumptions to this test case and code in general
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift. This routine assumes that the drift is perfectly cylindrical and straight and that the rock fall occurs as a square 1 x 1 x 1meter block at the spring line of the drift.

- Electronic files identified by name and location (include disc if necessary)
  The routine, test files and its description can be found on pp. 153 and 126, from S/N YMP-LBNL-CFT-GL-1 and pp. 112-117 from S/N YMP-LBNL-CFT-GL-1A Reference Binder. The routine (mddf_cs8.fV1.0), input file (MESH) and output file (MESHSF_cs8) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf_cs8/

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 153 and 126 for S/N YMP-LBNL-CFT-GL-1; and pp. 112-117 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

p153

Δ 1 cubic meter rock-fall from spring line:
code, mddf_cs8.f, modified from mddf.f (see page 33-36, 131, 146) to cut out 2x2x2 grids from spring line in mesh file: (version 1.0) G.C. 7/18/00)
mddf-cs8.f (under guomin/0999/prog_ir/)

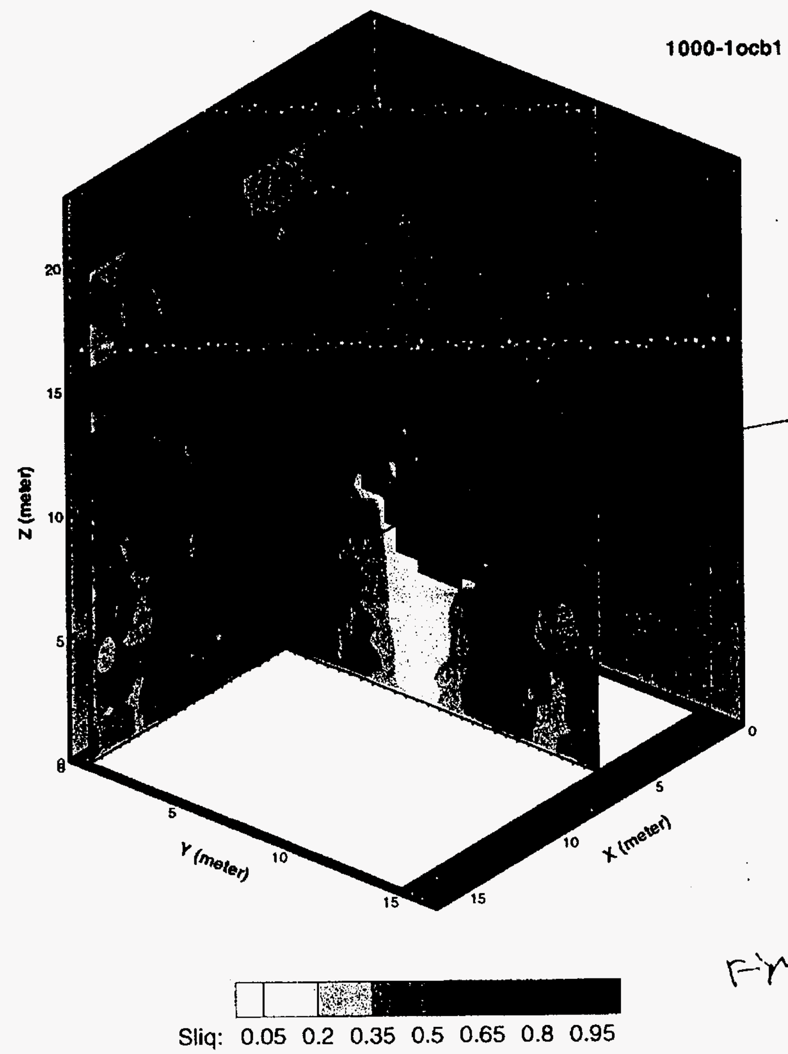
```
c check radius
        rr=sqrt(dy*dy+dz*dz)
        if(rr.lt.rdrift) goto 10

     if(x1.gt.2.2.and.x1.lt.3.0)then
     if(y1.gt.3.9.and.y1.lt.4.9)then
     if(z1.gt.7.5.and.z1.lt.8.5)then

        go to 10

     end if
     end if
     end if


c          if(neall/nz*nz.eq.neall)then
c          text='2'
```

— cut out a round tunnel

— cut out 2x2x2 grids from spring line

The figure on page 126 shown one of this kind results.
(Version 1.0) G.C. 7/18/00

Figure 2 shows the saturation contours on vertical plates for 1 m^3 rock-fall around spring line.



rock-fall position

Figure 2

The data files are saved under a directory on hydra:
guomin/0799/cb

Seepage rates compare with the old case (before rock fall).

Case	Old	1 m^3 rock-fall from crown	1 m^3 around spring line
Seepage rate	35.43%	35.75	36.04

SIGNATURE [signature] DATE 8-8 1999
READ AND UNDERSTOOD ______ DATE ______ 19__

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li
4. Document Title: Scientific Notebook: page 33-36, 153, 126 for Macro/Routine mddf-c58.f V1.0 (mc 12/10/99)
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical (Taken from Attachment 5)
11. ☒ Specific Review Criteria:
☐ Source:
☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL / Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-30-99
Signature Date

19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:
22. Reviewer: [signature] 12/9/99
Signature Date
23. PM: [signature] 12/10/99
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

MDL-NBS-HS-000002 REV01

Attachment II-88

December 2000

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (page 33-36, 153, 126) YMP-LBNL-CFT-GL-1

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-~~CFT~~ GL-1 (G.L. 12-9-99)	pages 33-36, 153, 126

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 33-36, 153, 126			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
	~~NM~~ hhl 11-30-99	~~no comment~~ hhl 11-30-99 Checked visually code and no error was found checked visually test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin LI
4. Document Title: Documentation for Routine mddf_cs8.f 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 N/A (Taken from Attachment 5)
11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name
18. [signature] 2-28-00
Signature Date
19. Mandatory Comments: ☐ Yes ☑ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No. NA Date:
22. Reviewer: [signature] 2-28-00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for mddf_cs8.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mddf_cs8.f 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-CFT-GL-1 Scientific Notebook	pp. 153 & 126
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 112-117
Routine Documentation Sheet	pp. 1-2

mddf.f 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 :
   mddf.f 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 takes an existing ITOUGH2 V3.2_drift MESH file and removes model elements within a defined radius and XYZ location (i.e. cuts out a cylindrical drift) to create an updated MESH file.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 92-97 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     First, the MESH will be cut with a cylinder with radius R through the center of the original 3D MESH. Second, the elements that are within the radius will be renamed to indicate their position. Third, the connections will be defined for those elements on the drift wall. This connection information for the drift neighboring elements will be used to form a new MESH file named MESHSF. The test will be checked by successfully running the code without error messages and by visually checking the MESH file as well as a 3D rendering of the output MESH to verify that the changes in formatting are correct. The visual check will consist of verifying that the elements at the XYZ coordinates specified in the input are in fact removed correctly from the output. The 3D visual-check method is also used because the output data is very large and it is most effective to visually check the results in 3D rather than check the output data line by line.

   - Specify the range of input values to be used and why the range is valid:
     The input is the original MESH file and a radius value of 2.75. This test case input range is deemed valid because the input data set is the data set used to model the drift scale problem.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The output from the test is the file MESHSF. A graphic display of this MESH is printed on p. 146 , S/N YMP-LBNL-CFT-GL-1 and file MESHSF is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf/. Any ITOUGH2 V.3.2_drift MESH file of comparable size to this model could possibly be used. Any radius used for a problem would have to be small enough so that the cylinder or drift would not intersect the outer boundary of the MESH.

   - Description of how the testing shows that the results are correct for the specified input:
     Visual inspection of both the input and output data files provided on the accompanying CD, as well as a 3D visualization of the final output (MESHSF) shows that the routine successfully removes the elements represented by the drift and that

all connections and elements are redefined properly. In addition, the test was successful because the routine successfully ran without error messages and the new MESHSF was successfully imported into ITOUGH2 V3.2_drift without errors. Therefore, the test case and routine are acceptable.

- List limitations or assumptions to this test case and code in general:
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift. This routine assumes that the drift is perfectly cylindrical and straight.

- Electronic files identified by name and location (include disc if necessary):
  The routine (mddf.fV1.0) and test files (MESH and MESHSF) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mddf/.

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

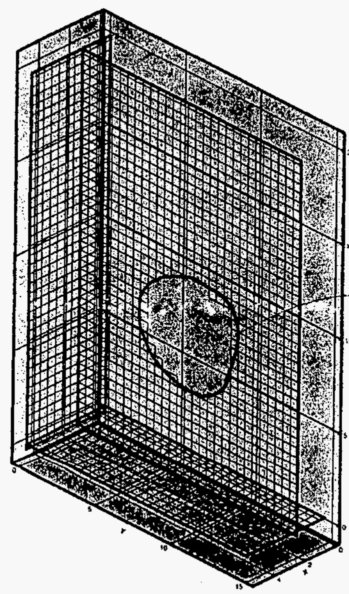
   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 146 for S/N YMP-LBNL-CFT-GL-1; and pp. 92-97 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

PROJECT NAME ______ NOTEBOOK NO. ______

(version 1.0) G.L. 2/18/00

Mddf.f (See the description on page 131):
the part of the macro was listed on page 33-36.
Whole code is listed on pp.71-76 S/N YMP-LBNL-CFT-GL-1A.
This macro was used to cut a round drift
with radius R (This report, R=2.75 meter) in
3D Mesh. Then a new mesh was generated without drift.

Following figures clearly show the macro successfully
cut out a round tunnel with radius 2.75 meter.



The figure can be
produced from the
data file named
500_a1h_2.plt
under a directory
on PC: (LBL/DOE
6335458) G.L. 12/9/99
C:\0999fig\

SIGNATURE ______ DATE ______ 19 ______
READ AND UNDERSTOOD ______ DATE ______ 19 ______

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li mc 12/10/99

4. Document Title: Scientific Notebook, page 33-36, 131, 146 for Macro/Routine mddf.f V1.0

5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A

8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical
(Taken from Attachment 5)

11. ☒ Specific Review Criteria:
☐ Source:
☒ Attached: YMP-LBNL Software Routine/Macro Documentation - Option 1
☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL/Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-29-99
Signature Date

19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Donald Mangold [signature] 11/29/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:

22. Reviewer: [signature] 12/9/99
Signature Date

23. PM: [signature] 12/10/99
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook: (pages 33-36, 131, 146) YMP-LBNL-CFT-GL-1

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-CFT-GL-1	33-36, 131, 146

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 33-36, 131, 146			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually the code and no error is found.		
		checked visually the test results and found that they are acceptable.		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin Li
4. Document Title: Documentation for Routine mddf.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature Date

19. Mandatory Comments: ☐ Yes ☑ No

CONCURRENCE:

21. Document Draft No: NA Date:
22. Reviewer: [signature] 2-28-00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for mddf.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mddf_.f 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-CFT-GL-1 Scientific Notebook	pp. 146
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 92-97
Routine Documentation Sheet	pp 1+2

meshbd.f 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:
   meshbd.f 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 routine and describe what it does:
     This routine reformats the ITOUGH2 V3.2_drift MESH file by doing 3 things. In the ELEM section of the MESH file it renames the boundary condition term for each element and changes the "Z" direction. In the CONN section of MESH file it changes the top boundary layer area value to a number in the routine. The new MESH file is saved to a new filename which is the output.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 86-87 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     During the test the routine will take one of 3 element type names (DRAIN, SOIL and BUNOF) and assign a term to the proper ITOUGH2 element based on the element's boundary condition. The test will also change the sign of the "Z" direction from positive to negative by adding a "-" sign. Lastly, the test will replace the "area" value for each element at the top boundary interface to "0.1E+03". The routine test will be checked by visually comparing a sampling of rows from the output with the input to verify that the changes in formatting are correct.

   - Specify the range of input values to be used and why the range is valid:
     The range of input values includes several lines of the ELEM section of the MESH file. These lines of text are printed on p. 129, S/N YMP-LBNL-CFT-GL-1. This test case input range is deemed valid because the routine's formatting changes can be successfully inspected using only a small sampling of lines from the very large input and output files.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The output from the test is printed on p. 129, S/N YMP-LBNL-CFT-GL-1. Since this routine only performs administrative formatting of the MESH file it is assumed that the routine is valid for use with any ITOUGH2 MESH file as input provided the Z values of the input file are positive.

   - Description of how the testing shows that the results are correct for the specified input:
     By visual inspection of the formatting of the input and output files, it can be seen that the routine successfully replaces the boundary condition term, changes the "Z" direction and modifies the top boundary layer area. Therefore, the test case and routine are acceptable.

   - List limitations or assumptions to this test case and code in general:

meshbd.f v.1.0

Routine/Macro Documentation Form

The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift.

- Electronic files identified by name and location (include disc if necessary):
  The routine is printed on pp. 86-87 from S/N YMP-LBNL-CFT-GL-1A Reference Binder and is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /meshbd/. The test input and output are printed on pp. 129, S/N YMP-LBNL-CFT-GL-1.

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 128-129 for S/N YMP-LBNL-CFT-GL-1; and pp. 86-87 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

PROJECT NAME (version 1.0) G.L. 2/18/00 NOTEBOOK NO.

Code, meshbd.f, is developed to replace the bottom and top boundary, change mesh order, of z direction from "-" to "+"; and interface at top boundary:

```
c
c change mesh order
c change z direction from "-" to "+"
c change interface at top boundary
c
      implicit double precision (a-h,o-z)
      integer nc,ne
      integer me,mc,nh
      parameter (me  = 88500)
      parameter (mc  =310000)
      parameter (nh  = 1000)
      double precision voll(mc),aa(mc)
      character*5 dddd,ccc,cccc
      character*5 texte
      character*1 text
      character*5 wrd,wrd2
      nx=12
      ny=30
      nz=42
c
      open(unit=2,file='MESH',status='unknown')
      rewind(2)
      texte='ELEME'
      write(2,'(a)')texte
c
      open(unit=1,file='meshm.mes',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEME') then
         stop 'no eleme in MESH'
      endif
c
      ne = 0
      nesum = 0
      locat = 1
      do i=1,nx
        do j=1,ny
         do k=1,nz
           ne=ne+1
           read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     dddd,texte,voll(ne),v1,x1,y1,z1
         nesum = nesum + 1
           if(k.eq.nz)then
             texte='BUNOF'
           elseif(k.eq.1)then
             texte='DRAIN'
           voll(ne)=1.0e+50
           else
             texte='SOILF'
           endif
           write(2,'(a,10x,a,2e10.4,10x,3e10.4)')
     &     dddd,texte,voll(ne),v1,x1,y1,-z1
```

JEH 11/16/01

SIGNATURE [signature] DATE 2-18 2000

READ AND UNDERSTOOD DATE 19

PROJECT NAME ____ NOTEBOOK NO. ____

```
            enddo
          enddo
        enddo
c
      read(1,*)
      read(1,'(a)')cccc
      write(2,*)
      cccc='CONNE'
      write(2,'(a)')cccc

      nc=0
      locat =1
30    read(1,'(2a,19x,a,4e10.4)',end=40)wrd,wrd2,text,v1,v2,aa(nc+1),v3
      if(wrd.ne. '     ' .and.wrd.ne.'+++  ')then
       if(wrd(1:2).eq.'B7'.and.wrd2(1:2).eq.'B7')aa(nc+1)=100.0
      write(2,'(2a,19x,a,4e10.4)')wrd,wrd2,text,v1,v2,aa(nc+1),v3
         nc=nc+1
         goto 30
      endif

c
      texte='     '
      write(2,'(a)')texte
      close(1)
      close(2)
      stop
   40 stop'Premature End of File'
      end
```

The code is tested by check the input and output files.

input data →

```
ELEME   NX=  12  NY=  30  NZ=  42
A11 1             10.1150E-070.5750E-01         0.5750E-010.2500E+00-.1000E-06
......
B71 1             10.1150E-060.5750E-01         0.5750E-010.2500E+00-.2000E+02
A12 1             10.1150E-070.5750E-01         0.5750E-010.7500E+00-.1000E-06
A22 1             10.2875E-010.0000E+00         0.5750E-010.7500E+00-.2500E+00
......

CONNE
A11 1A11 2                  10.5750E-010.2500E+000.1000E-06
......
B71 1B71 2                  10.5750E-010.2500E+000.1000E-05
......
```

G. L. 2-29-00

output data

```
ELEME
A11 1           DRAIN0.1000E+510.5750E-01       0.5750E-010.2500E+000.1000E-06
......
B71 1           BUNOF0.1150E-060.5750E-01       0.5750E-010.2500E+000.2000E+02
A12 1           DRAIN0.1000E+510.5750E-01       0.5750E-010.7500E+000.1000E-06
A22 1           SOILF0.2875E-010.0000E+00       0.5750E-010.7500E+000.2500E+00
......

CONNE
A11 1A11 2                  10.5750E-010.2500E+000.1000E-060.0000E+00
......

B71 1B71 2                  10.5750E-010.2500E+000.1000E+030.0000E+00
......
```

SIGNATURE [signature] DATE 8-15 19 99

READ AND UNDERSTOOD ____ DATE ____ 19 ____

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li 12/10/99
4. Document Title: Scientific Notebook page 128-129 for Routine/macro MeshBdf V1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical (Taken from Attachment 5)
11. ☒ Specific Review Criteria:
☐ Source:
☒ Attached: YMP-LBNL Software Routine/Macro Documentation - Option 1
☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H. H. Liu	LBNL/hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99
16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name
18. [signature] 11-30-99
Signature Date
19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:
22. Reviewer: [signature] 12/9/99
Signature Date
23. PM: [signature] 12/10/99
Signature Date

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

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook YMP-LBNL-CFT-GL-1

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-CFT-GL-1	128-129

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 128-129	2. Page 1 of 1

3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually code and error is not found. checked visually the test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin LI
4. Document Title: Documentation for Routine meshbd.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature Date

19. Mandatory Comments: ☐ Yes ☑ No

CONCURRENCE:

21. Document Draft No: NA Date:

22. Reviewer: [signature] 2-28-00
Signature Date

23. PM: [signature] 2/29/00
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for meshbd.f 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.		

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for meshbd.f 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-CFT-GL-1 Scientific Notebook	p. 129
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 86-87
Documentation sheet	pp. 1&2

mininipresf.f 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 :
   mininipresf.f 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 creates a portion of the ITOUGH2 V3.2_drift INCON file by taking input from the MESH file and a second file containing permeability values. The routine takes data from the two files and reformats it into the INCON file. The only calculation that takes place is converting the $\log_{10}$k values in the input permeability file to non-log numbers in the final INCON file.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 88-91 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     The routine will merge the permeability data into the INCON file in the appropriate column and the values will be converted from log to non-log to 4 units of precision. The routine will be checked by visually checking the certain lines of the output INCON file against the input MESH and permeability file to verify that the changes in formatting and log to non-log calculation is correct.

   - Specify the range of input values to be used and why the range is valid:
     Since the routine reformats text and performs one inverse log calculation, the routine will be verified using a sampling of the input and output files. This sampling is printed on p. 145, S/N YMP-LBNL-CFT-GL-1 under the headings of "part of input file". This test case input range is deemed valid because the routine's formatting 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 output from the test is printed on p. 145, S/N YMP-LBNL-CFT-GL-1 under the heading "part of output file". This output is a sampling of the INCON file. Since this routine only reformats text and does one inverse log calculation, it is assumed that the routine is valid for use with any range of values acceptable as a ITOUGH2 V3.2_drift MESH file and any set of $\log_{10}$k permeability values as input.

   - Description of how the testing shows that the results are correct for the specified input:
     By visual inspection of the formatting of the input and output files and a hand calculation of the log to inverse log calculation to 4 point precision (see p. 145), it can be seen that the routine successfully creates the portion of the INCON file as designed. Therefore, the test case and routine are acceptable.

   - List limitations or assumptions to this test case and code in general:

The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift. The log to non-log conversion was only carried out to 4 point precision.

- Electronic files identified by name and location (include disc if necessary):
  The input and output test data are printed on pp. 145, S/N YMP-LBNL-CFT-GL-1. The routine is printed on pp. 88-91 from S/N YMP-LBNL-CFT-GL-1A Reference Binder and is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mininipresf/. The test input and output are printed on pp. 145, S/N YMP-LBNL-CFT-GL-1.

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 145 for S/N YMP-LBNL-CFT-GL-1; and pp. 88-91 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

PROJECT NAME ______ NOTEBOOK NO. ______

9-22-99 (Version 1.0) G.L. 2/18/00

Description and Testing of Software Routine or Macro

Minipresf.f ~~(see page 13a)~~ G.M.L. 2-24/00

```
......
c read and write incon
      open(unit=1,file='MESH',status='old')
      rewind(1)
      open(unit=2,file='inconsf.out',status='unknown')
      rewind(2)
c
      read(1,'(a)')dddd
      write(2,*)'INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY '
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a,14x,a,2e10.4,10x,3e12.6)')name
c      sat=sini

      if(k.eq.1)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,2,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
      goto 99
      endif

      if(k.eq.nz)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,nz-1,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,nz,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500
      endif
      goto 99
      endif

      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,k,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,k-1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
 99   continue
c
      por=porm
      write(2,'(a5,2i5,e15.9,5e10.4)')name,idum,idum,porm,xkf,alfa0
      write(2,'(2e20.14)')sat
      enddo
      enddo
      enddo
      enddo
      texte='
      write(2,'(a)')texte
      write(2,*)
      close(1)
      close(2)
      stop
      end
```

See pp. 88-91 ~~15~~ in YMP-LBNL-CFT-GL-1A for whole code.

Part of input file MESH

```
ELEME
......
A21 1          SOILF0.2875E-010.0000E+00          0.5750E-010.2500E+000.2500E+00
......
B7U12          BUNOF0.1150E-060.5750E-01          0.5173E+010.1475E+020.2000E+02
......
```

part of input file permcut.dat

```
12x30x42 values
......
-0.14350E+02
......
```

→ $\log_{10} K$ $K = 0.4467 \cdot 10^{-14}$

part of output file inconsf.out

```
INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY
......
A21 1     0     00.124000000E-030.4467E-140.1000E+04
0.11000000000000E-01
......
```

The check also applies to minipresf_ir.f. G.L. 2/18/00

The macro is easily to be tested by visually checking the input and output files

SIGNATURE [signature] DATE ~~2-18~~ ~~19~~ ~~2000~~ G.L. 3/15/00

READ AND UNDERSTOOD ______ DATE ______ 19 ______

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li
4. Document Title: Scientific Notebook Page 130, 145 for Routine/Macro mininipresf.f V1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria: Technical (Taken from Attachment 5)

11. ☒ *Specific Review Criteria:*
- ☐ Source:
- ☒ Attached: YMP-LBNL Software Routine/Macro Documentation - Option 1
- ☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL/Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-29-99
Signature Date

19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:

22. Reviewer: [signature] 12/9/99
Signature Date

23. PM: [signature] 12/10/99
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook: YMP-LBNL-CFT-GL-1

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-CFT-GL-1	130, 145

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 130, 135

2. Page 1 of 1

3. Document No. YMP-LBNL-CFT-GL-1

4. Revision/ Change/Mod:

5. Draft

6. ☒ Q ☐ NQ

7. Reviewer: H. H. Liu

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked ~~code~~ visually and found no error checked visually the test results and found that they are acceptable.		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin LI
4. Document Title: Documentation for Routine mininipresf.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature Date

19. Mandatory Comments: ☐ Yes ☑ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No. NA Date:

22. Reviewer: [signature] 2-28-00
Signature Date

23. PM: [signature] 2/29/00
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: Routine Documentation for mininipresf.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mininipresf.f 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-CFT-GL-1 Scientific Notebook	pp. 145
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 88-91
Routine Documentation Sheet	pp. 1 & 2

mininipresf_ir.f 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 :
   ***mininipresf_ir.f* v1.0 (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 creates a portion of the ITOUGH2 V3.2_drift INCON by taking input from the MESH file and a file containing permeability values. The routine takes data from the property set and the MESH and reformats it into the INCON file. The code takes the original permeability set (A) and multiplies it by a factor to create a second (B) property set. The routine applies the A and B property sets such that property set B is applied to the elements nearest the drift and property set A is applied to the rest of the model elements. The routine also converts the property values (permeability) which are $\log_{10}$k values to non-log numbers in the final INCON file.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 102-105 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     First the test will enable the routine to merge the permeability data into the INCON file in the appropriate column based on the elements XYZ coordinate. Secondly, the code will create 2 sets of permeability values from the input permeability file. Next the B permeability property set will be applied to the elements nearest the drift and property set A is applied to the rest of the model elements. The values will be converted from log to non-log to 4 units of precision. The routine will be checked by visually comparing the output INCON file against the input MESH and two property sets files. The permeability data will also be visualized in 3D to inspect completeness and to verify that the changes in formatting and log to non-log calculation is correct.

   - Specify the range of input values to be used and why the range is valid:
     The 2 distinct permeability sets are applied to 2 distinct spatial areas of the model, so the entire input (MESH and the property file) will be used as the test input range so that correct spatial distribution of properties is accomplished. Since the routine also reformats text and performs one inverse log calculation, the routine will be verified using a sampling of the input and output files. This sampling is printed on p. 145, S/N YMP-LBNL-CFT-GL-1 under the headings of "part of input file". The input files (MESH and permcut.dat) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mininipresf/. This test case input range is deemed valid because the routine's formatting 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):

A portion of the output from the test is printed on p. 145, S/N YMP-LBNL-CFT-GL-1 under the heading "part of output file" and is provided in the INCON file (inconsf.out) on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mininipresf_ir/. The output on p. 145 is a sampling of the INCON file. Since this routine only reformats text and does one inverse log calculation, it is assumed that the routine is valid for use with any range of values acceptable as a ITOUGH2 MESH file and any set of $\log_{10}$k permeability values as input.

- Description of how the testing shows that the results are correct for the specified input:
  By visual inspection of the formatting (see p. 145) of the input and output files and a hand calculation of the log to inverse log calculation to 4 point precision (see p. 145, S/N YMP-LBNL-CFT-GL-1), it can be seen that the routine successfully creates the portion of the INCON file as designed. The 3D visualization of the final INCON file results on p. 152, S/N YMP-LBNL-CFT-GL-1 demonstrates that the 2 permeability data sets are properly assigned to the model elements by observing that the lower liquid saturation values (therefore higher permeability) of set B are nearest the drift. Therefore, the test case and routine are acceptable.

- List limitations or assumptions to this test case and code in general:
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift or greater. The log to non-log conversion was only carried out to 4 point precision.

- Electronic files identified by name and location (include disc if necessary):
  The routine (mininipresf_ir.fV1.0) and test files (MESH, permcut.dat) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mininipresf_ir/.

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 145 and 152 for S/N YMP-LBNL-CFT-GL-1 and pp. 102-105 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

 PROJECT NAME ______ NOTEBOOK NO. ______

9-22-99 (version 1.0) G.L. 2/18/00

Description and Testing of Software Routine ~~or~~ Macro

Minipresf.f ~~(see page 130)~~ G.M.L. 2-24/00

```
......
c read and write incon
      open(unit=1,file='MESH',status='old')
      rewind(1)
      open(unit=2,file='inconsf.out',status='unknown')
      rewind(2)
c
      read(1,'(a)')dddd
      write(2,*)'INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY '
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a,14x,a,2e10.4,10x,3e12.6)')name
c      sat=sini

      if(k.eq.1)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,2,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif
      goto 99
      endif

      if(k.eq.nz)then
c permeability of top element equal next element
      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,nz-1,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,nz,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500
      endif
      goto 99
      endif


      if(kk.eq.1)then
      xkf=(10.0**xfield(i,j,k,kk))
      porm=0.000124
      sat=0.011
      alfa0=1000.
      else
      xkf=xfield(i,j,k-1,kk)
      porm=0.089
      sat=0.92
      alfa0=1562500.
      endif

   99 continue
c
      por=porm
      write(2,'(a5,2i5,e15.9,5e10.4)')name,idum,idum,porm,xkf,alfa0
      write(2,'(2e20.14)')sat
      enddo
      enddo
      enddo
      enddo
      texte='    '
      write(2,'(a)')texte
      write(2,*)
      close(1)
      close(2)
      stop
      end
```

See pp. ~~15~~ 88-91 IN YMP-LBNL-CFT-GL-1A for whole code.

Part of input file MESH

```
ELEME
......
A21 1          SOILF0.2875E-010.0000E+00           0.5750E-010.2500E+000.2500E+00
......
B7U12          BUNOF0.1150E-060.5750E-01           0.5173E+010.1475E+020.2000E+02
......
```

part of input file permcut.dat

```
12x30x42 values
......
-0.14350E+02
......
```

-0.14350E+02 → $\log_{10} K$ $K = 0.4467 \cdot 10^{-14}$

part of output file inconsf.out

```
INCON -- INITIAL CONDITIONS FOR DUAL PERMBILITY
......
A21 1    0    00.124000000E-030.4467E-140.1000E+04
0.11000000000000E-01
......
```

The check also applies to minipresf_ir.f. G.L. 2/18/00

The macro is easily to be tested by visually checking the input and output files

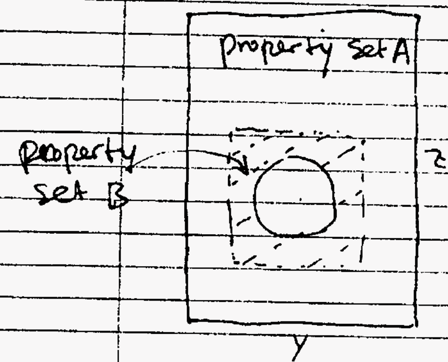
SIGNATURE [signature] DATE ~~2-18-19~~ G.L. 2/18/00

READ AND UNDERSTOOD ______ DATE ______ 19 ______

10-27-99

Effect of frature dilation

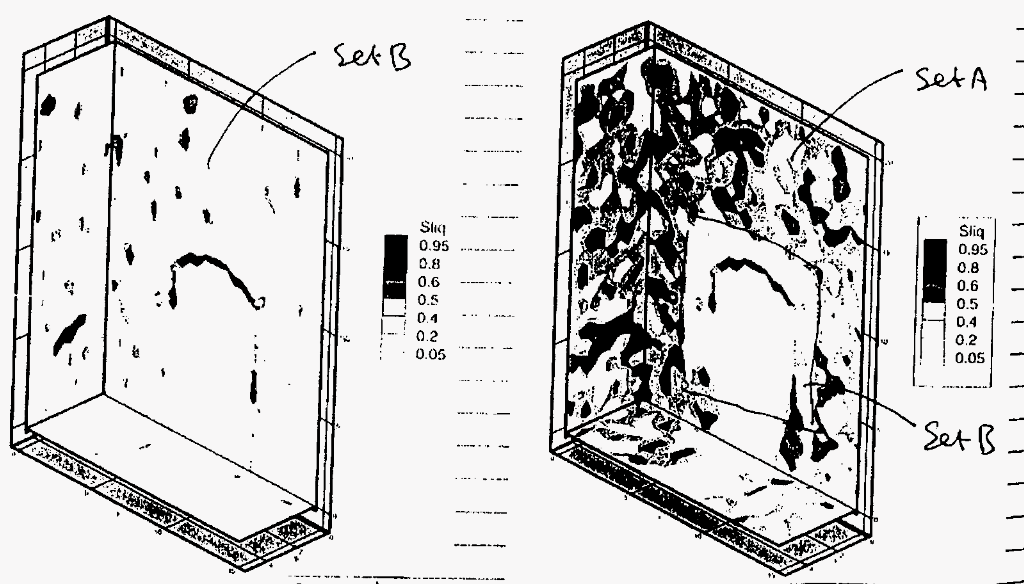
Model miniipresf_ir.f (under guomin/a999/prog-i




```
......
yyy=(j-1)*0.5+0.25
zzz=(k-2)*0.5+0.25

if(kk.eq.1)then
if((yyy.gt.3.0.and.yyy.lt.11.5).and.
)    (zzz.gt.3.5.and.zzz.lt.12.0))then
xkf=10.0*(10.0**((xfield(i,j,k,kk)+13.05)*0.860-13.05))
  alfa0=100.
else
xkf=(10.0**xfield(i,j,k,kk))
  alfa0=1000.
end if
porm=0.000124
sat=0.011
else
xkf=xfield(i,j,k-1,,kk)
porm=0.089
sat=0.92
alfa0=1562500.
endif
......
```

(vers. 1.0) G.C. 2/18/00

The code, minipresf_ir.f is modified from minipresf.f. This routine is used to reform property set B around drift (11.5 > y > 3.0, 12.0 > z > 3.5 meter) and property set A elsewhere. The figure on page 147 shows the saturation contours with property set A. The figure bellow on left shows the saturation contours with property set B. And the figure on right shows the saturation contours of the new model.



	Case A	Case B	New model
Seepage rate	9.53	4.47	9.53

All data files saved under guomin/a999/drift_geo/drift_kzone/

SIGNATURE [signature] DATE 10-27 19 99

READ AND UNDERSTOOD ______ DATE ______ 19 ______

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li — MC 12/10/99
4. Document Title: Scientific Notebook: page 145, 152 for Macro/routine miniprosf_ie.f v1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical (Taken from Attachment 5)
11. ☒ Specific Review Criteria:
☐ Source:
☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL/Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-29-99
Signature Date

19. Mandatory Comments: ☐ Yes ☐ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:

22. Reviewer: [signature] 12/9/99
Signature Date

23. PM: [signature] 12/10/99
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook: (page 145, 152) YMP-LBNL-CFT-GL-1

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 G.L. 12-9-99	Relevant Sections/Pages
YMP-LBNL-CFT-GL-1	pages 145, 152

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 145, 152	2. Page 1 of 1

3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually the code and no error is found. checked (visually) the test results and found that they are acceptable.		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin LI
4. Document Title: Documentation for Routine mininipresf_ir.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature Date

19. Mandatory Comments: ☐ Yes ☑ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date: 2-28-00
22. Reviewer: [signature] 2-28-00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: Routine Documentation for mininipresf_lr.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mininipresf_ir.f 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-CFT-GL-1 Scientific Notebook	pp. 145 & 152
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 102-105
Routine Documentation Sheet	pp 1 + 2

minrefine3d.f 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:
   minrefine3df.f 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:
     The routine will reform the ITOUGH2 V3.2_drift file INCONsf and remove the grid cells in the cut "drift" domain. Two input files will be needed: MESHsf.new generated from the routine mddf.f v1.0 inconsf.out generated from the routine mininipresf.f v1.0.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 124-125 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     The test or running of the routine will reform INCONsf and remove the grid cells in the cut "drift" domain. Two input files will be needed: MESHsf.new generated from the routine mddf.f v1.0 and inconsf.out generated from the routine mininipresf.f v1.0. This is done by simply identifying the elements removed in the MESH file and ensuring that the same elements are removed from the INCON information.The routine will be verified by visually checking raw data files as well as the 3D plot of the ITOUGH2 V3.2_drift output. If the macro has any problem, the simulation will produce an error result. The visual-check method is preferred because the output data is very large and it is most effective to visually check the results in 3D space rather than check the output data line by line. The visual check will consist of verifying that the elements at the XYZ coordinates specified in the input are in fact removed correctly from the output.

   - Specify the range of input values to be used and why the range is valid:
     The range of input values are the input files: MESHsf.new generated from the routine mddf.f v1.0 and inconsf.out generated from the routine mininipresf.f v1.0 which are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /minrefine3df/. No special range of input values is necessary to perform the macro. This macro is used to reform a new INCON file from two existing ITOUGH2 V3.2_drift files.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The resulting INCON data is written to the file INCONsf which is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /minrefine3df/. Since this routine simply reformats the INCON data, it is assumed that the routine is valid for use with any range of values acceptable as a ITOUGH2 V3.2_drift MESH file and any set of similar model characteristics.

- Description of how the testing shows that the results are correct for the specified input:
  The running of the routine and then importing the INCON file into ITOUGH2 successfully shows that the routine does not produce errors. Secondly, a line by line visual inspection of the output was conducted and it can be seen that the routine successfully produced the INCON properties for the for the cut out "drift". Thirdly, The 3D visualization of the model results on pp. 147, S/N YMP-LBNL-CFT-GL-1 indicates that the routine is successfully removed the "drift" properties. Therefore, the test is valid and the routine is acceptable.

- List limitations or assumptions to this test case and code in general:
  The routine was tested using an input data set that is comparable to that of 3D ITOUGH2 V3.2_drift models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift.

- Electronic files identified by name and location (include disc if necessary):
  The input files (MESHsf.new and inconsf.out) and output (INCONsf) are provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /minrefine3df/.

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.

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 146-147 f or S/N YMP-LBNL-CFT-GL-1; pp. 124-125 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

(Version 1.0) G.L. 2/18/00

- Minrefine3dff.f (See the description on page 131)

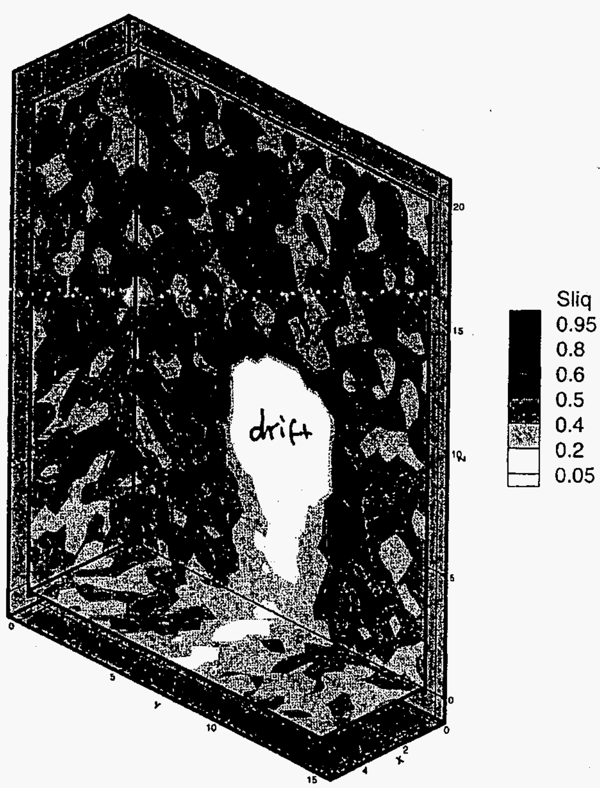
It is used to reform a new file of initial grid's properties from the old one "inconsf.out". The new file named INCONsf corresponds the grids listed in the new mesh file without the drift.

The new incon file and new mesh file should be used to perform the simulation by the software ITOUGH2 V3.2 drift. If the "minrefine3df.f" had any problem, the simulation should have produced an error result with the improper initial condition (Incon file). Otherwise, we could get a calculation results. The following figure can provide the identify of the macro.

SIGNATURE [signature] DATE 2-18 19-2000
READ AND UNDERSTOOD ____________ DATE ________ 19 ____

PROJECT NAME ______________________ **NOTEBOOK NO.** ________

```
c
      implicit double precision(a-h,o-z)
      character*5 name,wrd
      character head*60
      character*1 text
      character*5 irock
      dimension x(160000),y(160000),z(160000)
      dimension por(70,45,55,5),xperm(70,45,55,5),
     j      xalfa(70,45,55,5)
      dimension xsat(70,45,55,5)
      character*5 id(160000)
      character*5 iinc(70,45,55,5)
c
c read refined mesh

      ndual=1

      open(unit=1,file='MESHsf.new',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .no. 'ELEME') then
         stop 'no eleme in MESH'
      endif
      ne = 0
   10 read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &      id(ne + 1),irock,vol,vl,xl,yl,zl
      if(id(ne+1) .eq. '     ') goto 100
      ne = ne + 1
      x(ne) = xl
      y(ne) = yl
      z(ne) = zl
      goto 10
  100 close(1)
c
c read incon    (not refined)
      nx=12
      ny=30
      nz=42
c
      open(unit=1,file='inconsf.out',status='old')
      rewind(1)
      read(1,'(a60)')head
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      read(1,'(a5,2i5,e15.9,2e10.4)')
     &iinc(i,j,k,kk),idum,idum,por(i,j,k,kk),xperm(i,j,k,kk),
     j   xalfa(i,j,k,kk)
      read(1,'(e20.14)')xsat(i,j,k,kk)
      enddo
      enddo
      enddo
      enddo

c
      open(unit=2,file='INCONsf',status='unknown')
      rewind(2)
      write(2,'(a60)')head
      do i=1,nx
      do j=1,ny
      do k=1,nz
      do kk=1,ndual
      do nn=1,ne
      if(id(nn).eq.iinc(i,j,k,kk))then
          write(2,'(a5,2i5,e15.9,2e10.4)')
     &     id(nn),idum,idum,por(i,j,k,kk),-xperm(i,j,k,kk),
     &     xalfa(i,j,k,kk)
          write(2,'(e20.14)')xsat(i,j,k,kk)
        endif
      enddo
      enddo
      enddo
      enddo
      enddo


c
      write(2,*)
      close(1)
      close(2)
      stop
 40   stop 'Premature EOF on MESH'
      end
```



Saturation contours on vertical plates in 3D block.

This figure is produced from the data file named 500_a1k_0.plt under a directory on PC:

C:\0999fig\

SIGNATURE ____________ DATE ~~2-1-8 19~~ 6/2 3/25/00
READ AND UNDERSTOOD ____________ DATE ________ 19 ____

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li
4. Document Title: Scientific Notebook: page 131, 146-147 for Macro/Routine minrefine3dff v1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria Technical (Taken from Attachment 5)
11. ☒ Specific Review Criteria:
    ☐ Source:
    ☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
    ☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL/Hydrol.	Technical			

COMMENTS DUE:	REVIEW BY:	CONCURRENCE:
15. Due Date: 11/29/99	17. Hui Hai Liu (Print Name)	21. Document Draft No: N/A Date:
16. Originator/Review Coordinator: Donald Mangold (Print Name)	18. [signature] (Signature) 11-29-99 (Date)	22. Reviewer: [signature] (Signature) 12/9/99 (Date)
	19. Mandatory Comments: ☐ Yes ☒ No	23. PM: [signature] (Signature) 12/10/99 (Date)
	ORIGINATOR/REVIEW COORDINATOR (After response completed): 20. Donald Mangold [signature] (Print Name/Signature) 12/9/99 (Date)	DISPUTE RESOLUTION: (if applicable) 24. PM: (Signature) (Date)

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (page 131, 146-147) YMP-LBNL-CFT-GL-1

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.

GL. 12-9-11

Document(s) Title/Data	Relevant Sections/Pages
YMP-LBNL-CFT-GL-1	pages 131, 146-147

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 131, 146-147			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked visually the code and no error is found. checked visually the test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin Li
4. Document Title: Documentation for Routine minrefine3df.f 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 N/A (Taken from Attachment 5)
11. ☐ Specific Review Criteria:
    ☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
    ☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000
16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name
18. [signature] 2·28·00
Signature Date
19. Mandatory Comments: ☐ Yes ☑ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: NA Date:
22. Reviewer: [signature] 2·28·00
Signature Date
23. PM: [signature] 2/29/00
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: **Routine Documentation for minrefine3df.f 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.		

YMP-LBNL
APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for minrefine3df.f 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-CFT-GL-1 Scientific Notebook	pp. 146-147, 131
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 124-125
Reference Documentation Sheet	pp. 1&2

mk_gener.f 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 :
   mk_gener.f v1.0 (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:
     The routine produces percolation flux values for every node at the top boundary of the 3D model. This routine creates a portion of the ITOUGH2 V3.2_drift input (the GENER data) by taking input from the MESH file and a user defined percolation flux value.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 98-99 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     The test will run the routine and produce individual percolation flux values for nodes at the top boundary of the 3D model given a single average percolation flux. The code will take the top boundary area for the each element and multiply this area by the average percolation flux to come up with element specific percolation flux value. This routine will create a portion of the ITOUGH2 input (the GENER data) by taking input from the MESH file and the user defined percolation flux value. Since the routine's calculations can be successfully checked using sample data that do not cover the full range of possible top boundary areas, only a select number of elements will be tested.

   - Specify the range of input values to be used and why the range is valid:
     The input range is an overall percolation flux of 5 mm/yr and 3 sample elements from the original MESH (see left margin p. 148, S/N YMP-LBNL-CFT-GL-1). This test case input range is deemed valid because the routine's formatting 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 output from the test is printed on p. 148, S/N YMP-LBNL-CFT-GL-1 under the heading "TESTING". 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 (shown on p. 148, S/N YMP-LBNL-CFT-GL-1).

   - List limitations or assumptions to this test case and code in general:

The input percolation flux is valid from 0 to infinity. The routine was tested using an input data set that is comparable to that of 3D models necessary to model drift scale type problems. The routine is only valid for files compatible with ITOUGH2 V3.2_drift.

- Electronic files identified by name and location (include disc if necessary):
  The routine is printed on pp. 98-99 from S/N YMP-LBNL-CFT-GL-1A Reference Binder and is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mk_gener/. The test input and output are printed on pp. 145, S/N YMP-LBNL-CFT-GL-1.

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

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 148 for S/N YMP-LBNL-CFT-GL-1; and pp. 98-99 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

△ MK_gener.f (See the description on page 131)
(Version 1.0) G.L. 2/18/00

This macro is used to add the percolation flux at the top boundary grid.
It can be tested by checking the input and output files.

```
      implicit double precision (a-h,o-z)
      integer ne,ixyz
      integer me,mc,nh
      parameter (me  =160000)
      parameter (mc  =700000)
      parameter (nh  = 2500)
      character*5 id(me)
      character*5 tfeld(me)
      double precision x(3,me)
      double precision a(mc),voll(me)
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      call rmesh
     &(rdrift,ne,id,tfeld,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz,voll)
      stop
      end
c
      subroutine rmesh
     &(rdrift,ne,id,tfeld,x,ec,e,a,cc,hsh,ind,me,mc,nh,ixyz,voll)
      implicit double precision (a-h,o-z)
      character*5 id(me)
      character*5 texte
      character*5 tfeld(me)
      double precision x(3,me)
      double precision a(mc)
      integer ec(me)
      integer e(2,mc)
      integer cc(2,mc)
      integer hsh(nh)
      integer ind(me)
      double precision voll(me)
      character*5 wrd
c
      write(*,*)'Infiltration Rate in mm/a'
      read(*,*)rinf
c
      open(unit=2,file='GENERsf',status='unknown')
      rewind(2)
      texte='GENER'
      write(2,'(a)')texte
      iw1=0
      iw2=0
c
      open(unit=1,file='MESHSF',status='old')
      rewind(1)
      read(1,'(a)',end=40) wrd
      if(wrd .ne. 'eleme' .and. wrd .ne. 'ELEMS') then
         stop 'no eleme in MESH'
      endif
c
      ne = 0
      nesum = 0
      locat = 1
 10   read(1,'(a,10x,a,2e10.4,10x,3e10.4)',end=40)
     &     id(ne + 1),texte,voll(ne+1),v1,x1,y1,z1
      nesum = nesum + 1
      if(id(ne+1) .ne. '     ') then
c        if(vol .eq. 0.) goto 10
         if(texte.eq.'BUNOF')ne = ne + 1
       goto 10
      endif
c
      volsum=0.0
      do i=1,ne
      volsum=volsum+voll(i)
      enddo
c
      do i=1,ne
      fakt=voll(i)/volsum
      write(2,'(2a,i4,25x,a,e10.4)')
     &id(i),'I',i,'WATE ',fakt*rinf*78.45*3.171e-08
      enddo
c
      close(1)
      close(2)
      stop
   40 stop'Premature End of File'
      end
```

← part of input file MESHSF

```
ELEME
B77 2 ... BUNOF0.5000E-060.2500E+00 0.3650E+000.3250E+010.2000E+02
B78 2 ... BUNOF0.5000E-060.2500E+00 0.3650E+000.3750E+010.2000E+02
B79 2 ... BUNOF0.5000E-060.2500E+00 0.3650E+000.4250E+010.2000E+02
```

Testing:
input the percolation flux 5 mm/yr

For a grid with a surface area 0.5x0.5 m^2, the number of the percolation flux should be added.

5 mm/yr x 0.25 m^2

= 0.005 x .25 (m^3) / 365 x 24 x 3600 (s)
= 0.39645 (kg/s) x10^{-7} G.L. 2/18/00

The output file also shown the correct results. (The name is GENERsf) G.L. 6-29-00

```
GENER
......
B77 2I  37                    WATE 0.3964E-07
B78 2I  38                    WATE 0.3964E-07
B79 2I  39                    WATE 0.3964E-07
......
```

SIGNATURE [signature] DATE 9-22 1999
READ AND UNDERSTOOD ______ DATE ______ 19__

MDL-NBS-HS-000002 REV01

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li
4. Document Title: Scientific Notebook: page 31-32, 131, 148 for macro/Routine ml_gener.f v.10
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A
8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. [X] Standard Review Criteria Technical (Taken from Attachment 5)
11. [X] Specific Review Criteria:
[ ] Source:
[X] Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
[X] Scientific notebook/data associated with this review as noted on Attachment 3
12. Comment Documentation:
[X] Comment Sheets
[ ] Review Copy Mark-up
13. YMP-LBNL Project Manager (PM): Gudmundur S. Bodvarsson

14.

Reviewer	Org./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL / Hydrol.	Technical			

COMMENTS DUE:
15. Due Date: 11/29/99
16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:
17. Hui Hai Liu
Print Name
18. [signature] 11-29-99
Signature Date
19. Mandatory Comments: [ ] Yes [X] No

CONCURRENCE:
21. Document Draft No: N/A Date:
22. Reviewer: [signature] 12/9/99
Signature Date
23. PM: [signature] 12/10/99
Signature Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):
20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

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

Attachment II-145

December 2000

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (pages 31-32, 131, 148) YMP-LBNL-CFT-GL-1

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-CFT-GL-1	pages 31-32, 131, 148

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 31-32, 131, 148			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked ~~the~~ visually code and no error is found. Checked ~~the~~ visually test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin LI

4. Document Title: Documentation for Routine mk_gener.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature Date

19. Mandatory Comments: ☐ Yes ☑ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:

22. Reviewer: [signature] 2-28-00
Signature Date

23. PM: [signature] 2/25/00
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: Routine Documentation for mmk_gener.f 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.		

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mk_gener.f 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-CFT-GL-1 Scientific Notebook	pp. 148
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 98-99
Routine Documentation Form	pp 1&2

mk_scale_k.f 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:
   mk_scale_k.f 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 scale a heterogeneous field by changing the parameter A in the following formula: $K' = (K - \underline{K})A + \underline{K}$ where, K = old log permeability; $\underline{K}$ = old mean log permeability; K' = new log permeability; A = scaled factor. Special conditions for A: unchanged heterogeneous field when A = 1, K' = K; homogeneous field when A = 0, K' = K; higher heterogeneous field when A>1; or a lower heterogeneous field if A < 1.

   - Source code: (including equations or algorithms from software setup (LabView, Excel, etc.):
     pp. 100-101 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

   - Description of test(s) to be performed (be specific):
     The routine is checked by taking a set of permeability values as input, and then comparing the results with a hand calculation of standard deviation. These results will be checked by hand calculating the output and input data to verify that the standard deviation of log permeability has been correctly scaled.

   - Specify the range of input values to be used and why the range is valid:
     The range of input values are the permeability values in file (permd5_r1.dat) which is provided on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mk_scale_k/.

4. **Test Results.**

   - Output from test (explain difference between input range used and possible input):
     The output file from the test is saved as perm.new on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mk_scale_k/. Since this routine does one standard deviation calculation that is valid on real numbers, it is assumed that the routine is valid for use with any range of values acceptable as a ITOUGH2 V3.2_drift MESH file and any set of similar permeabilities.

   - Description of how the testing shows that the results are correct for the specified input:
     When the value of the input parameter A is 1.292, the standard deviation of the log permeability is 2.503 (see p. 149, S/N YMP-LBNL-CFT-GL-1, from the output file perm.new). By hand calculation of the standard deviation it is apparent that the code correctly scales the permeability values. Therefore, the test case is valid.

   - List limitations or assumptions to this test case and code in general:
     The limitation of the input value of the scale factor: A >= 0.0.

- Electronic files identified by name and location (include disc if necessary):
  The output file (perm.new) and input file (permd5_r1.dat) are saved on the accompanying CD entitled YMP-LBNL-CFT-GL-1 (routines) in directory /mk_scale_k/.

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.

   MAINTAIN NOTEBOOK PAGES IN THIS ORDER:
   pp. 149, 123 for S/N YMP-LBNL-CFT-GL-1; pp. 100-101 from S/N YMP-LBNL-CFT-GL-1A Reference Binder

PROJECT NAME ______ NOTEBOOK NO. ______

9-24-99

Δ Description and testing the software routine for scaling the heterogeneous field

See page 123 and 133–134. The following routine is used for scaling the heterogeneous field by the formula listed on page 123.

mk-scale-k.f (version 1.0) G.L. 2/18/00

G.L. 2/24/00

```
      implicit double precision(a-h,o-z)
      character name*5,head*80
      dimension xfield(100,100,100,20),class(100)
      nz=42
      ny=30
      nx=12
      ndual=1
c read kfield
      open(unit=1,file='permd5_r1.dat',status='old')
      rewind(1)
      read(1,*)
      do k=1,nz
      do j=1,ny
      do i=1,nx
      read(1,*)xfield(i,j,k,1)
      enddo
      enddo
      enddo
      close(1)

      do k=1,nz
      do j=1,ny
      do i=1,nx
      xmeans=xmeans + xfield(i,j,k,1)
      enddo
      enddo
      enddo
      xmeans=xmeans/dble(12*30*42)
      do k=1,nz
      do j=1,ny
      do i=1,nx
      sss=sss+(xfield(i,j,k,1)-xmeans)*(xfield(i,j,k,1)-xmeans)
      enddo
      enddo
      enddo

      sss=sss/dble(12*30*42)
      sssd=sqrt(sss)
      open(unit=3,file='perm.new',status='unknown')
      rewind(3)
      write(3,*)'MEAN IN Log10 ',xmeans
      do k=1,nz
      do j=1,ny
      do i=1,nx
      scalek=(xfield(i,j,k,1)-xmeans)*1.292+xmeans
      write(3,*)scalek
      enddo
      enddo
      enddo

      close(3)
      stop
      end
```

Testing:

Input file permd5_r1.dat with $\sigma(\ln k) = 1.937$, $\log_{10} k = -13.045$

output file perm.new (Scaling by factor A = 1.292) with $\sigma(\ln k) = 2.503$, $\log_{10} k = -13.045$

SIGNATURE [signature] DATE ~~2-18~~ ~~19~~ ~~2000~~ G.L. 3/25/00
READ AND UNDERSTOOD ______ DATE ______ 19 ______

PROJECT NAME ______ NOTEBOOK NO. ______

8-2-99

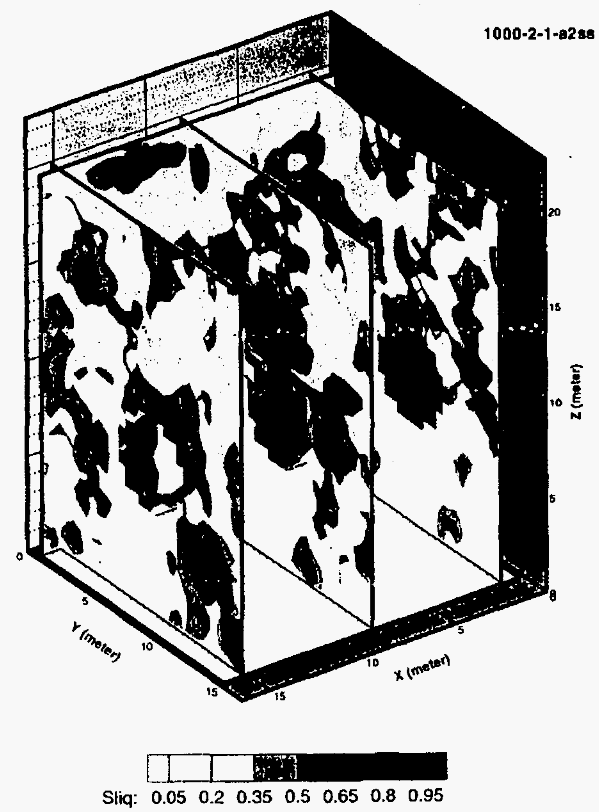
Presentation of the saturation contours on vertical planes for 2 correlation lens upscaled by simple factor.

We try to upscale the heterogeneity field by a simple formula bellow:

$$K' = (K - \bar{K}) * A + \bar{K}$$

Where K — old log permeability, $\bar{K}$ — mean log₁₀ permeability, K' — new log₁₀ permeability. A — upscaled factor. A = 1, K' = K; same heterogeneity field;
A = 0, $K' = \bar{K}$, Homogeneous field;
A > 1, higher heterogeneous field generated;
A < 1, lower " " "

Follow figures show the saturation contours for 2 upscaled heterogeneity fields with the factor A of 0.5 and 2.



Percolation flux 1000 mm/yr;
Steady State;
A = 2.

SIGNATURE [signature] DATE 2-18 19 2000
READ AND UNDERSTOOD ______ DATE ______ 19 ______

YMP-LBNL
REVIEW RECORD

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

3. Originator: Guomin Li G. Li 12/1/99
4. Document Title: Scientific Notebook: page 123, 133-134 & 149 for Macro/Routine mk_scale-k.f V1.0
5. Document Number: YMP-LBNL-CFT-GL-1 6. Revision/Mod.: N/A 7. Draft: N/A

8. Governing Procedure Number: AP-SI.1Q 9. Revision/Mod: 2/1

REVIEW CRITERIA

10. ☒ Standard Review Criteria: Technical (Taken from Attachment 5)

11. ☒ Specific Review Criteria:
- ☐ Source:
- ☒ Attached: YMP-LBNL Software Routine/Macro Documentation – Option 1
- ☒ 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./Dicipline	Review Criteria	Reviewer	Org./Discipline	Review Criteria
H.H. Liu	LBNL / Hydrol.	Technical			

COMMENTS DUE:

15. Due Date: 11/29/99

16. Originator/Review Coordinator: Donald Mangold
Print Name

REVIEW BY:

17. Hui Hai Liu
Print Name

18. [signature] 11-29-99
Signature Date

19. Mandatory Comments: ☐ Yes ☒ No

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Donald Mangold [signature] 12/9/99
Print Name/Signature Date

CONCURRENCE:

21. Document Draft No: N/A Date:

22. Reviewer: [signature] 12/9/99
Signature Date

23. PM: [signature] 12/10/99
Signature Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature Date

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Scientific Notebook : (pages 123, 133-134, 145) YMP-LBNL-CFT-GL-1

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 G.L. 12/9/99	Relevant Sections/Pages
YMP-LBNL-CFT-GL-1	pages 123, 133-134, 145

YMP-LBNL COMMENT SHEET

QA: L

1. Document Title: Scientific Notebook page 123, 133-134, 148			2. Page 1 of 1
3. Document No. YMP-LBNL-CFT-GL-1	4. Revision/ Change/Mod:	5. Draft	6. ☒ Q ☐ NQ
7. Reviewer: H. H. Liu			

8. NO. CODE	9. SECT./PARA./P#	10. COMMENT	11. RESPONSE	12. ACCEPT
		checked ~~th~~ visually code and no error is found. checked ~~th~~ visually test results and found that they are acceptable		

YMP-LBNL
REVIEW RECORD

1. QA: L
2. Page 1 of 1

3. Originator: Guomin Li
4. Document Title: Documentation for Routine mk_scale.f 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 N/A (Taken from Attachment 5)

11. ☐ Specific Review Criteria:
☑ Source: AP-SI.1Q/Rev. 2/ICN4, Sec. 5.1.1 (One time use routine)
☐ 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
Randall Hedegaard	LBNL/Hydrogeologist	Technical			

COMMENTS DUE:

15. Due Date: 25 FEB 2000

16. Originator/Review Coordinator: Guomin Li
Print Name

REVIEW BY:

17. Randall F. Hedegaard
Print Name

18. [signature] 2-28-00
Signature   Date

19. Mandatory Comments: ☐ Yes ☑ No

CONCURRENCE:

21. Document Draft No: NA   Date:

22. Reviewer: [signature] 2-28-00
Signature   Date

23. PM: [signature] 2/29/00
Signature   Date

ORIGINATOR/REVIEW COORDINATOR (After response completed):

20. Guomin Li [signature] 2-28-00
Print Name/Signature   Date

DISPUTE RESOLUTION: (if applicable)

24. PM:
Signature   Date

YMP-LBNL
COMMENT SHEET

QA: L

1. Document Title: Routine Documentation for mk_scale.f 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.		

YMP-LBNL

APPLICABLE REFERENCE INFORMATION

Document No.and Title: Notebook pages for Routine Documentation for mk_scale_k.f 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-CFT-GL-1 Scientific Notebook	pp. 149
YMP-LBNL-CFT-GL-1A Scientific Notebook for Reference Binder	pp. 100-101
Routine Documentation Form	pp1-2-

ATTACHMENT III – ADDITIONAL CASES WITH PARAMETER SET B′

With reference to Section 6.3.4, an additional parameter Set B′ is defined:

$k_{FC} = 1.86 \times 10^{-11}$ m^2

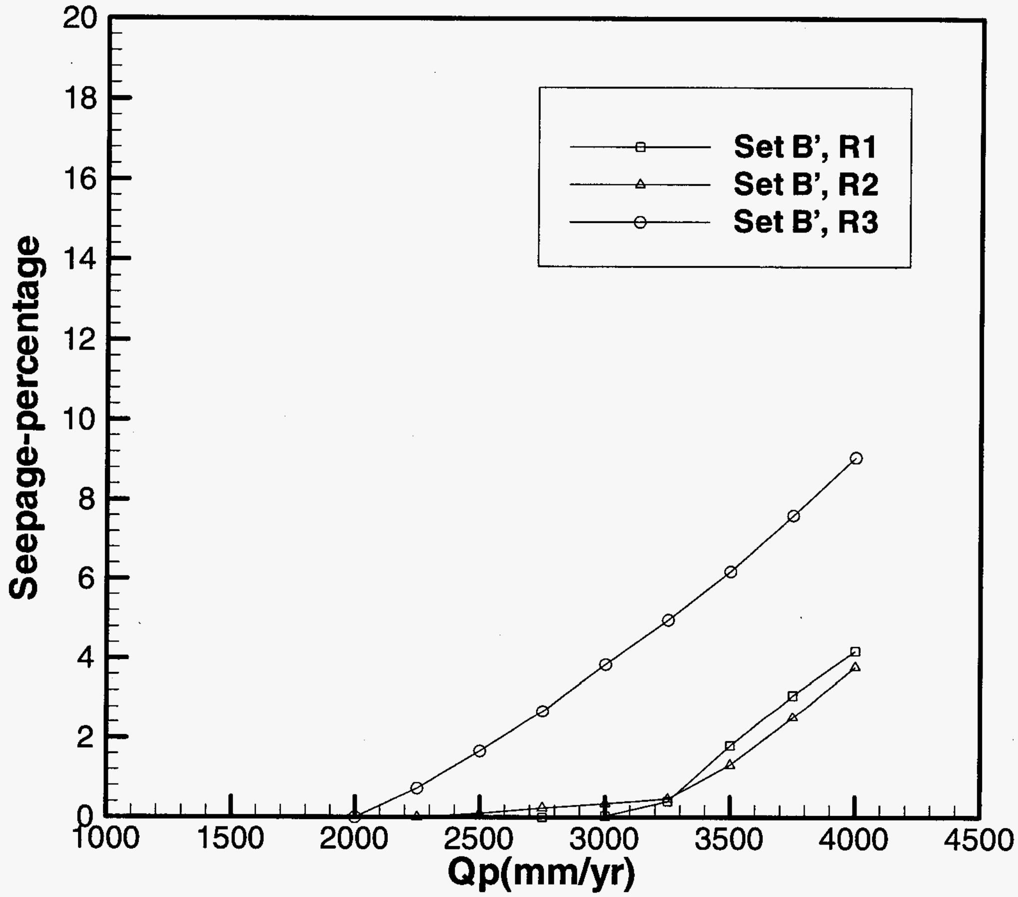
$1/\alpha = 537$ Pa

$n = 2.57$

$\sigma = 1.93$

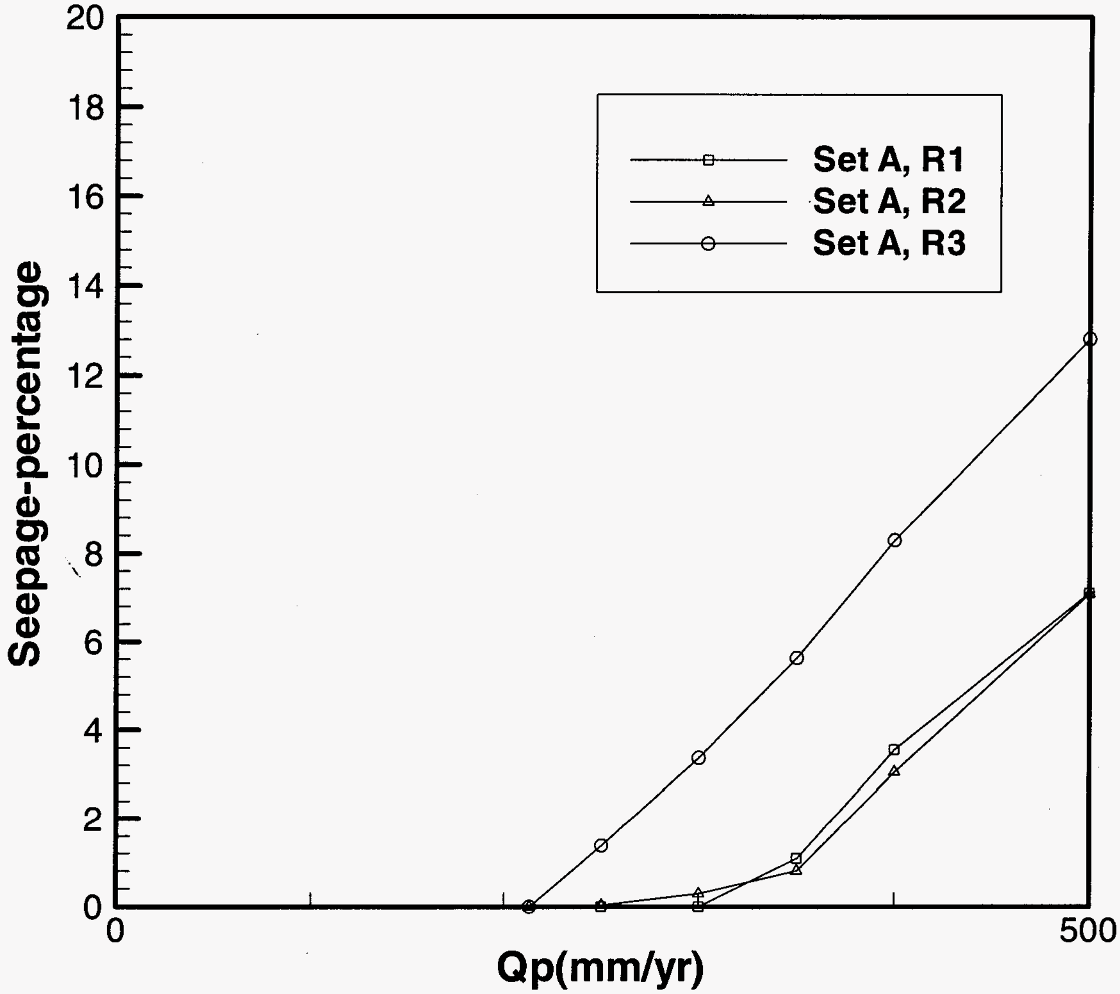
This parameter set is same as that of Set B, except for the $1/\alpha$ is reduced to account for the effects of the lithophysal cavities on seepage. As discussed in the SCM report (CRWMS M&O 2000 [153045], Section 6.3.3.3) lithophysal cavities tend to increase seepage. Since SMPA does not include lithophysal cavities explicitly, it is necessary to represent this effect by a reduced $1/\alpha$ value. One calibration case was run with and without lithophysal cavities in the model and the reduction of the $\log(1/\alpha)$ value caused by the presence of lithophysal cavities is found to be 0.21 (CRWMS M&O 2000 [153045], Section 6.3.3.3), suggesting a value of $\log(1/\alpha)$ of 2.73, which translates to the $1/\alpha$ value of 537 Pa.

With parameter Set B′, seepage percentages are calculated as a function of percolation flux for the three realizations R1, R2, and R3. The results are presented in Figure A3-1. For comparison, similar calculations are also done for Parameter Set A (see Section 6.3.4) and results are shown in Figure AIII-2.



DTN: LB0012SMDCATT3.002, LB0012SMDCATT3.001

Figure AIII-1. Seepage Percentage as a Function of Q_p for Parameter Set B′.



DTN: LB0012SMDCATT3.002, LB0012SMDCATT3.001

Figure AIII-2. Seepage Percentage as a Function of Q_p for Parameter Set A.