OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

1. QA: QA

Page: 1 of: 50

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 Model; ☐ 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
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9.	Checker	Robert Baca	Robert J. Baca	4/14/2000
10.	Lead/Supervisor	James Houseworth	James E Houseworth	4/17/00
11.	Responsible Manager	Clifford Ho	R. N. W. for Cl Ho	4/17/00

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

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ATTACHMENTS

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TABLES

ACRONYMS

AMR	Analysis and Model Report
AP	administrative procedure
ASTM	American Society for Testing and Materials
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
DOE	United States Department of Energy
DTN	data tracking number
ECRB	enhanced characterization of the repository block
ESF	exploratory studies facility
FEP	features, events, and processes
NRC	Nuclear Regulatory Commission
QAP	Quality Administrative Procedure(s)
SZ	saturated zone
SCFZ	Solitario Canyon fault zone
TBV	to be verified
TSPA	total-system performance assessment
TSPA-SR	total-system performance assessment – site recommendation
TSPA-VA	total-system performance assessment – viability assessment
UZ	unsaturated zone
VA	viability assessment
YMP	Yucca Mountain Site Characterization Project

1. PURPOSE

The purpose of this analysis is to evaluate the potential for changes to the hydrogeologic system caused by fault displacement to affect radionuclide transport in the unsaturated zone at Yucca Mountain. The potential repository is bounded on the west by the Solitario Canyon fault and on the east by the Bow Ridge fault. The northern boundary of this structural block is bounded by the Drill Hole Wash fault. In addition, there are intrablock faults consisting of the Ghost Dance, Sundance, and Dune Wash faults. For the purposes of this analysis, the focus is on two possible effects of fault displacement along the bounding faults: (1) uniform change in fracture properties throughout the UZ flow model domain and (2) change in fracture properties within the faults only. These two hypothetical end-member cases relate to the mechanical strain that's either uniformly distributed throughout the strata bounded by the faults, or localized to the individual fault zones. In the physical system, the strain would be spatially distributed in some manner that lies between these end-member cases. This evaluation used the bounding case estimates to determine if fault displacement can be excluded from consideration with respect to unsaturated zone (UZ) transport in total system performance modeling.

These two end-member cases were evaluated by simulating the flow and transport in the unsaturated zone (UZ) for a pulse input tracer at the potential repository location. For a specific cross-section, computer simulations were performed assuming: (1) a change in fracture properties throughout the UZ model domain (which assumes all fracture apertures are uniformly altered), and (2) a change in fracture properties in the fault zones only. Simulations were performed for the present-day climate and a wetter longer-term average climate case. Tracer breakthrough curves computed at the water table were used to examine the potential impact induced on transport in the UZ.

This evaluation supports the analysis of Features, Events, and Processes (FEPs) that may affect total system performance. The evaluation of FEPs are conducted to comply with the specifications in the DOE Interim Guidance (Dyer 1999) for justifying the inclusion or exclusion of FEPs from the total system performance assessment (TSPA). The specific issue of the effects of fault displacement on UZ transport encompasses four FEPS:

- Faulting (1.2.02.02.00)
- Seismic activity (1.2.03.01.00)
- Hydrologic response to seismic activity (1.2.10.01.00)
- Changes in stress produce change in permeability of faults (2.2.06.02.00)

The numbers in parentheses indicate the numerical identification used in the TSPA FEPs database (CRWMS M&O 1999a). The evaluation and screening of the other aspects of the FEPs listed above are documented in the UZ FEPs Analysis and Model Report (AMR) (CRWMS M&O 2000b) and saturated zone (SZ) FEPs AMR (CRWMS M&O 2000c).

Constraints and limitations of this work include the preliminary status of the input data and software used in the analysis (see Sections 3, 4, and 5). Once these source data and software are qualified, the results of this analysis can be considered qualified. Until then, the information developed from this analysis must be considered unqualified. This report has been prepared in accordance with the work plan, "Fault Displacement Effects on Transport in the Unsaturated Zone " (CRWMS M&O, 2000d).

2. QUALITY ASSURANCE

The quality assurance program is applicable to this report. The Performance Assessment Operations responsible manager has evaluated this activity in accordance with QAP-2-0, *Conduct of Activities*. The QAP-2-0 activity evaluation (CRWMS M&O 1999b) determined that the development of this AMR is subject to the *Quality Assurance Requirements and Description* (DOE 2000) requirements. This report is prepared in accordance with AP-3.10Q, *Analyses and Models*.

The unsaturated and saturated zone natural barriers have not been classified per QAP-2-3, *Classification of Permanent Items*. However the natural barriers have been classified by hydrogeologic units in the current project Q-List (YMP/90-55Q Rev. 5, 1998). In this document, the following hydrogeologic units in the UZ were identified as important to waste isolation: Tiva Canyon Welded, Paintbrush Nonwelded, Topopah Spring Welded, Calico Hills Nonwelded. In addition, the SZ was listed as a natural barrier important to waste isolation.

3. COMPUTER SOFTWARE AND MODEL USAGE

The computer software and models used in this report are listed below in Table 1:

Table 1. Computer Software and Software Routines Used in this Report

Software Name	Version	SCM Identifier	Computer Type	Documentation
TOUGH2	V1.3	10061-1.3-00	HP Workstation J2240	Mishra, 1998
FEHM	V2.00	10031-2.00-00	Dell Poweredge PC PII	Zyvoloski, 1999b
extract_xd.f	V1	software routine	HP Workstation J2240	Attachment II
va_ini_ext.f	V1	software routine	HP Workstation J2240	Attachment III
alt_tough2_aper.f	V1	software routine	HP Workstation J2240	Attachment IV
fehm_post.f	V1	software routine	HP Workstation J2240	Attachment V
T2FEHM2	V1	software routine	HP Workstation J2240	Attachment VI

TOUGH2 V1.3 and FEHM V2.00 are software for modeling unsaturated zone flow (TOUGH2) and radionuclide transport (FEHM) in the unsaturated zone. TOUGH2 V1.3 is qualified for use on the SUN Ultra Sparc and DEC/Alpha computers only, therefore, its use in this analysis on the HP Workstation J2240 computer is unqualified. Similarly, FEHM V2.00 is qualified for use on the SUN Ultra Sparc computer only, therefore, its use in this analysis on the Dell Poweredge PC PII computer is unqualified.

The selection of TOUGH2, T2FEHM2, and FEHM to evaluate UZ flow and transport is based on the fact that these software codes have been developed on the Yucca Mountain Project for just this purpose. The use of TOUGH2 V1.3 for site-scale flow and T2FEHM2 for conversion of the TOUGH2 flow field output for input to FEHM V2.00 is documented in CRWMS M&O (1998a). The use of FEHM V2.00 for site-scale radionuclide transport is documented in CRWMS M&O (1998b). Installation tests cases were performed for both of these software codes and the T2FEHM2 software routine.

3.1 QUALIFIED SOFTWARE

No software qualified in accordance with AP-SI.1Q, *Software Management*, (with the exception of software routines discussed in Section 3.3) was used in the development of this AMR.

3.2 SOFTWARE UNDER CONFIGURATION MANAGEMENT CONTROL

TOUGH2 V1.3 and FEHM V2.00 are software for modeling UZ flow (TOUGH2) and radionuclide transport (FEHM) in the UZ. Both of these software codes were obtained from configuration management in accordance with Section 5.11 of AP-SI.1Q, *Software Management*, and were determined to be appropriate for their respective applications. The software was installed and used in accordance with the available software documentation, indicated in Table 1.

3.3 SOFTWARE ROUTINES

T2FEHM2 is a software routine that was developed independently (Ho, 1997, see Attachment V). This software routine is appropriate for the application used in this analysis and is used only within the range of validation established for the software routine.

Additional pre- and post-processing routines listed in Table 1 were specifically developed for use in this analysis (extract_xd.f, va_ini_ext.f, alt_tough2_aper.f, fehm_post.f). These software routines are qualified through the documentation given in attachments to this analysis, as shown in Table 1. The executables of these software routines have been obtained using the HP FORTRAN 90/S700 compiler (version: B.10.20.00).

All software routines are documented in accordance with AP-SI.1Q, *Software Management*, and have been verified through visual inspections and/or hand checks as shown in Attachments I through V.

4. INPUTS

4.1 DATA AND PARAMETERS

The data and parameter inputs for UZ flow calculations using TOUGH2 presented in this analysis are contained in the total system performance assessment – viability assessment (TSPA-VA) three-dimensional UZ flow and transport model (DTN: LB971212001254.001). UZ flow properties affected by fracture aperture were varied for the sensitivity study reported in this analysis. For the UZ transport calculations, diffusion and sorption were assigned a value of 0. Dispersion has been shown to have little effect on transport results in the UZ over a wide range of dispersivities investigated (CRWMS M&O 1998b; Section 7.6.1.2.6). A dispersivity of 25 m is the nominal value used for these calculations.

4.2 CRITERIA

A criterion established by the NRC that is relevant to this analysis concerns whether or not an event is sufficiently unlikely to be excluded from further consideration. According to the DOE's Interim Guidance Section 102(j) (Dyer 1999), if the probability of occurrence for an event is less than 10^{-4} per 10^{4} years, then the event may be excluded from further consideration in the total system performance assessment. In this analysis, events with probability of occurrence less than this magnitude are excluded from further consideration.

4.3 CODES AND STANDARDS

The applicable standard for this work is ASTM D 5718 – 95, Standard Guide for Documenting a Ground-Water Flow Model Application. Not all aspects of this standard are applicable to the present investigation. In particular, calibration of the UZ flow model was performed in an earlier study, and the sensitivity analysis performed here is for the purpose of identifying model sensitivity alone, rather than identifying differences in calibration sensitivity compared with model sensitivity.

This AMR was prepared to comply with DOE's Interim Guidance (Dyer 1999) which specifies guidance to be used for evaluations in the absence of the NRC's final Yucca Mountian regulation. Subparts of this guidance that are particularly applicable to the data in this investigation include Subpart B, Section 15 (Site Characterization) and Subpart E, Section 114 (Requirements for Performance Assessment). Subparts applicable to models are outlined in Subpart E, Sections 114 (Requirements for Performance Assessment) and 115 (Required Characteristics of the Reference Biosphere and Critical Group).

5. ASSUMPTIONS

5.1 ASSUMPTION 1

The sensitivity studies on a two-dimensional, vertical cross-sectional model are assumed to be adequate to reveal any important effects of fault displacement on UZ flow and transport. This assumption is used in Sections 6.2.1 and 6.2.1.4

Basis: Transport in the UZ is dominated by the degree of matrix interaction that can take place. The transport behavior identified in the cross-sectional analysis (Section 6.2.2.2) demonstrates that there is at least some matrix transport that occurs in the base-case model because the travel times to the water table are too long for fracture-only transport. The selected cross-section contains all the major units that are important to transport, excluding zones of perched water, and the range of infiltration in this cross-section is reasonably representative of the range for the three-dimensional model. Perched water zones were found to result in rapid, fracture-dominated transport to the water table (CRWMS M&O 1998b; Section 7.6.1.2.7). Therefore, the current cross-sectional model should be more responsive and sensitive to the appearance of early breakthrough as a result of changes in fracture properties. It follows that testing the sensitivity of transport to changes in fracture properties in this cross-sectional model is biased in a conservative direction. Therefore, this assumption does not require further verification.

5.2 ASSUMPTION 2

Fault displacement effects on radionuclide transport behavior in the UZ are assumed to be entirely the result of changes to fracture properties in fault zones and/or in the surrounding rock. The effects of fault displacement on matrix properties are assumed to be negligible. This assumption is used in Sections 6.2 and 6.2.1.

Basis: Several fracture properties (permeability, capillary pressure, porosity) are a function of fracture aperture, which can be changed significantly by small strains if these strains are allocated entirely to the fracture apertures. The sensitivity of fracture aperture to mechanical strain is due to the small porosity of the fracture continuum. The matrix, on the other hand, has much greater porosity than the fractures in general, and its properties are not expected to be as sensitive to mechanical strain. This assumption is reasonable given the fact that fracture porosity is much less than matrix porosity at Yucca Mountain. Therefore, further verification of this assumption is not required.

5.3 ASSUMPTION 3

Changes in fracture properties are related to dilation or compression of existing fractures rather than the generation of new fractures. This assumption is used in Section 6.2.1.

Basis: This assumption relies on the fact that the rock at Yucca Mountain is highly fractured and that fractured rock is mechanically weaker along existing fractures than intact rock. This assumption is supported by the results of the Probabilistic Seismic Hazard Analysis, which show that the probability for fault displacement to occur along existing fractures is more likely than for intact rock (CRWMS M&O, 1998c; Section 8.2.1). Therefore, strain due to fault displacement is likely to occur along existing fractures rather than initiate new fractures. This assumption is reasonable and does not require further verification.

5.4 ASSUMPTION 4

The effects of fault displacement on mountain-scale UZ transport can be evaluated from the response for a simulated non-diffusing, non-sorbing tracer. This assumption is used in Section 6.2.1.

Basis: Transport of a non-sorbing tracer is more sensitive to changes in fracture aperture because fracture/matrix interaction is dominated by the effects of fracture aperture for such a tracer (given fixed matrix properties). For a non-sorbing tracer, the effects of diffusion are generally small (CRWMS M&O 1998b; Section 7.6.1.1.6). This assumption is reasonable and does not require further verification.

5.5 ASSUMPTION 5

Changes to fracture properties are assumed to be uniform, either throughout the UZ domain or localized to the fault zones. This assumption is used in Section 6.2.1

Basis: A large change in fracture properties over the entire UZ domain (fault zones and fractured rock) is one bound for the possible effects of fault displacement. Isolating the effects of fault displacement to the fault zones provides another bound which emphasizes the effects of property contrasts between the fault zones and the fractured rock. Clearly, this assumption bounds the expected extremes for the spatial distribution of changes to fracture properties as a result of fault displacement. This assumption is conservative and does not require further verification.

5.6 ASSUMPTION 6

The transient effects of changes in fracture properties can be neglected (i.e. transport for steady flow equilibrated to the changed conditions bounds the effects of the change). This assumption is used in Section 6.2.1.

Basis: This assumption is analogous to the assumption that transient flow effects are negligible. Tests of transient flow processes related to climate change have shown that transport in a transient flow environment is accurately approximated using a quasi-steady flow approximation (CRWMS M&O 1998b; Section 7.4.4.1 and Figures 7-12 and 7-13). Therefore, the transient effects of changes in fracture aperture are likewise expected to be inconsequential compared with the resulting changes in steady flow and transport associated with the change. Verification of this assumption by analogy with the transient flow problem is reasonable and does not require further verification.

5.7 ASSUMPTION 7

Water table elevation is unchanged by any fault displacement. This assumption is used in Section 6.2.1.

Basis: This assumption provides a fixed reference point for comparisons of the effects of fault displacements on radionuclide transport. This assumption is reasonable as a basis for comparison of the effects of fault displacement. Therefore, further verification of this assumption is not required. The effects of fault displacement on water table rise is analyzed in CRWMS M&O (2000b), and the effects are found to be negligible.

5.8 ASSUMPTION 8

The viability assessment (VA) model for UZ flow (CRWMS M&O 1998a) is adequate to represent UZ flow in this sensitivity study. This assumption is used in Section 6.2.1.

Basis: A new UZ flow model is being developed for use in TSPA-SR. This new flow model includes a different treatment of fracture/matrix interaction than used in the VA model. Because the results of the mountain-scale UZ flow and transport analyses are potentially sensitive to the treatment of fracture/matrix interaction, this assumption is to be verified (TBV) and will require a re-evaluation with the new UZ flow model.

5.9 ASSUMPTION 9

Fault displacements may result in changes to perched water. However, the effects of these changes in perched water on potential radionuclide transport are assumed to be negligible. This assumption is used in Section 6.2.1.

Basis: The sensitivity of radionuclide transport to different perched water models has been shown to be small (CRWMS M&O 2000a). Furthermore, the potential release of the perched water (and associated radionuclides) due to some disruptive event is expected to have a negligible effect on radionuclide releases at the water table (CRWMS M&O 2000b). This assumption is based on TBV information and, therefore, is also TBV.

5.10 ASSUMPTION 10

Thermal-hydrologic processes due to waste heat from the potential repository will affect UZ flow and transport. However, the effects of thermal-hydrologic processes are expected to be negligible with respect to the sensitivity study conducted in for this report on the effects of fault displacements on mountain-scale UZ transport. This assumption is used in Section 6.2.1.

Basis: Waste heat from the potential repository will perturb the UZ flow fields and potentially alter hydrogeologic and transport properties in the UZ. However, these effects are assumed to be small in comparison with effects caused by the changes in fracture aperture and different climate conditions (infiltration rates) investigated here. If so, the conclusions based on an isothermal analysis should also be valid for a thermally-perturbed condition. This assumption requires further verification and, therefore, is TBV.

6. ANALYSIS/MODEL

As stated in Section 1, the purpose of this report is to describe the potential for fault displacement events during the potential repository postclosure period that affect performance through changes in radionuclide transport in the UZ at Yucca Mountain. In particular, the effects of fault displacement on potential repository performance will be addressed in terms of changes in the simulated breakthrough at the water table of a pulse input of tracer at the potential repository.

The approach for the analysis of fault displacement effects on transport in the UZ is divided into two distinct components: a review of site description information which provides a basis for defining bounding conditions and for understanding the physical significance of the results (Section 6.1); and a modeling component to provide quantitative analysis of the sensitivity of the UZ flow system to changes in hydrologic parameters (Section 6.2).

6.1 SITE DESCRIPTION INFORMATION

The spatial and temporal patterns of faulting and fracturing of the volcanic bedrock are the fundamental elements of the structural geology of the potential repository for high-level radioactive wastes at Yucca Mountain. To document and discuss these patterns, a comprehensive program of geologic mapping and fractured rock mass studies has been conducted as an integral part of the site characterization. Of particular importance to this analysis are geologic observations related to displacement in fault zones and observations of the characteristics of the faults zones made during the excavation of the Exploratory Studies Facility (ESF) and in the enhanced characterization of the repository block (ECRB) Cross Drift. The observations are briefly described in Section 6.1.1. These observations provide a basis for determining the reasonableness and appropriateness of the range of inputs used in the modeling analysis in Section 6.2 and for interpreting the level of conservatism represented by the models.

However, the primary controlling factor for amount of flux through the UZ is the amount of precipitation available to infiltrate and percolate through the UZ. This variable is highly dependent on climate conditions. To address this variable, present day average and long term average climate conditions (CRWMS M&O 1998a, Section 2.4.1.1) were used as bounding conditions. The differences in these climate states are briefly explained in Section 6.1.2.

6.1.1 Geologic Setting

The Yucca Mountain area is cut by steeply dipping, north-south-striking normal faults which separate the Tertiary volcanics into blocks one to four kilometers wide (Scott 1990). The potential repository lies in the central block of the central Yucca Mountain structural domain. The central block is bounded on the west by the Solitario Canyon fault, on the east by the Bow Ridge fault, and on the north by the northwest-striking Drill Hole Wash fault. The southern boundary is marked by a transition to structural styles that accompany greater magnitudes of extension and continue south. Intrablock faults include the Ghost Dance, Sundance, and the Dune Wash faults.

The potential repository area is bounded by the Solitario Canyon fault to the west and the Ghost Dance fault to the east. Both faults dip steeply toward the west, and displacement, amount of brecciation, and number of associated splays vary considerably along their trace. (Scott and Bonk 1984; Day et al. 1998a). The two-dimensional cross-section used for the basis of the modeling for this analysis (Section 6.2.1.4) intersects the Solitario Canyon, Ghost Dance, and Dune Wash faults.

Surface geologic mapping (Scott and Bonk 1984; Day et al. 1998a), underground mapping of the ESF, geophysical surveys, and borehole studies show that the Yucca Crest subblock is little deformed, and cut only by widely spaced intrablock faults (Ghost Dance and Dune Wash). Within structural blocks, small amounts of strain are accommodated along intrablock faults. In many cases, intrablock faults appear to represent local structural adjustments in response to displacements on the block-bounding faults. Many of the intrablock faults within this part of Yucca Mountain are short, discontinuous, have minor cumulative displacement (1 to 10 m), and represent the localization of slip along pervasive preexisting weaknesses in the rock mass (Potter, Day et al. 1996a, 1996b). In some cases, intrablock faults are expressions of hanging wall or footwall deformation that affect the block within a few hundred meters of the block-bounding faults. The eastern and southern edges of the central block, however, are cut by numerous faults associated with block margin deformation (Solitario Canyon and Bow Ridge faults).

6.1.1.1 Fracture Attributes

The fracture network acts as a significant preexisting weakness in the rock mass that can accommodate extensional strain through distributed slip along many reactivated joints. Evidence for reactivation of joints includes the presence of thin breccia zones along cooling joints and observable slip lineations along joint surfaces (Sweetkind, Potter, and Verbeek 1996). Cooling joints originally formed as tensional openings, having only face separation, not shear. However, thin selvages of tectonic breccia are often present along the trace of cooling joints, indicating later slip. Subsequent analyses performed here (see Sections 6.2.1 and 6.2.2.1) will consider the dilation or compression of any hydraulically connected fractures at Yucca Mountain, regardless of whether the fractures originated as tensional openings during cooling of the rock or from past seismic activity and regardless of distance from the fault.

There are a number of primary controls on fracture characteristics within the Paintbrush Group that are related to stratigraphy, upon which any later tectonic signature (such as fault displacement) is superimposed. Fracture characteristics in the pyroclastic flows at Yucca Mountain are primarily controlled by variations in the degree of welding (CRWMS M&O 1998d, Section 3.6). The intensity of fracturing increases with degree of welding within the welded pyroclastic flows because of the presence of cooling joints, and because increasing brittleness of the rock favors an increase in the number of tectonic joints. Lithophysal development, alteration, and pumice content are secondary controls important in specific stratigraphic intervals. These lithostratigraphic controls affect fracture spacing, type, number of sets, continuity of individual fractures within each lithostratigraphic zone, and they also affect the fracture connectivity of the network as a whole (Sweetkind and Williams-Stroud 1996, pp. 60 to 66; Sweetkind, Barr et al. 1997, pp. 62 to 67).

Each lithostratigraphic zone at Yucca Mountain has characteristic fracture attributes, including predominant orientations, spacing, trace length, and joint type (Sweetkind, Barr et al. 1997, p. 76); each is unique in its ability to deform by distributed slip. The result is stratigraphic control of structural geometry—what may be a discrete break in one lithostratigraphic unit may be a broad zone of distributed deformation in another.

An analysis of fracture apertures is available from the ECRB Cross Drift Study (DTN GS990408314224.001 and GS990408314224.002). The largest aperture recorded was 520 mm. Approximately 64 percent of the observed fractures exhibited zero aperture. Of the over 1800 fractures measured, only 40 apertures were measured as greater than 20 mm, or about 2 to 3 percent. The remaining apertures were less than 20 mm.

The relationship of fractures smaller than 1 m in length to faults was evaluated by visual examination of every fault in the ESF (Sweetkind, Barr et al. 1997, p. 68) that could be correlated with a fault mapped at the surface (Day et al. 1998a). Four principal conclusions were reached, based on observations in the ESF (Sweetkind, Barr et al. 1997, pp. 68, 71).

The first conclusion is that the width of the zone of influence on fracture frequency in the immediate vicinity of a fault is, in general, quite narrow, ranging from less than 1 m to about 7 m from the fault.

The second conclusion regarding the relationship between faults and fracture attributes is that the width of the zone of influence in the immediate vicinity of a fault correlates, in a general way, with the amount of cumulative fault offset. Therefore, faults with the largest potential future displacement are the most likely to influence the potential repository block. Intrablock faults with very small amounts of cumulative offset (1 to 5 m) have zones of influence that are 1 to 2 m in width. Block-margin faults with tens of meters of cumulative offset (faults at ESF Stations 11+20 and 70+58) have zones of influence that range up to 6 to 7 m wide. The limited available data from block-bounding faults are not definitive regarding the nature of attendant fracturing.

The third conclusion is that the width of the zone of influence around a fault does not appear to be related to depth, at least within the ESF. The width of the zones of influence is similar for small faults observed along the North Ramp, where overburden is 50 to 60 m thick, as it is for small faults observed elsewhere in the ESF, where overburden thickness is two to three times greater. However, upward-splaying faults can result in apparent broad zones of influence at the surface because of the overlap of fractured zones surrounding individual fault splays.

The fourth conclusion is that the amount of deformation associated with faults appears, in part, to be dependent upon which lithologic unit is involved in the faulting. In the ESF, overall variability in the frequency of fractures 1 m long or longer is primarily a function of lithology, not proximity to faults (Sweetkind, Barr et al. 1997, p. 68). Fracture intensity correlates to lithologic differences, lowest in lithophysal units and nonwelded to partially-welded tuffs, and highest in densely welded, nonlithophysal rock. Faults within nonwelded to partly welded portions of the crystal-poor vitric zone of the Tiva Canyon Tuff are generally sharp, discrete breaks with minimal fault gouge or secondary shear surfaces. Individual pumice clasts along some faults can be traced to the fault surface without visible sign of breakage, and wall rocks show little evidence of deformation. In comparison to brittle, welded rocks, nonwelded units apparently can accommodate a greater amount of extensional strain before failing by fracture.

6.1.1.2 Fault Attributes

Information on the significant faults present in the repository area follow. The three faults that are included in the two-dimensional cross-section used in this analysis (Solitario Canyon, Ghost Dance, Dune Wash) are specifically described. Neither the Bow Ridge nor the Sundance faults are included in the two-dimensional cross-section used for the modeling portion of the analysis. However, information for these faults is pertinent for discussion about the reasonableness of bounding conditions.

In the following descriptions fault length refers to the maximum length of a given fault or fault zone as reported or shown on maps in published references (e.g., Piety 1996). Unless otherwise indicated, the following descriptions for regional faults, including temporal and behavioral data, are from Piety (1996), and the field reconnaissance work is from Anderson, Bucknam et al. (1995) and Anderson, Crone et al. (1995). Piety's report (1996) is an excellent synthesis of most of the data available for characterizing regional faults, and contains an extensive list of published references.

The Solitario Canyon Fault Zone (SCFZ) The SCFZ is the most laterally continuous fault and displays the most total offset of any structure in the immediate vicinity of Yucca Mountain. Day et al. (1998a, p. 6) consider the SCFZ to be one in a series of major north-south trending, block-bounding faults. The fault has been extensively investigated by trenching at the surface in Solitario Canyon (Ramelli et al. 1996). The Solitario Canyon fault has normal down-to-the-west displacement of about 260 m near the potential repository block and is the most significant of the faults involved in this analysis.

The main trace of this fault extends southward from Yucca Wash for about 18 km. It is located about 1 km from the western boundary of the potential repository site (Simonds et al. 1995). Total bedrock displacement varies from 61 m down-to-the-east at the northern end, to more than 500 m down-to-the-west at the southern end (Scott and Bonk 1984). Average dip of the fault plane is 72°W. Slickensides indicate a component of left-lateral slip.

A continuous 14 km-long Quaternary tectonic and erosional scarp is present at the bedrock-surficial deposit contact. Trenching evidence suggests four to six mid- to late-Quaternary surface-rupture events. The evidence for these events provides an estimated cumulative dip slip of 2.2 ± 0.4 m (Ramelli et al. 1996). Preliminary average slip rates range from 0.01 to 0.02 mm/yr (Ramelli et al. 1996). Minimum and maximum individual displacements range from 0 to 1.4 m, based on data for events more recent than 500 ka.

Map patterns demonstrate that tectonic mixing of various Paintbrush Group lithologies has occurred within the most intensely deformed parts of block-bounding fault systems. This is most apparent in the Solitario Canyon fault system (Scott and Bonk 1984; Day et al. 1998a). In this system, which is up to 400 m wide, there are domains in which lenses from stratigraphically diverse parts of the Tiva Canyon Tuff are juxtaposed; similar zones in which slices of Topopah Spring Tuff are mixed; and several areas where lenses from more than one Paintbrush Group formation are tectonically mixed (Day et al. 1998a). Individual fault strands within these tectonically-mixed zones are highly brecciated, and in some cases, the fault-bounded lenses have a high degree of internal brecciation.

The SCFZ was not crossed during the ESF excavation. In the ECRB Cross Drift, the SCFZ was expected to be composed of two major normal fault strands; the first (eastern strand) was projected as the "main splay" with a predicted total offset of about 230 m. The second (western strand) was projected with a predicted cumulative offset of about 165 m (CRWMS M&O, 1998e). Between these two larger strands, several smaller faults were expected to be associated with the SCFZ faulting. The tunnel boring for the ECRB Cross Drift was stopped between the two strands based on programmatic considerations, and the western strand was not intersected.

The as-built geologic cross-section for the ECRB Cross Drift (DTN GS990408314224.006) shows that the eastern strand was encountered at Station 25+85 (Station 25 means 2500 m from the start of the survey line and +85 means 85 m from that Station point) and has approximately 260 m of cumulative normal offset. Shears and small faults increase in intensity prior to (east of) of Station25+00. The SCFZ influences rock in the footwall of the fault to about Station 25+00 (or approximately 85 m from the fault proper) in the form of increased shear intensity. Spacing of faults and shears decreases, while continuity and amount of cumulative offset increases with proximity to the eastern strand of the SCFZ. At Station 25+30, a small fault oriented 200/83 is intercepted by the tunnel. Although the cumulative offset along the fault is approximately 1 m or less, the rock is intensely fractured after (west of) Station 25+40. The rock from Station 25+80 to 25+82 (between 3 and 5 m from the fault) is a clast-supported breccia. The rock is shattered to the point of not having recognizable structure. From Station 25+82 to 25+85, the rock is a clast-supported breccia. The main plane of displacement along the eastern strand of the SCFZ is at Station 25+85, (left wall, springline). The fault plane is defined by an 8 to 12 cm thick zone of fault gouge composed of about 85 percent clay and about 15 percent fine to medium sand. The gouge is firm and was slightly damp at the time of excavation in October 1998, but dry by February 1999. On the west (hanging wall) side of the fault plane described above, there is a zone of matrix-supported breccia that extends along the left wall from Station 25+85.5 to 25+89.90. The farthest western zone along the eastern strand of the SCFZ is composed of a clast-supported breccia extending along the left wall from Station 25+89.9 to 25+99.15 (or a distance of approximately 14 m west of the fault). This zone is bounded on the west side by a thin, discontinuous, matrix-supported breccia about 10 to 20 cm thick.

Ghost Dance Fault Zone–The Ghost Dance fault is in the central part of the potential repository block. It is mapped for approximately 3 km as a zone of numerous splays that not only parallel the main north-trending trace of the zone, but locally branch away from the main trace. In general, it is a north-striking normal fault zone, dipping steeply west (75° to 85°) with down-to-the-west displacement. The Ghost Dance fault bifurcates; one branch connects with the Abandoned Wash fault to the southwest (Scott and Bonk 1984; Day et al. 1996), and a second branch trends southeast, but does not appear to connect with the Dune Wash fault (Day et al. 1996) subdivided the fault into three sections on the basis of cumulative offset and brecciation.

Along the northern segment, north of Split Wash, the fault is a relatively narrow zone (2 to 4 m wide) with as much as 6 m of down-to-the-west total displacement.

The central segment of the Ghost Dance fault zone has greater down-to-the-west displacement than the northern segment, and extends from Split Wash to Broken Limb Ridge. On Antler Ridge, there is 13 to 20 m of cumulative displacement across several splays of the Ghost Dance that are distributed over a map width of approximately 100 to 150 m (Day et al. 1998a, p. 9). Individual splays are characterized by 1 to 2 m-wide breccia zones.

To the south on Whale Back Ridge, the fault zone is about 55 m wide and has about 30 m cumulative down-to-the-west offset. There, the zone is bounded by two north-striking faults. The eastern fault is the main trace of the Ghost Dance. Locally, the immediate hanging wall of the principal splay of the Ghost Dance fault is highly fractured. On the south-facing slope of Broken Limb Ridge, the cumulative offset is less than 6 m, and intense fracturing in the hanging wall extends about 15 m to the west.

The amounts of displacement and brecciation along the southwestern projection of the Ghost Dance fault across Highway Ridge are considerably less than those preserved along the central segment. Cumulative offset on the fault increases to the southwest from Ghost Dance Wash, becoming about 17 m down-to-the-west in Abandoned Wash on the eastern splay of the Abandoned Wash fault (Day et al. 1998a, p. 10).

In the Ghost Dance Wash area (near the southern bend in the ESF), displacement on the fault is less than 3 m both on the surface and in the ESF, and deformation is also confined to a relatively narrow zone (2 m) of intense fracturing and brecciation.

The Geotechnical Baseline Report (CRWMS M&O 1998e, p. 4-15) stated that the Ghost Dance fault might be encountered in the ECRB Cross Drift, but the fault should have minimal cumulative offset. The geologic cross section from the Baseline Report accurately predicted the fault in the vicinity of Station 4+80. A shear (i.e., less than 0.1m displacement) was encountered at Station 4+99 (left wall, springline) which has been identified as the northern distal end of the Ghost Dance fault. This feature is the only north-trending, conspicuous discontinuity in this portion of the tunnel. The feature consists primarily of a 1 to 10-cm thick zone of silty/sandy gouge with clasts. The gouge thickens slightly in the crown to 10 cm, but is only 2 to 4-cm thick elsewhere. The gouge is surrounded by a zone of intensely fractured and crushed rock. On the right wall, this fractured zone is approximately 0.4 m thick on the east side of the feature, and 0.6 m thick on the west side of the feature (DTN GS990408314224.003).

Dune Wash Fault–This south- and southeast-trending fault is mapped along the eastern side of the potential repository site for a distance of 3 km. It is mapped in exposures of bedrock as a west-dipping normal fault with down-to-the-west displacement. Toward the northern end of the fault, Tertiary volcanic rocks are displaced a total of 50 to 100 m (Day et al. 1996, 1998b; Scott and Bonk 1984). However, no evidence of Quaternary movement has been found in surficial deposits that bury the fault toward the south, and no per-event displacement data are available.

The Dune Wash fault is exposed in the ESF near Station 67+88, where the cumulative offset is 65 m (Sweetkind, Barr et al. 1997, Table 21), and the zone of increased fracture frequency in the vicinity of the fault is 6 to 7 m wide. This fault was not encountered in the Cross Drift.

Sundance Fault–The Sundance fault is located in the north-central portion of the potential repository block and lies northward of the line of the two-dimensional model cross section used in the model for this analysis.

A detailed investigation of the Sundance fault has been conducted by Potter, Dickerson et al. (1999). The maximum width of the Sundance fault zone is about 75 m, and the cumulative down-to-the-northeast vertical displacement across the fault zone does not exceed 11 m. The faults in this zone are almost exclusively characterized by down-to-the-northeast displacement (Potter, Dickerson et al. 1999, pp. 5 to 6). Even though some horizontal slickensides have been observed, significant strike-slip displacement along the Sundance fault zone is not evident. Potter, Dickerson et al. (1999, p. 9) concluded that the Sundance fault zone has a significantly smaller along-strike extent than had been suggested by previous workers.

Individual faults in the Sundance fault zone and elsewhere at Yucca Mountain are vertically and laterally discontinuous; one or more mechanisms of strain accommodation must operate in the Tiva Canyon Tuff to accommodate displacements in the rock volume between the discontinuous discrete fault segments. Two probable mechanisms are: distributed brittle deformation associated with diffuse breccia bodies, and minor cumulative offsets along numerous preexisting cooling joints (Potter, Dickerson et al. 1999, pp. 13 to 14).

The ESF passes beneath the southeastern end of the Sundance fault zone, as mapped by Potter, Dickerson et al. (1999), where displacement is minimal on the south flank of Live Yucca Ridge. In the ESF, the fault is identified within a broad zone of discontinuous minor northwest-striking faults and joints in the middle nonlithophysal zone of the Topopah Spring Tuff. The exposure in the ESF is similar in character to the fault zone mapped at the surface near its southeastern termination on the south-facing slope of Live Yucca Ridge (Potter, Dickerson et al. 1999, p. 8; Day et al. 1998a).

The Geotechnical Baseline Report (CRWMS M&O, 1998e, p. 4-15) predicted the Sundance fault to be near Station 10+70 to11+00. The Sundance fault was encountered along the left wall at Station 11+35.40 to 11+36.70 (DTN GS990408314224.003). The fault intercepts the right wall at Station 11+35 to 11+36.2, approximately 35 m southwest of the location predicted. The amount of displacement is thought to be on the order of several meters, but is indeterminate. The margins of the fault zone were unaltered except in the immediate area of the fault, which exhibits some iron oxide stainings along the right wall. All portions of the Sundance fault were dry at the time of excavation.

The fault zone is composed of three distinct zones along the left wall. Zone 1 is adjacent to the footwall plane, and is a matrix-supported, uncemented breccia. Zone 1 is approximately 20 cm thick on the left wall, thinning to 4 cm on the right wall. Zone 2 along the exposure of the Sundance fault is approximately 0.7 m thick and is a matrix-supported breccia. Zone 3 varies in thickness from 0.3 m on the left wall, to zero on the right wall. Despite the very sharp and distinct plane of the fault at the footwall, distinct slickensides are not evident. Faint, low-angle slickensides can be interpreted on the left wall, and undulations in the fault plane with low-angle plunges occur at the boundary between Zones 1 and 2. The footwall rock is intact, even within 10 cm of the fault plane. The hanging wall is slightly more fractured, with an intensely fractured zone about 1 m thick.

Bow Ridge Fault–This fault is a prominent north-striking, west-dipping, normal-oblique (sinistral) slip fault. It is about 10 km long and lies along the east side of the potential repository area. The fault is buried beneath alluvium and colluvium for most of its extent along the western margin of Midway Valley. The best topographic expression of the fault occurs where a 760-m-long section follows the base of the west side of Exile Hill (Simonds et al. 1995; Menges and Whitney 1996; Menges et al. 1997). Tertiary volcanics are displaced at least 125 m down-to-the-west at this locality. The fault dips 65°E to 75°E.

Trenches on the surface and the ESF expose a complex fault zone in highly-fractured Tertiary volcanic bedrock and colluvial deposits that have been subjected to multiple Quaternary faulting events. At least two and possibly three surface-rupture events are evident in late to middle Pleistocene colluvial deposits at trench 14D (Menges and Whitney 1996; Menges et al. 1997). A minimum age of 48 ± 20 ka is established for the most recent surface-rupture event. Displacements range from 14 to 44 cm for individual faulting events, and cumulative displacement is from 30 to 70 cm for all events younger than 500 ka. Average recurrence intervals vary from 70 to 215 ky. Recurrence intervals for individual events vary more widely from 40 to 350 ky. Average slip rates are 0.002 to 0.007 mm/yr (Menges and Whitney 1996; Menges et al. 1997).

The Bow Ridge fault has very little attendant fracturing despite the 100 m cumulative offset and its exposure near the surface (approximately 35 m of overburden). Lack of deformation around the fault zone probably results from the presence of nonwelded pre-Rainier Mesa Tuff in the hanging wall of the fault.

6.1.1.3 Significance of Geologic Setting to the Analysis

The descriptions in Sections 6.1.1.1 and 6.1.1.2 suggest that an analysis of fault displacement effects needs to be considered from two perspectives: the impact on fractures throughout the potential repository as a whole, and the effect on fractures in the immediate vicinity of the faults only. Furthermore, the range of fault characteristics that was described supports the idea that movement on the Solitario Canyon fault may be considered the bounding scenario.

As stated in Section 6.1.1.1, the fracture network at Yucca Mountain acts as a significant preexisting weakness in the rock mass that can accommodate extensional strain through distributed slip along many reactivated joints. Evidence for reactivation of joints includes the presence of thin breccia zones along cooling joints and observable slip lineations along joint surfaces (Sweetkind, Potter, and Verbeek 1996). There are a number of primary controls on fracture characteristics within the Paintbrush Group that are related to stratigraphy, upon which any later tectonic signature (such as fault displacement) is superimposed. The existence of distributed slip suggests that changes in strain (such as would be associated with a significant fault displacement) are likely to be propagated throughout the repository area. Also, some fault zones (such as the Ghost Dance and Solitario Canyon) may be on the order of 100 to 400 m wide. Although strain is expected to diminish with distance from the fault, these observations suggest that the effect of strain distributed in the fractures throughout the potential repository should be considered (Sections 6.2.2.1 and 6.2.2.2).

The presence of gouge and brecciated zones only in limited proximity to the fault planes, however, suggests that much of the strain will be mechanically dissipated within or near the fault plane itself. For instance, as described in Section 6.1.1.2, in the Solitario Canyon fault zone in the ECRB Cross Drift, the total displacement is approximately 260 m, but the gouge and brecciated zones are limited to less than 20 m. Similarly, the Dune Wash fault as exposed in the ESF exhibits a cumulative offset of 65 m (Sweetkind, Barr et al. 1997, Table 21), but the zone of increased fracture frequency in the vicinity of the fault is only 6 to 7 m wide. A third example is the observation of the Sundance fault in the ECRB Cross Drift; with an assumed, though indeterminate displacement of several meters, the footwall rock is intact, even within the 10 cm of the fault plane. The hanging wall is slightly more fractured, with an intensely fractured zone about 1 m thick. Consequently, an analysis of fault displacement should also consider a case where the effects of strain are limited to the immediate vicinity of the fault zone (Section 6.2.2.3).

6.1.2 Fault Displacement Hazards

Fault displacement hazards at Yucca Mountain have been investigated in detail in the report "Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada" (CRWMS M&O, 1998c). Several original approaches to characterizing the fault displacement potential were developed by the seismic source expert teams. The approaches were based primarily on empirical observations of the pattern of faulting at the site during past earthquakes (determined from data collected during fault studies at Yucca Mountain). Empirical data were fit by statistical models to allow use by the experts. The results of this analysis were curves representing probabilistic predictions of fault displacements.

Nine locations within the preclosure controlled area were identified to demonstrate the fault displacement methodology. The term "preclosure controlled area" is defined in DOE's Interim Guidance (Dyer 1999). These locations were chosen to represent the range of potential faulting conditions. Two of the nine sites each had four identified faulting conditions. Some of these locations lie on faults that may experience both principal faulting and distributed faulting. The other points are sites only of potential distributed faulting.

With the exception of the block-bounding Bow Ridge and Solitario Canyon faults (sites 1 and 2, respectively), the mean displacements are 0.1 cm or less at a 10^{-5} annual exceedance probability, and on the order of 1 m or less at 10^{-8} annual exceedance probability (CRWMS M&O 1998c, Figures 8-4 through 8-14). For the Ghost Dance fault, the range of displacements per event is 0.6 m to about 1.5 m at 10^{-8} mean annual exceedance probability (CRWMS M&O 1998c, Figure 8-5). Thus, sites not located on a block-bounding fault, such as sites on the intrablock faults, other small faults, shear fractures, and intact rock, are estimated to have displacements significantly less than 0.1 cm for mean annual exceedance probabilities of 10^{-5}.

For Solitario Canyon fault and Bow Ridge fault (CRWMS M&O 1998c, Figures 8-2 and 8-3), the mean displacements are 7.8 and 32 cm, respectively, for these two faults at a 10^{-5} annual exceedance probability. At lower annual exceedance probabilities, the fault displacement hazard results are driven by the upper tails of uncertainty distributions and are close to 5 m.

For purposes of determining the appropriateness of the choosen bounding conditions based on the Probabilistic Seismic Hazard Assessment, per-event displacements can be used as a comparison. As described in Section 6.1.1 above, the largest estimate of per event displacement for the faults intersected by the 2-D cross section used for the analysis is 1.4 m along the Solitario Canyon fault. A displacement of 1.2 m corresponds to the 15th fractile curve at a 10^{-8} annual exceedance probability. (CRWMS M&O 1998c, Figures 8-3). As described in Section 6.2.1.5, strains associated with a displacement of 10 m are used as bounding conditions. Given that the assumed bounding condition is about a factor of 10 greater than measured displacement and the probabilistic displacement event suggested by the 15th fractile curve, the values used in this analysis are judged to be extremely conservative.

6.1.3 Climate Data

The primary controlling factor for flow through the UZ is the amount of infiltration through the system. This variable is highly dependent on precipitation and climate conditions. To address this constraint, present-day average and long-term average conditions were used as bounding conditions.

Present day climate conditions represent relatively dry, interglacial conditions, while the long term average conditions represent typical conditions at Yucca Mountain between the wet and dry extremes based on available paleoclimate data. (CRWMS M&O 1998a, Section 2.4.1.1). Because these two sets of conditions represent relatively stable (i.e., long-term conditions) rather than extreme conditions (i.e., short-duration climatic states such as superpluvial periods), they were chosen as representative conditions for this analysis.

The primary difference in these conditions is a doubling of the precipitation rate, with an approximately 6- to 8- fold increase in the average net base infiltration rates (CRWMS M&O 1998a, Table 2-5 and Table 2-16). The total water influx used for the two-dimensional model for the present-day climate is 0.11471 kg/s (3.2 mm/yr), while the total water influx to the model for the long-term average climate is 0.98413 kg/s (27.3 mm/yr).

6.2 EFFECTS OF FAULT DISPLACEMENTS ON UZ FLOW AND TRANSPORT

As discussed in Section 6.1, fault displacements are expected to occur along existing faults in the vicinity of Yucca Mountain. The movement produced by a fault displacement will result in changes in the rock stress in the vicinity of the fault. Obviously, the change in rock stress will decrease with distance from any given fault that does move. However, the magnitude of the changes in rock stress as a function of distance from the fault depends on the specific details of the fault displacement (e.g., magnitude of fault motion, direction of fault movement, extent of the fault that participates in the movement) and the mechanical properties of the surrounding rock (e.g., fracture spacing, fracture stiffness, geomechanical properties of the rock matrix). Given some change in rock stress, the fractured rock mass will respond to the change in stress through deformation, or strain, in the rock. Of particular importance is the fact that this induced strain can affect the geometry of fractures in the rock, as discussed in Section 5.2. The effects of changes in properties of the rock matrix (as opposed to the fractures) are assumed to have a negligible effect on UZ flow and transport (Section 5.2). In theory, the effects of a given fault displacement could be evaluated using process-level calculations for the effects of the induced stress and strain on fracture geometry. Then the effects of this change in fracture geometry on the fluid-flow properties of the fracture network could be evaluated. However, this method was not used in this analysis due to the large uncertainty and complexity of the problem.

Some of the effects of previous fault displacements at Yucca Mountain can be examined directly. Previous fault displacements have resulted in observable changes to the structure of the surrounding rock (Section 6.1.1). However, geologic observations are not adequate to assess the effects of some of the changes caused by fault displacements that could be important to UZ flow and transport. In particular, the effects of previous fault displacements on the present-day fracture apertures at Yucca Mountain are difficult to determine by observation. For example, it is difficult to determine by geologic observation that a given fracture with an effective hydraulic aperture of, say 200 μm, may have had an effective hydraulic aperture of 150 μm at some point in the past prior to a fault displacement event. In fact, it is difficult to determine the effective hydraulic apertures of the present-day fractures at Yucca Mountain by direct observation (Sonnenthal et al. 1997, Section 7.5.4). Fracture apertures at Yucca Mountain are determined through pneumatic flow tests (giving the fracture permeability) and a theoretical model relating fracture frequency (determined by observation of fractures), fracture permeability, and fracture aperture (Sonnenthal et al. 1997, Section 7.5.4).

6.2.1 Analysis Approach

In the absence of definitive, predictive process modeling or definitive geologic observational evidence, a bounding approach is used to assess the potential effects of fault displacement on potential repository performance. As a corollary to the assumptions in Section 5.2 and 5.3, the problem is assumed to be bounded if large enough changes in fracture aperture are evaluated. Here, "large enough changes" are defined to be changes that can be justified as larger than any expected changes resulting from any fault displacements (in the vicinity of Yucca Mountain) that have an annual exceedance probability greater than 10^{-8}. Given an assumed change in aperture, it is possible to estimate the change in fracture hydraulic properties using theoretical models that relate the changes in fracture properties to the changes in fracture aperture (see Section 6.2.1.3). The effects of the modified fracture properties on transport behavior between the potential repository and the water table can be evaluated using the UZ site-scale flow and transport models. Changes in transport are identified through the use of breakthrough curves (see Section 6.2.1.2) for a simulated nondiffusing, nonsorbing tracer as described in Section 5.4. If the identified changes in transport are small, then it can concluded that the effects of fault displacement on potential radionuclide transport are negligible and can be excluded from further consideration in TSPA.

For such a method to be valid, the assumed changes in fracture aperture must be shown to represent a bounding change in fracture aperture for the effects of any fault displacement in the vicinity of Yucca Mountain. The justification that the assumed changes in fracture aperture bound the range of expected changes is given in Section 6.2.1.3.

The spatial distribution of changes to fracture aperture within the modeling domain is treated using two end-member scenarios (Section 5.5):

1. All fracture apertures are altered uniformly throughout the UZ model domain (both fault zones and fractured rock) (Section 6.2.2.1).

2. Only fracture apertures in the faults zones are altered (Section 6.2.2.2).

The first scenario bounds the most widespread disturbance possible. The second scenario considers the possibility that the effects of fault displacement remain local to the fault zones. The second scenario is also used to investigate the potential sensitivity associated with an enhanced contrast in properties between the fault zones and the fractured rock.

Sensitivity calculations are performed for both the present-day (dry) climate and the wetter long-term-average climate (CRWMS M&O 1998a; Section 2.4.1.1). The average infiltration rates for these climates represent the range of average infiltration behavior expected at Yucca Mountain over the next 10,000 years (CRWMS M&O 1998a; Section 2.4.1.3 and 2.4.2.7). Over the potential repository block, the average infiltration rates used in the model for the present-day climate is 7.7 mm/yr and for the long-term average climate is 42 mm/yr (CRWMS M&O 1998a; Section 2.4.2.7).

The site-scale models for UZ flow and radionuclide transport are based on a three-dimensional spatial domain. For computational efficiency, one-dimensional and two-dimensional portions of the three-dimensional domain were used for the sensitivity calculations performed in this study (Sections 5.1 and 6.2.1.4).

Several additional assumptions are also implicitly used in this modeling approach. These implicit assumptions, and the bases for these assumptions, are given in Sections 5.5 through 5.10.

6.2.1.1 Dual-Permeability Concept

The conceptual model for unsaturated flow and transport used in this analysis is called the dual-permeability model. In the version of the dual permeability model used in this analysis, there are two continua representing the fracture and matrix that overlap in the macroscopic flow continuum. At every macroscopic "point" we have separate hydrologic conditions, properties, and other factors, for a the fracture continuum and for the matrix continuum. Therefore, at every macroscopic "point" there is also a defined flux of water (flow rate of water per unit area) in the fracture continuum and in the matrix continuum. Practically speaking, the macroscopic point (or length scale) is defined by the grid discretization. At the microscopic (or sub-grid) scale, the fractures and matrix are spatially distinct, with length scales that define the microscopic geometric arrangement of the fracture and matrix continua. Given this microscopic geometry of the continua and the properties and conditions defined in each continuum, a flux of fluid at each macroscopic point between the fracture and matrix continua is also defined. In other words, there is also an exchange of flow between the fracture and matrix continua as well as flow through each continuum at each macroscopic point.

Although the dual-permeability model has been described above in terms of a flow model, an analogous description can also be made for the transport model. That is, transport takes place at each macroscopic point in both the fracture and matrix continua (each continuum having its own transport properties and conditions), and there is, likewise, a transport exchange between the fracture and matrix continua.

The dual-permeability model for flow and transport can be used in either three, two or one dimension. For example, a one-dimensional problem would have flow and transport in one linear direction only. This is easiest to understand for a problem in which flow occurs along one axis, say the z axis. Assume that the rock properties and conditions at the boundaries of the model are independent of the remaining two spatial coordinates, x and y. Then the only spatial variations that could possibly occur in the problem are in the z direction. The spatial evolution of the problem can be completely described in terms of z. The x and y dimensions only enter the problem in a trivial sense to scale the total quantity of flow and transport that take place in the real three-dimensional domain. This simple scaling can be done after analyzing the spatial (and temporal) variations in the problem. Numerically, the one-dimensional dual-permeability model is configured using a stack of paired grid cells as shown in the one-dimensional connection diagram give in Figure 1. One stack represents the fracture continuum and one stack represents the matrix continuum. The dual-permeability connection diagram can be extended to two dimensions as shown in Figure 2. In three dimensions, the conceptual nature of the dual-permeability model (with overlapping continua) becomes more apparent in so far as a connection diagram is concerned. In this case, there is no "extra" dimension for the fracture/matrix node pairing, so the fracture/matrix node pairs must overlap spatially in a three-dimensional connection diagram.

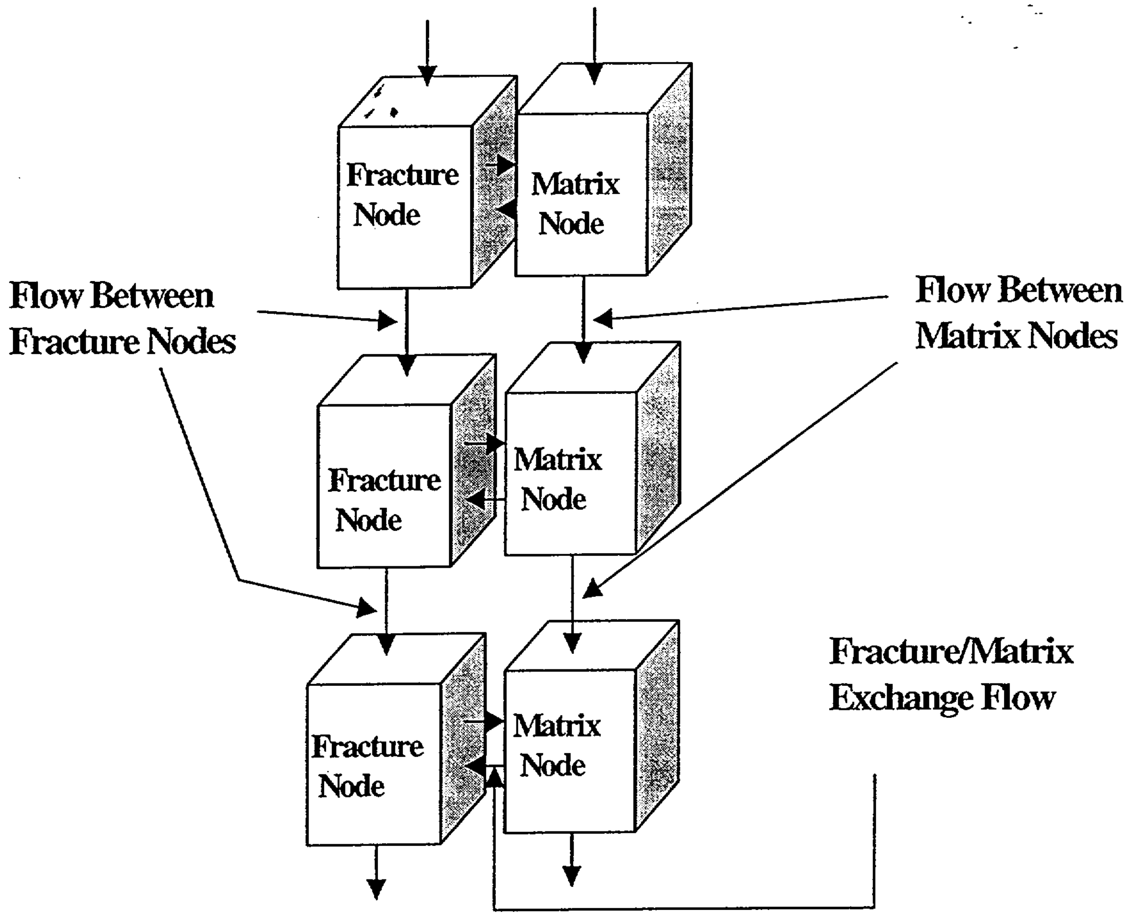

Figure 1. Conceptual Connection Diagram for a One-Dimensional Dual-Permeability Model

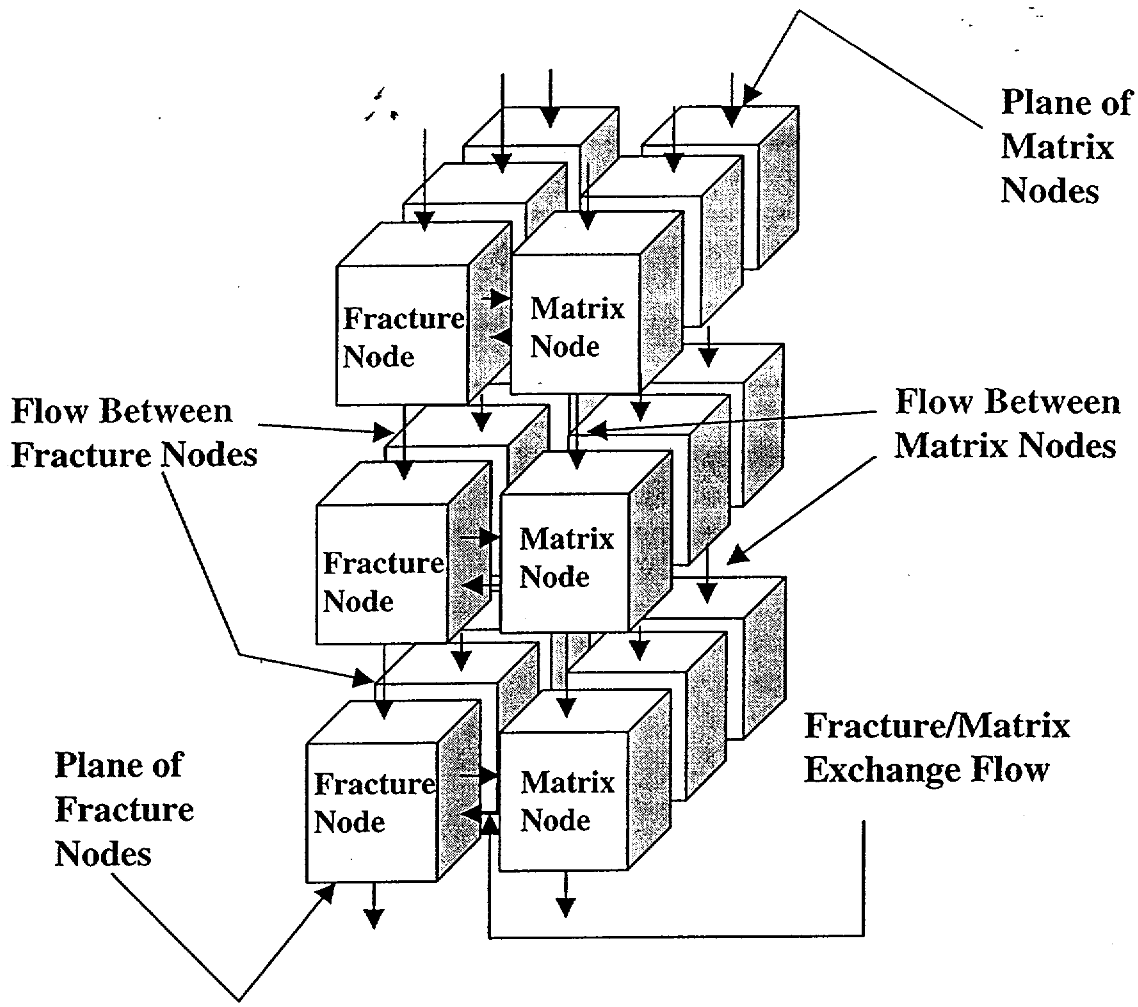

Figure 2. Conceptual Connection Diagram for a Two-Dimensional Dual-Permeability Model

6.2.1.2 Site-Scale Models for UZ Flow and Transport

The site-scale model for UZ flow uses the software TOUGH2 V1.3 (Section 3.). TOUGH2 is a multi-purpose numerical model that, among other problems, can solve fluid flow problems in geologic materials (Pruess 1991; Section 1). The standard differential conservation equations describing flow are cast in an integrated form for the numerical solution methods used in TOUGH2 (Pruess 1991; Appendices A and B). The solution to these conservation equations is obtained by discretization of problem in space and time. In this analysis, TOUGH2 is used to solve the equations for unsaturated flow in a fractured rock domain representative of Yucca Mountain. Unsaturated flow is defined to be the flow of water only in a geologic material with pore spaces partially filled with water and partially filled with air. In an unsaturated flow model (as opposed to a two-phase flow model), the air is assumed to be at static equilibrium. As discussed in Section 6.1.2.1, fractured rock is represented using a dual-permeability conceptual model.

The site-scale model for UZ transport uses the software FEHM V2.0 (Section 3). FEHM is a multi-purpose numerical model that, among other problems, can solve mass transport problems in geologic materials (Dash and Zyvoloski 1999; Section 1). The transport solution technique used in this analysis is a particle tracking method (Zyvoloski et al. 1995; Section 8.3.3.2). Particle tracking methods solve the transport problem by following the motions of simulated particles through geologic material. The motions of the particles are subject to the processes known to affect transport (i.e., flow (advection), diffusion, sorption, and dispersion). However, rather than solving for the effects of these processes through the conservation equations, the effects are determined directly through the motion of particles over the spatial and temporal domain of the problem.

6.2.1.3 Breakthrough Curves

Breakthrough curves are used in this analysis to describe the behavior of radionuclide transport in the unsaturated zone. A breakthrough curve is generated by releasing particles uniformly over the fracture nodes of all the grids cells within the potential repository. Particles are only released to the fracture nodes because fractures are expected to be the main transport pathway at the repository horizon. Particles are released over some time period (short relative to the transport time of the problem), approximating an "instantaneous" release of the particles. For this analysis, the particles are released uniformly over a period of one year. The breakthrough curve shows the total mass that has arrived at the water table (over the entire model domain) relative to the total mass released as a function of time, as shown in Figure 3.

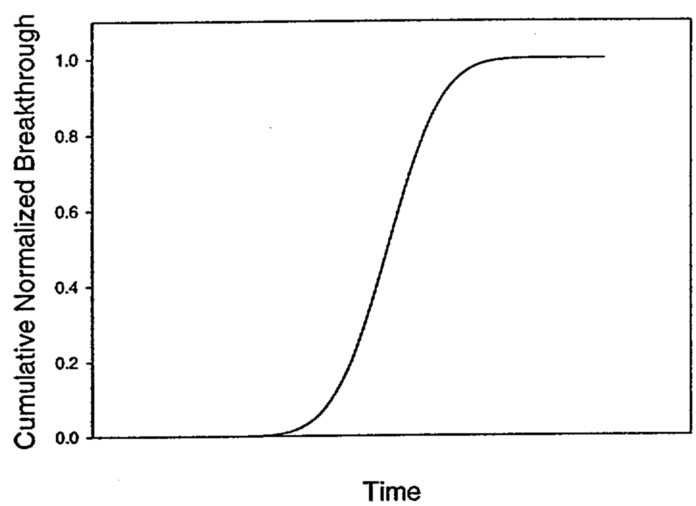

Figure 3. Schematic Diagram of a Breakthrough Curve

6.2.1.4 Problem Domain

The entire domain of the site-scale flow and transport models is shown in plan view in Figure 4 (TSPA-VA three-dimensional UZ flow and transport model; DTN: LB971212001254.001). In the vertical dimension, the models encompass the entire UZ between the ground surface and the water table. An east-west vertical cross-section and a one-dimensional column are extracted from this three-dimensional model for calculations performed for this analysis. Figure 4 shows the location of this cross-section (a-a) and column (•) within a plan view of the three-dimensional UZ grid. The selected cross-section passes through three of the four major faults in the region: counting from the west toward the east, the Solitario Canyon fault, Ghost Dance fault, and the Dune Wash fault.

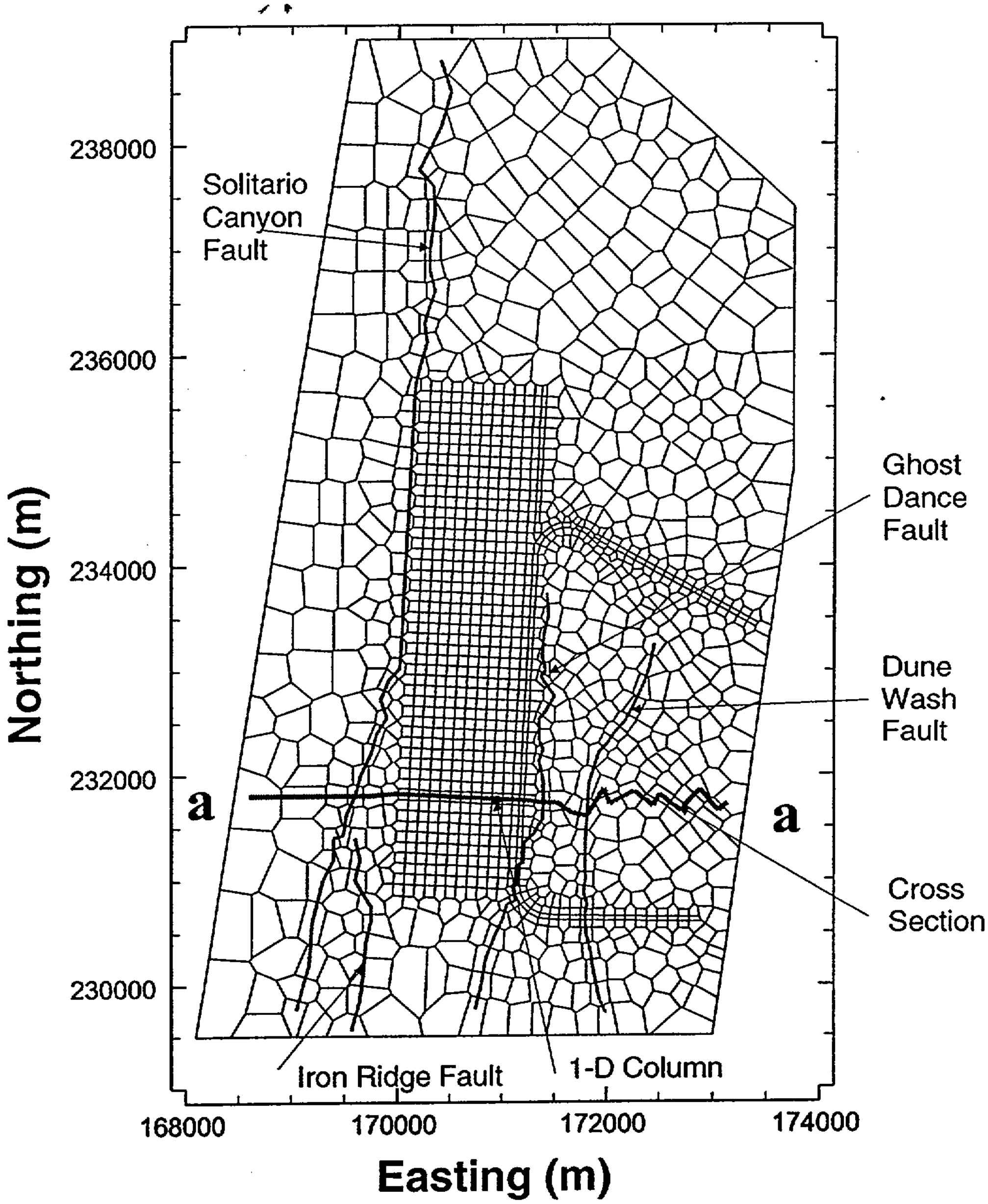

Figure 4. Plan View of the Locations of the Two-Dimensional Cross Section and Four of the Nearby Faults within the TSPA-VA UZ Grid. The Location of the One-Dimensional Column Is Shown with a •.

6.2.1.5 Bounds on the Change in Fracture Aperture

As discussed in Section 6.2.1, the approach used to investigate the effects of fault displacements is to evaluate the sensitivity of radionuclide transport in the UZ to changes in fracture apertures. This is investigated over a wide enough range to bound the potential changes in fracture aperture that could result from any fault displacement at Yucca Mountain with an annual exceedance probability of greater than 10^{-8}. As discussed in Section 6.1.1, the largest fault movement close to the potential repository is likely to be along Solitario Canyon fault. The general topic of seismic hazard at Yucca Mountain has been investigated in detail in the report "Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada" (CRWMS M&O, 1998c). For Solitario Canyon fault, the hazard analysis shows fault displacement 5 m (CRWMS M&O, 1998c, Figure 8.3) at an annual exceedance probability of 10^{-8}. We use 10 m as an extremely conservative fault displacement for bounding analyses.

Geomechanical models used to investigate the amount of strain induced by fault movements in the rock at Yucca Mountain show that changes in strain extend several kilometers from a fault movement (Gauthier, et al. 1995, National Research Council 1992; Appendix D). Using a three-dimensional elastic boundary element mode of Yucca Mountain, Gauthier et al. (1995) investigated the effects of a right-lateral, strike-slip fault displacement on a fault dipping 60°. The fault movement was 1 meter along a 30 km section of the fault. The results show strains of 10 microns per meter (10 micro-strain, or 10 μs) up to 8 km from the fault. Geomechanics calculations were also performed in the National Research Council (1992, Appendix D) report. This calculation was for a normal displacement along a fault dipping 60° to the vertical. The simulated fault movement was 1 meter along 30 km section from the surface to a depth of 10 km. The results of this calculation show 50 μs two kilometers from the fault plane and 10 μs about 6 km from the fault plane. If these models were used for a 10 m fault movement instead of 1 m, the strains would be amplified proportionally because of the linearity of the elastic model. Therefore, for a bounding fault movement of 10 meters along Solitario Canyon fault, an elastic model would predict strains up to 500 μs two kilometers from the fault and 100 μs six kilometers from the fault. If the conservative assumption is made that all the strain accumulates in the fractures, then an estimate of the change in aperture can be made. First, assume a lower bound aperture of 100 μm in the present-day system (Sonnenthal et al. 1997; Table 7.12) and a fracture spacing of approximately 1 m (Sonnenthal et al. 1997; Table 7.7). Then a tensile strain of 500 μs would result in a new fracture aperture of about 600 μm. For a compressive strain of 500 μs, then the fractures would essentially be closed and the rock matrix would necessarily be compressed.

These results suggest that a factor of 10 change in aperture would bound the effects of tensile strain. In fact, because the average aperture at Yucca Mountain is approximately 200 μm (Sonnenthal et al. 1997; Table 7.12), a factor of 10 change would result in fractures with an average aperture of 2000 μm, or 2 mm. With regard to the reduction in aperture under compressive strain, other limitations constrain the change in fracture aperture. Attempts were made to use a factor of 10 reduction in aperture, however, convergence problems were encountered with the flow model. This is likely the result of insufficient bulk permeability in the system to accommodate the imposed infiltration flow conditions. Therefore, reductions in aperture were limited to factors of 0.2, and in the case of a wetter climate, the lowest value that could be used was a factor of 0.5.

6.2.1.6 Affected Parameters

Given a change in aperture, theoretical models are available to quantitatively model the associated changes in fracture permeability, fracture capillary pressure, and fracture porosity. Fracture aperture enters flow and transport modeling in different ways. Aperture affects the permeability and capillary pressure used for steady-state unsaturated flow calculations. For radionuclide transport calculations, the fracture aperture affects the fracture porosity. Fracture aperture also affects matrix diffusion for radionuclide transport, but for these simulations the matrix diffusion coefficient was set to zero (Section 5.4). The fracture apertures used in these different parameters are not necessarily the same because the theoretical models strictly apply to idealized "parallel plate" fractures. Therefore, the aperture for permeability, capillary pressure, and porosity are generally different values. However, we will assume that an increase or decrease in aperture will affect these physical characteristics in proportion to the functional dependence on aperture in the theoretical models.

The relationship for permeability, known as the cubic law, (Freeze and Cherry, Section 2.12; Sonnenthal et al., 1997, Section 7.5.4) is the following:

$$k = \overline{f}\frac{b^3}{12} \qquad \text{(Eq. 1)}$$

where $\overline{f}$ is the average fracture frequency, k is the permeability, and b is the fracture aperture. As can be seen, the permeability is proportional to the cube of the fracture aperture.

The relationship for capillary pressure (van Genuchten 1980; Sonnenthal, et al., 1997; Section 7.5.5) is the following:

$$P_c = \frac{2\tau\cos\theta}{b\rho g}\left[S_e^{-1/m} - 1\right]^{1/(1-m)} \qquad \text{(Eq. 2)}$$

where τ is the surface tension of an air/water interface, θ is the contact angle between the air/water interface and the mineral surface, ρ is the density of water, g is the acceleration of gravity, S_e is the effective water saturation (normalized for the residual and maximum saturations), and m is the shape parameter for the variation in capillary pressure with water saturation. The collection of terms, $\frac{b\rho g}{2\tau\cos\theta}$, is known as the van Genuchten α parameter. The van Genuchten α parameter scales the overall capillary pressure in the system. The parameter m accounts for the distribution of fracture apertures that the air/water interface encounters as a function of water saturation. As can be seen, the van Genuchten α parameter is directly proportional to fracture aperture.

The relationship for porosity, ϕ_f, is the following:

$$\phi_f = fb \qquad \text{(Eq. 3)}$$

The porosity is also found to be proportional to the fracture aperture.

Now, assume b is changed to b^*, then correspondingly k, α, and ϕ_f are changed to k^*, α^*, and ϕ_f^*. These variables can be used to express the following relationships:

$$k^* = (b^*/b)^3 k \qquad \text{(Eq. 4)}$$

$$\alpha^* = (b^* / b)\alpha \qquad \text{(Eq. 5)}$$

$$\phi_f^* = (b^* / b)\phi_f \qquad \text{(Eq. 6)}$$

The factor of change in fracture aperture (b*/b) is then used to directly assign the new values of permeability, capillary pressure (α), and porosity. From these relationships, it is apparent that to determine the change in permeability, capillary pressure, and porosity, it is only necessary to know the aperture ratio, not the aperture itself. Aperture is used directly in the transport model formulation for matrix diffusion (Zyvoloski et al., 1999; Section 8.3.3.2). However, the value of the aperture is not important for transport calculations in this analysis because the matrix diffusion coefficient is assumed to be zero (Section 5.4).

6.2.1.7 Calculation Procedures

Each calculation involves two major computer programs: TOUGH2/version-1.3 (Pruess 1987, 1991; Mishra 1998) and FEHM/version-2.0 (Zyvoloski et al. 1999). TOUGH2 with its EOS9 module (for single-phase unsaturated flow) is used for computing unsaturated flow fields. Through transient simulations, steady-state flow fields are obtained and used in subsequent transport simulations. FEHM performs specified particle-tracking calculations on the flow field calculated by TOUGH2. The software routine T2FEHM2 (Ho, 1997; DTN: SNT05091597001.002) is used for organizing TOUGH2 output into files ready for restarting FEHM particle-tracking calculations. Installation tests were performed for both of these software codes and the T2FEHM2 software routine.

The matrix and fracture parameter values both for the hydrogeologic units and the faults are taken from the base-case TSPA-VA UZ flow model (DTN: LB971212001254.001) and treated as the base-case for this study. Sensitivity cases are conducted using fracture apertures modified as discussed in Sections 6.2.1, 6.2.1.5 and 6.2.1.6. Flow and transport modeling calculations are performed for present-day and long-term average climates (Section 6.2.1). The UZ flow results from the base-case TSPA-VA UZ flow calculation are processed to obtain the initial condition for calculations involving cases affected by fault displacement.

The utility computer routines involved in the calculations include:

(a) extract_xd.f: For extracting sub-dimensional models out of the three-dimensional UZ model. The extraction is performed upon TOUGH2 MESH and GENER input sections. Other input sections for TOUGH2 are processed separately.

(b) va_ini_ext.f: For preparing the INCON section of the TOUGH2 input by extracting data from a previously converged TOUGH2 output file for a given grid.

(c) alt_tough2_aper.f: For altering seismically affected parameters in a TOUGH2 input file, using the factor of change in fracture aperture as the primary parameter. For each selected factor, fracture porosity, permeability, and van Genuchten α parameters are changed in accordance with equation (5). As a practice of preserving the computational setups for dual-permeability models in TOUGH2, the pure fracture volumes used in the TOUGH2 MESH section are also changed.

(d) fehm_post.f: For processing FEHM particle-tracking results into concentration histories synthesized for the entire system outlet. This program is in essence the same as the program 'bkpm.f' (DTN: MO9807MWDOFEHM.000). Modifications were made mainly to make the program capable of handling multiple species with variable number of input particles (irrelevant to this study).

Further descriptions of these software routines, including the source listings, are provided in Attachments I through IV.

The calculation input and output files for the calculations presented in Section 6.2.2 are available from the technical data base under the data tracking number MO9910MWDUZT20.001.

6.2.2 Results

The next three subsections describe the effects of fracture aperture changes on flow in the unsaturated zone and mass releases at the water table. Results for cases in which the fracture apertures are varied are compared with the corresponding base cases. The first subsection, 6.2.2.1, describes the effects of a change in fracture aperture on the flow conditions and on transport. The one-dimensional modeling is carried out for illustrative purposes to examine changes in key flow variables and their implications on transport as a result of changes in fracture aperture. Only the present-day climate is used for the one-dimensional calculations. The second subsection, 6.2.2.2, describes the results for transport in a two-dimensional model when fracture apertures are changed uniformly throughout the modeling domain. These calculations are performed for present-day and the wetter long-term-average climates. The third subsection, 6.2.2.3, describes the results for transport in a two-dimensional model when fracture apertures are only changed in the fault zones, not in the fractured rock. These calculations are also performed for present-day and the wetter long-term-average climates. Mass transport calculations correspond to the continuous release of 10^4 particles at the potential repository for a period of one year.

6.2.2.1 Fracture Apertures Altered Uniformly Across the Repository Block; One-Dimensional Calculations for Present-Day Climate

A one-dimensional model was extracted from the three-dimensional model (TSPA-VA three-dimensional UZ flow and transport model; DTN: LB971212001254.001) using the software routine extract_xd.f. This one-dimensional column is located in the TSPA-VA three dimensional model (DTN: LB971212001254.001), as identified in Figure 4 (see also Figure 1). The total water influx to the model for the present-day climate is 0.175×10^{-3} kg/s, which, with the horizontal area of the column being 10^4 m^2, corresponds to an infiltration of about 0.55 mm/year. Flow calculations for the one-dimensional model were performed using TOUGH2 and these flow fields were converted to input for FEHM using T2FEHM2. The breakthrough curves were computed using FEHM and post-processed using fehm_post.f. Calculations for altered fracture aperture cases were conducted by modifying the input data for TOUGH2 using the software routine alt_tough2_aper.f. The initial condition for the TOUGH2 calculations for the altered aperture cases was obtained using the output of TOUGH2 for the base case, post-processed by the software routine va_ini_ext.f for use as input to TOUGH2.

Figure 5 shows the breakthrough curves at the water table for three cases. When compared with the base case, although the effects are minor, the factor-of-0.2 case shows delayed breakthrough, whereas the factor-of-10 case shows earlier arrival.

These differences can be attributed to water saturation and flux distributions in the fractures and the matrix. The overall breakthrough times are long in this one-dimensional model due to the low infiltration rate at the location of this column (see Figure 4) under present-day climate. Figures 6 and 7 show the water saturation distributions. Note that the potential repository is located at an approximate elevation of 1100 meters. When fracture apertures are altered from the base case, matrix saturations show little or no change, whereas fracture saturations can be changed significantly. Specifically, for the factor-of-10 case, fracture saturation decreases by more than one-half of the base case saturation in the Topopah Spring welded unit, and increases slightly in the Calico Hills unit. Figures 8 and 9 show the water flux distributions along the column.

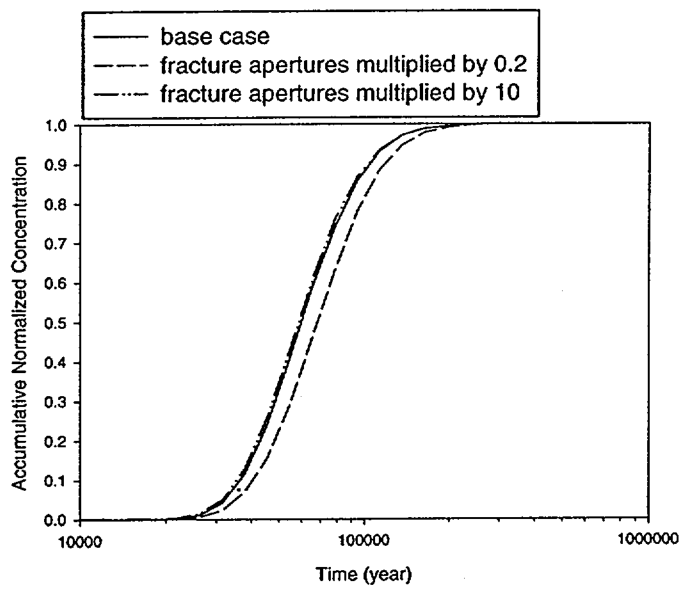

Figure 5. Breakthrough Curves for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

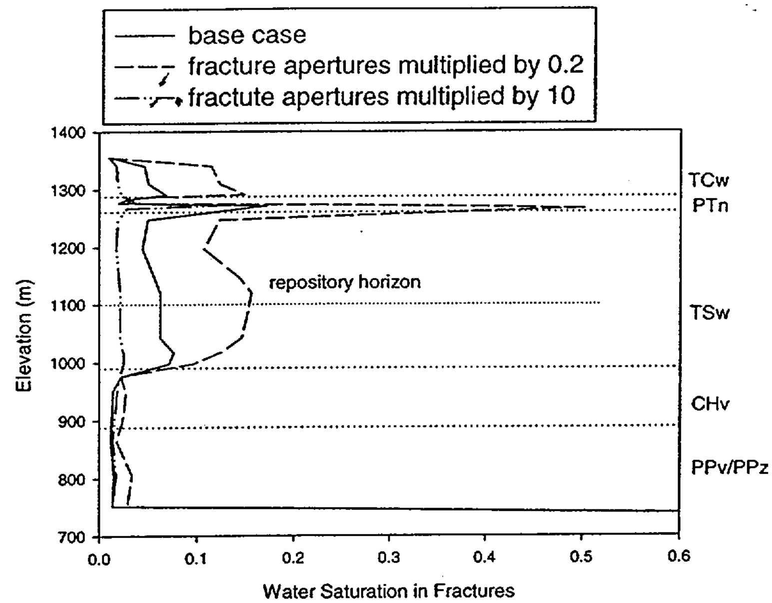

Figure 6. Water Saturation Distributions in the Fractures for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

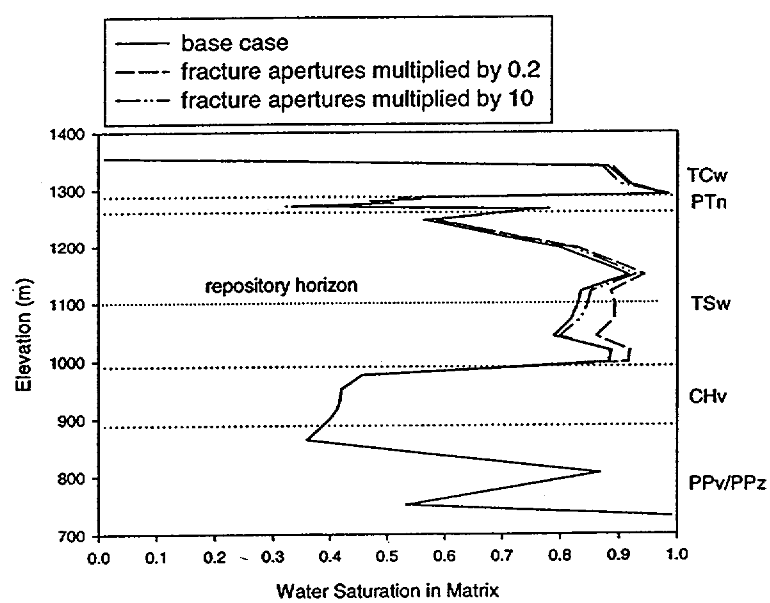

Figure 7. Water Saturation Distributions in the Matrix for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

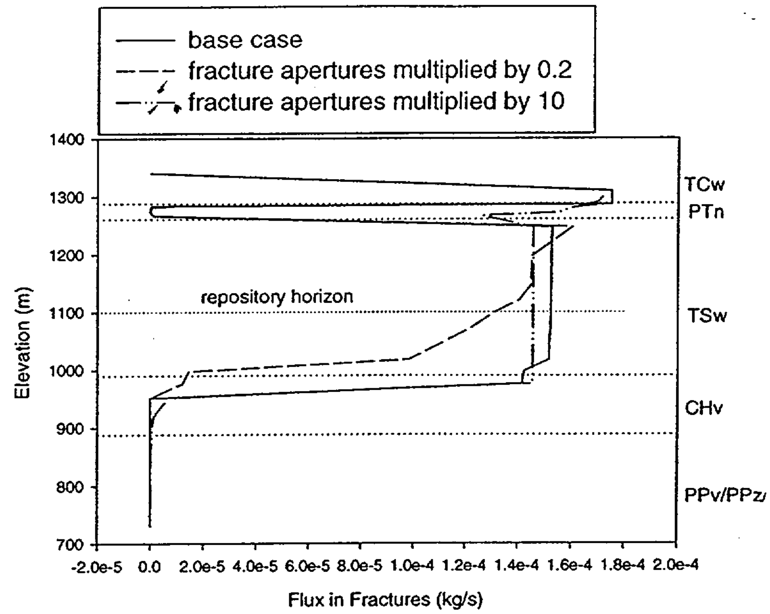

Figure 8. Water Flux Distributions in the Fractures for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

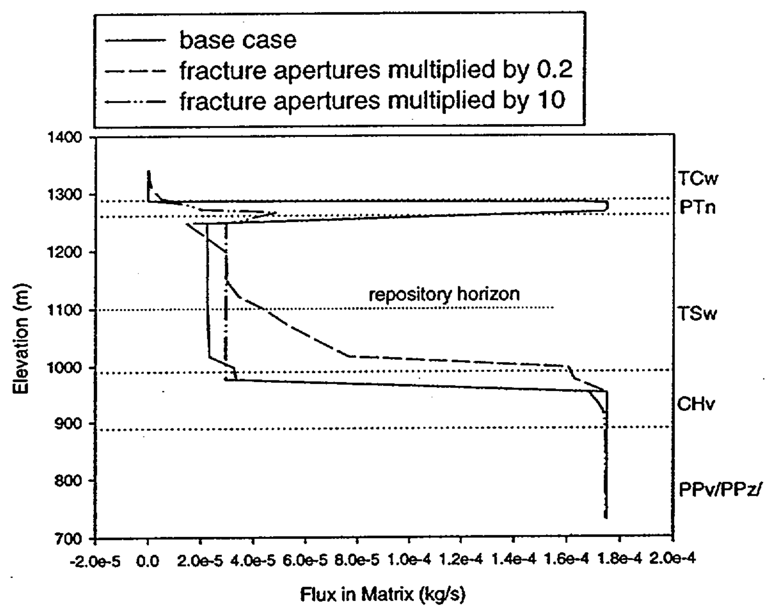

Figure 9. Water Flux Distributions in the Matrix for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

From these figures one can see that the matrix of the Calico Hills unit takes the majority of the total flux and thus controls the travel times of most particles. For the factor-of-0.2 case, the flux in the matrix of the Calico Hills unit is essentially identical to that for the base case. For the lower part of the Topopah Spring welded unit, there is more flux in the matrix (less flux in the fractures) than that for the base case. For the factor-of-10 case, there is a little less matrix flux and a little more fracture flux in the Calico Hills unit as compared with the base case. In the

Topopah Spring welded unit, the matrix flux is larger in the upper portion of the unit and smaller in the lower portion near the interface with the underlying Calico Hills unit, when compared with the base case. The reverse is true for fracture flux.

The driving force for partition of flux between the fractures and the matrix is the capillary pressure difference between the two media. Figures 10 and 11 show the capillary pressure distributions in the fractures and the matrix. Note that the plots stop just short of the water table at a nonzero capillary pressure. Shown in Figure 12 is the capillary pressure in the matrix minus the capillary pressure in the fractures. Specifically for the factor-of-10 case, capillary pressure in the matrix does not change much from the base case, whereas capillary pressure in the fractures has been reduced significantly. The capillary pressure difference between the matrix and the fractures increases in the Calico Hills unit, but remains almost unchanged in other units, when compared with the base case.

In summary, the Calico Hills unit is responsible for most of the travel time between the potential repository and the water table. As fracture aperture is increased, the amount of flux in the fractures of the Calico Hills unit increases slightly, with a corresponding decrease in the matrix flux. This increase in flux through the fractures in the Calico Hills for larger fracture apertures occurs despite the increase in the capillary pressure difference between the fractures and the matrix for larger fracture apertures. The explanation for this apparent anomaly is given in Section 6.2.3. The increase in fracture flux through the Calico Hills leads to a substantial decrease in travel time for a small fraction of the simulated tracer particles at the leading edge of the breakthrough curve and a small decrease in travel time for the vast majority of the simulated tracer particles.

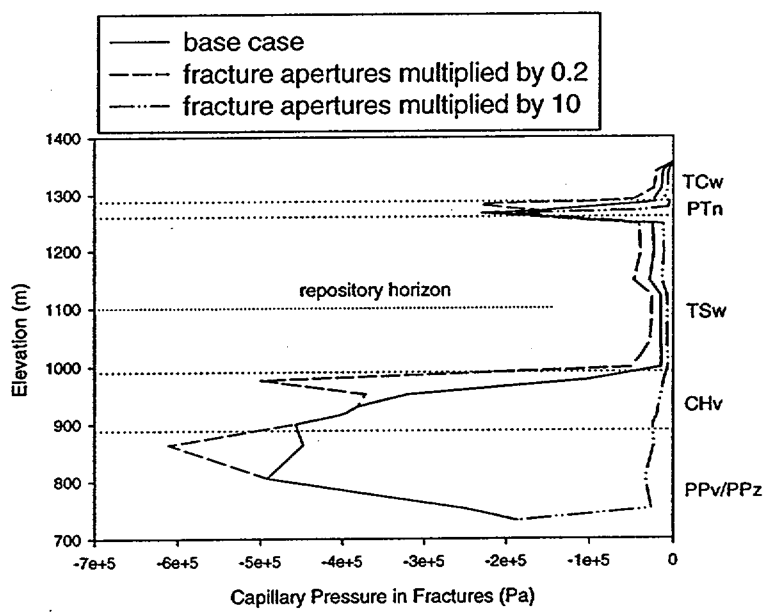

Figure 10. Capillary Pressure Distributions in the Fractures for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

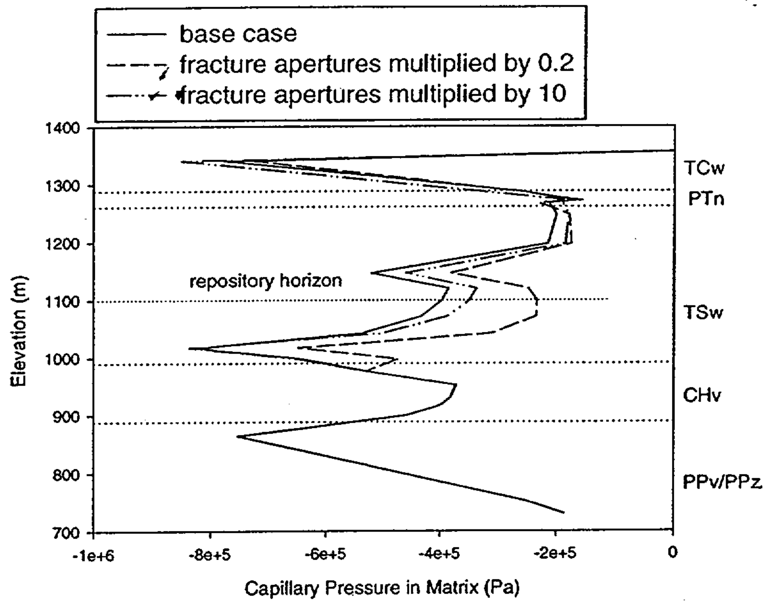

Figure 11. Capillary Pressure Distributions in the Matrix for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

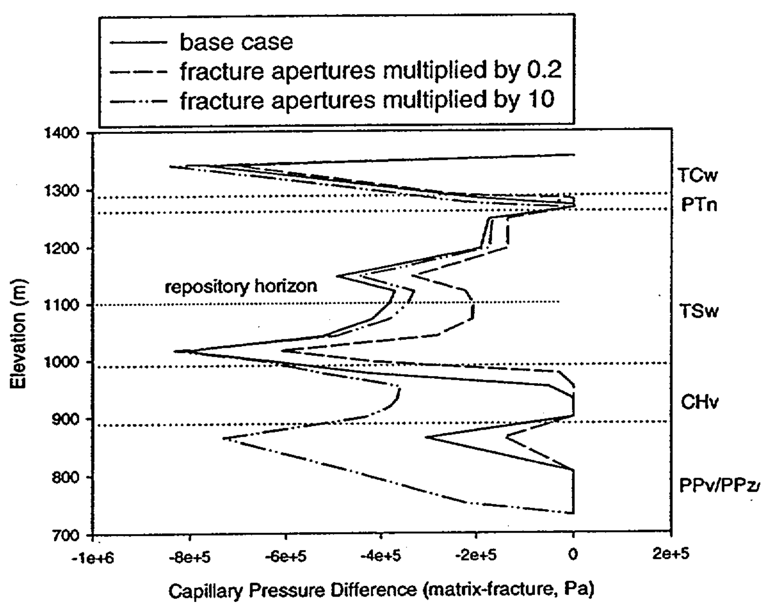

Figure 12. Capillary Pressure-Difference Distributions for the One-Dimensional Column Model under Present-Day Infiltration. DTN: MO9910MWDUZT20.001

6.2.2.2 Fracture Apertures Altered Uniformly Across the Repository Block; Two-Dimensional Calculations for Present-Day and Long-Term-Average Climate

Calculations for flow and transport were also conducted for the two-dimensional, vertical cross-section identified in Figure 4 (see also Figure 2). A two-dimensional model was extracted from the three-dimensional model (TSPA-VA three-dimensional UZ flow and transport model; DTN: LB971212001254.001) using the software routine extract_xd.f. As for the one-dimensional model, the transport calculations were performed for non-sorbing, non-diffusing particles released into the fracture nodes of the repository elements over a one-year period. The total water influx to the two-dimensional model for the present-day climate is 0.11471 kg/s (equivalent to 3.2 mm/yr on average). Flow calculations for the two-dimensional model were performed using TOUGH2 and these flow fields were converted to input for FEHM using T2FEHM2. The breakthrough curves were computed using FEHM and post-processed using fehm_post.f. Calculations for altered fracture aperture cases were conducted by modifying the input data for TOUGH2 using the software routine alt_tough2_aper.f. The initial condition for the TOUGH2 calculations for the altered aperture cases were obtained using the output of TOUGH2 for the base case, post-processed by the software routine va_ini_ext.f for use as input to TOUGH2.

Shown in Figure 13 are the cumulative breakthrough curves of four cases. Similar to the one-dimensional calculations, the factor-of-0.2 case has slightly delayed breakthrough, whereas the factor-of-5 and factor-of-10 cases have earlier arrivals when compared with the base case. Although the earlier arrival for the factor-of-5 case is barely visible on the scale of the figure, the earlier arrival for the factor-of-10 case has a plateau of about 4 percent of the total release. In other words, about 400 out of the 10^4 particles have bypassed the matrix of the Calico Hills unit and traveled through the aperture-increased fractures of the unit.

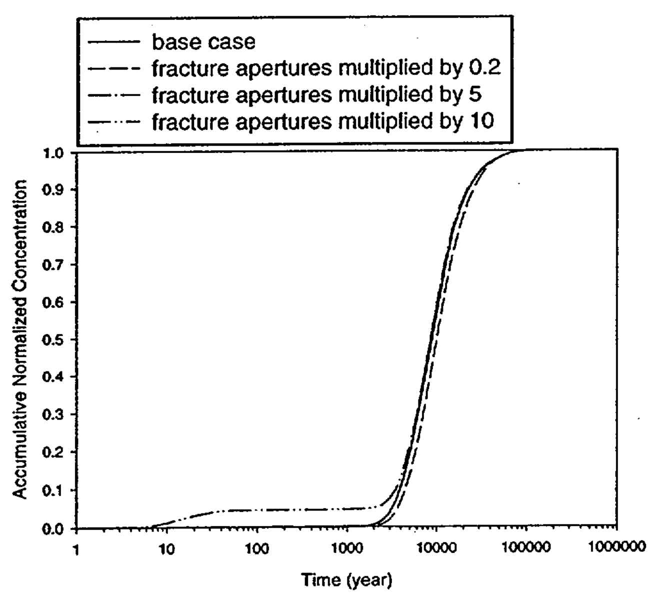

Figure 13. Breakthrough Curves for the Two-Dimensional Model under Present-Day Infiltration. Note that the x 5 curve overlies the base case. DTN: MO9910MWDUZT20.001

The total water influx to the model for the long-term-average climate is 0.98413 kg/s (equivalent to 27.3 mm/yr). As shown in Figure 14, due to the increase in water input, the travel times have decreased from those for the present-day climate. The results for different fracture apertures are similar in nature to those for the present-day climate, but the breakthroughs occur much earlier. For the factor-of-10 case, the plateau for early arrival becomes more pronounced, reaching about 12 percent of the total release. As compared with the present-day climate, the higher flux of this long-term-average climate has driven much earlier breakthroughs and has caused more particles to bypass the matrix through the fractures of the Calico Hills unit when fracture apertures are increased. As found for the present-day climate case, the effects of increased fracture aperture on the breakthrough characteristics are much less pronounced for the factor-of-5 case.

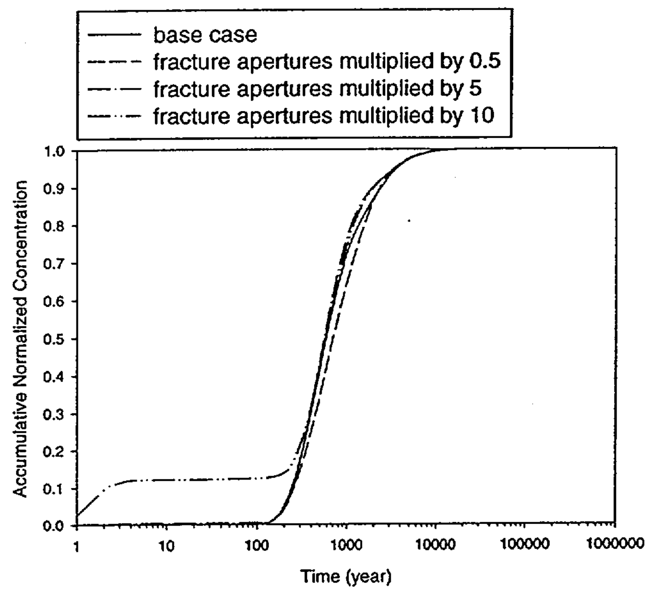

Figure 14. Breakthrough Curves for the Two-Dimensional Model under Long-Term-Average Infiltration. DTN: MO9910MWDUZT20.001

6.2.2.3 Fracture Apertures Altered in Fault Zones Only; Two-Dimensional Calculations for Present-Day and Long-Term-Average Climate

In this set of calculations, only the fracture apertures for the three fault zones are changed by given factors. Otherwise, the flow and transport calculations described in this section were performed in exactly the same manner as described in Section 6.2.2.2.

As shown in Figures 15 and 16, respectively, for the present-day climate and the long-term-average climate, the breakthroughs for the altered cases remain essentially unchanged from the base case. This indicates that if only the fault fracture apertures are affected by factors of 0.2 to 10, the impact to UZ flow and transport is negligible.

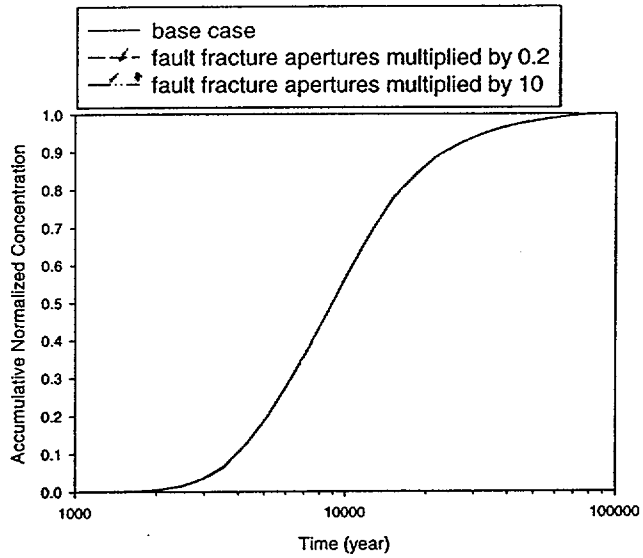

Figure 15. Breakthrough Curves for the Two-Dimensional Model under Present-Day Infiltration when Fault Fractures Are Altered. DTN: MO9910MWDUZT20.001

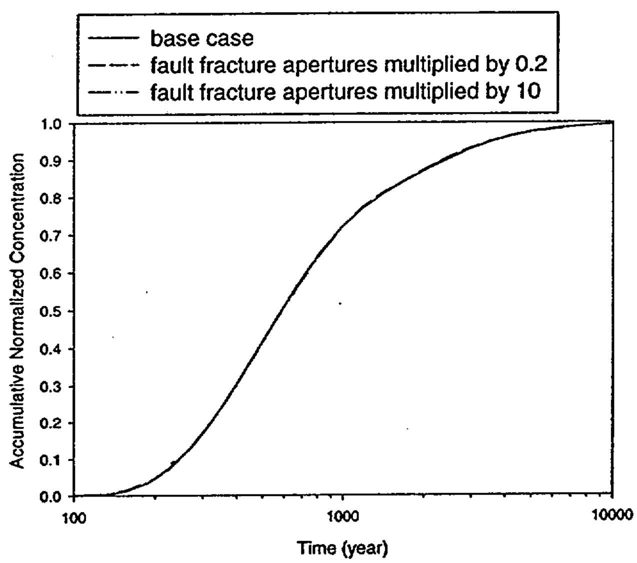

Figure 16. Breakthrough Curves for the Two-Dimensional Model under Long-Term-Average Infiltration when Fault Fractures Are Altered. DTN: MO9910MWDUZT20.001

6.2.3 Discussion

The effect of changing fracture apertures on the flow in different units is not consistent; in the Calico Hills unit the flow in the fractures increases with increased aperture, but the effects in the Topopah Spring unit are more complex. However, because travel time through the UZ is dominated by transport in the Calico Hills unit, the effect on mass transport reflects the trend observed in the flow; increased aperture leads to greater transport in fractures and shorter travel time to the water table. This leads to a consistent trend for simulated tracer breakthrough profiles at the water table. If the fracture apertures are decreased (increased), the travel times of the majority of the particles are only slightly increased (decreased), causing slightly delayed (earlier) breakthrough. In particular, when fracture apertures are increased, the travel times of some particles are dramatically decreased due to enhanced transport in the fractures, and the number of such faster-moving particles increases with increases in fracture apertures and input water flux. Within the current model, the matrix of the Calico Hills unit functions as the primary barrier to transport. When fracture apertures are enlarged to a sufficient degree, an increase in transport through fractures of the Calico Hills unit promotes visible changes to the breakthrough curves at early times. The two-dimensional model produced more significant early breakthroughs than the one-dimensional model, primarily because the input water flux is low in the one-dimensional model compared with the average input water flux in the two-dimensional model.

Capillary forces in the fractures of the dual-permeability model tend to work against fracture-matrix inter-flow and keep water flowing in the fractures. Note that fracture-matrix inter-flow is driven by the matrix-fracture capillary pressure difference. Assuming the inter-flow is from the fractures to the matrix, larger fracture apertures tend to promote fracture-to-matrix flow due to decreased fracture capillary pressure and essentially unchanged matrix capillary pressure (i.e. an increased matrix-fracture capillary pressure differential). The decreased capillary pressure in the fractures is roughly inversely proportional to the fracture aperture. However, due to the use of upstream weighting of the relative permeability in the numerical scheme of TOUGH2, the fracture relative permeability is used with the matrix absolute permeability to estimate the effective permeability of the fracture/matrix interface for fracture to matrix flow. The fracture relative permeability is the effective permeability for the fracture system at the given flow rate divided by the absolute permeability of the fracture system (i.e. a saturated fracture system). Thus, when the fracture apertures are increased, the fracture relative permeability (for about the same amount of fracture flow) decreases roughly in proportion to the cube of the aperture ratio. This is due to the fact that the effective permeability is roughly set by the amount of flow and the saturated permeability is proportional to the cube of the fracture aperture (see equation 1). Therefore, the fracture/matrix interface effective permeability is also reduced by this ratio. This reduction of the fracture/matrix interface effective permeability leads to greater flow and transport in the fractures of the Calico Hills when fracture apertures are increased.

7. CONCLUSIONS

Sensitivity studies for UZ flow and transport presented in this analysis suggest that transport between the potential repository and the water table is only weakly coupled to changes in fracture aperture. Overall, small changes in transport behavior are found for large changes in fracture aperture. Changes in fracture aperture confined to the fault zones show virtually no effect on transport behavior. Changes in fracture aperture, up to a five-fold increase over the entire UZ domain, show virtually no effect on transport behavior. Some early breakthrough, on the order of 10 percent or less, is found for a ten-fold increase in fracture aperture applied over the entire UZ domain. Such a large change in fracture apertures over the entire UZ domain is an extremely conservative scenario. Therefore, models for TSPA may exclude the effects of fault displacement on UZ transport.

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This analysis relies on several assumptions (Sections 5.8 through 5.10) which require verification, software which is still under development and has not been qualified (TOUGH2 v1.3 and FEHM v2.00), and uses unverified input data (LB971212001254.001). Therefore the resulting output and conclusions stated here require verification.

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ATTACHMENT I

SOFTWARE ROUTINE 'extract_xd.f'.

ATTACHMENT I

Software routine 'extract_xd.f v.1'

This routine is used for extracting sub-dimensional models out of the TSPA-VA three-dimensional UZ model. The extraction is performed upon TOUGH2 MESH and GENER input sections. Other input sections for TOUGH2 are processed separately. The code listing given below and files referred to in this Attachment may be found in the technical data base under the data tracking number MO9909MWDUZT20.000.

(1) Code listing:

```
c
c     To extract a (e.g., 2-D) grid out of a given (e.g., 3-D) grid.
c
c     input files: MESH file for the given grid.
c                  GENER file for the given grid.
c     output files: MESH file for the extracted grid.
c                   GENER file for the extracted grid.
c
c     kode =1, start extraction using two parameters: rloc & bound.
c          =2, start extraction from a given file of 'column indictors':
c              'zx_id?.txt'.
c          =3, start extraction from a given (1-D) column indicator:
c              colc & coln.
c
      double precision VOLX
      parameter(kode=2, rloc=2.32e05, bound=100.0)
      character dumele*5,EL*3,MA1*3,MA2*2,EL1*3,EL2*3
      character ELG*3,SL*3,TYPE*4,ITAB*1
      character colc*1
      data colc/'B'/,coln/40/
c  input files:
      open(11,file='mesh_bas.2k',status='old')
      open(21,file='qb.inf',status='old')
      if(kode.eq.2) open(31,file='zx_ida.txt',status='old')
c  output files:
      open(12,file='MESH.ext2a')
      open(13,file='MESH.tmp2a')
      open(14,file='GENER.ext2a')

      read(11,'(a5)') dumele
      write(12,'(a5)') dumele
50    read(11,'(a5)') dumele
      if(dumele.eq.'CONNE') then
        write(13,'(a3)') '+++'
        goto 120
      endif
      if(dumele.ne.'CONNE') backspace(11)
      read(11,100) EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
c       write(6,100) EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
100   FORMAT(A3,I2,2I5,A3,A2,2E10.4,10X,3f10.3)
      if(kode.eq.1) then
        if(abs(Y-rloc).le.bound) then
```

```
          write(12,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
          write(13,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
        endif
        goto 50
      endif
      if(kode.eq.2) then
        rewind (31)
102     read(31,'(A3,I2)') EL1,NE1
c          write(6,'(A3,I2)') EL1,NE1
        if(EL1.eq.'+++') goto 50
        if(EL1(3:3).eq.EL(3:3).and.NE1.eq.NE) then
          write(12,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
          write(13,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
          goto 50
        endif
        goto 102
      endif
      if(kode.eq.3) then
        if(EL(3:3).eq.colc.and.NE.eq.coln) then
          write(12,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
          write(13,100)EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
        endif
        goto 50
      endif
120   write(12,*)
      write(12,'(a5)') dumele
150   read(11,200) EL1,NE1,EL2,NE2,NSEQ,NAD1,NAD2,ISOT,D1,D2,
     +     AREAX,BETAX,ifm
200   FORMAT(A3,I2,A3,I2,4I5,4E10.4,I5)
      if(EL1.eq.'+++') then
        write(12,*)
        goto 360
      endif
      kode1=0
      kode2=0
      rewind(13)
250   read(13,100) EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
      if(EL.eq.'+++') goto 150
      if(EL.eq.EL1.and.NE.eq.NE1) kode1=1
      if(EL.eq.EL2.and.NE.eq.NE2) kode2=1
      if(kode1.eq.1.and.kode2.eq.1) then
         write(12,200) EL1,NE1,EL2,NE2,NSEQ,NAD1,NAD2,ISOT,
     +       D1,D2,AREAX,BETAX,ifm
         goto 150
      endif
      goto 250
360   read(21,*)
      write(14,'(a5)') 'GENER'
380   READ(21,400) ELG,NEG,SL,NS,NSEQ,NADD,NADS,LTAB,TYPE,ITAB,GX,EX,HX
400   FORMAT(A3,I2,A3,I2,4I5,5X,A4,A1,3E10.4)
      if(ELG.eq.'+++')  then
        write(14,*)
        close (12)
        close (14)
        stop
      endif
      rewind(13)
```

```
420    read(13,100) EL,NE,NSEQ,NADD,MA1,MA2,VOLX,AHTX,X,Y,Z
       if(EL.eq.'+++') goto 380
       if(ELG.eq.EL.and.NEG.eq.NE) then
         write(14,400)ELG,NEG,SL,NS,NSEQ,NADD,NADS,LTAB,TYPE,ITAB,GX,EX,HX
         goto 380
       endif
       goto 420

       end
```

(2) Example Input Files:

(a) mesh_bas.2k

A TOUGH2 MESH file for the TSPA-VA present-day climate 3-D UZ grid, containing ELEM and CONNE sections for element and connection definitions.

```
ELEME
Fi   1          tswF10.1206E+030.1000E+01           168400.500229900.000 1044.6900
Mi   1          tswM10.1352E+070.0000E+00           168400.000229900.000 1044.6900
Fj   1          tswF20.1046E+040.1000E+01           168400.500229900.000 1030.5200
...
FjB35           tswF20.4496E+020.1000E+01           171238.670231752.800 1199.3700
MjB35           tswM20.3485E+060.0000E+00           171238.170231752.800 1199.3700
...

CONNE
Fj   1Fi   1    0    0    0    30.1215E+020.2024E+010.3203E+060.1000E+01    1
Mj   1Mi   1    0    0    0    30.1215E+020.2024E+010.3203E+060.1000E+01    0
Fi   1Fi   2    0    0    0    10.3509E+030.3509E+030.1869E+040.1823E+00    1
...
FjB35FiB35      0    0    0    30.1688E+020.2814E+010.1031E+050.1000E+01    1
MjB35MiB35      0    0    0    30.1688E+020.2814E+010.1031E+050.1000E+01    0
...
```

(b) qb.inf

A TOUGH2 GENER file for the TSPA-VA present-day climate.

```
GENER - Infiltration: 4.9 mm/yr.
Fi   1                                      COM1 0.5333E-020.7561E+05
Fa   2                                      COM1 0.1250E-010.7561E+05
Fa   3                                      COM1 0.2611E-010.7561E+05
...
FaB35                                       COM1 0.9211E-030.7561E+05
FaB36                                       COM1 0.2337E-030.7561E+05
...
```

(c) zx_ida.txt

List of grid-blocks containing column identifiers for the 2-D cross section (Figure 1) sub-model to be extracted from the TSPA-VA 3-D UZ grid.

```
TP   4
TP  29
```

```
TP 49
TP 70
TP 90
TPB49
TPB48
TPB47
TPB46
TPB45
TPB44
TPB43
TPB42
TPB41
TPB40
TPB39
TPB38
TPB37
TPB36
TPB35
TP229
TP259
TP3 0
TP349
TP397
TP413
TP475
TP522
TP541
TP589
TP6 7
TP633
TP669
TP683
+++
```

(3) Example Output Files:

(a) mesh.ext2a

A TOUGH2 MESH file for the extracted 2-D sub-model.

```
ELEME
Fa   4      0      0tcwF10.2968E+040.1000E+01          168600.500231800.000  1344.840
Ma   4      0      0tcwM10.1274E+080.0000E+00          168600.000231800.000  1344.840
Fb   4      0      0tcwF20.3809E+040.1000E+01          168600.500231800.000  1285.550
...
FjB35       0      0tswF20.4496E+020.1000E+01          171238.672231752.797  1199.370
MjB35       0      0tswM20.3485E+060.0000E+00          171238.172231752.797  1199.370
...

CONNE
Fb   4Fa   4     0    0    0    30.2964E+020.2964E+020.2229E+060.1000E+01    1
Mb   4Ma   4     0    0    0    30.2964E+020.2964E+020.2229E+060.1000E+01    0
Fa   4Fa  29     0    0    0    10.3000E+030.3000E+030.1693E+05-.1926E+00    1
...
FjB35FiB35       0    0    0    30.1688E+020.2814E+010.1031E+050.1000E+01    1
MjB35MiB35       0    0    0    30.1688E+020.2814E+010.1031E+050.1000E+01    0
...
```

(b) gener.ext2a

A TOUGH2 GENER file for the extracted 2-D sub-model.

```
GENER
Fa 4   0  0  0  0  1   COM1 0.3585E-010.7561E+050.0000E+00
Fa 29  0  0  0  0  1   COM1 0.1149E-010.7561E+050.0000E+00
Fa 49  0  0  0  0  1   COM1 0.1253E-060.7561E+050.0000E+00
...
FaB35  0  0  0  0  1   COM1 0.9211E-030.7561E+050.0000E+00
FaB36  0  0  0  0  1   COM1 0.2337E-030.7561E+050.0000E+00
...
```

(4) Verification:

'FjB35', 'FjB35FiB35' and their associated data in the output file 'mesh.ext2a' are picked up by the program from the input file 'mesh_bas.2k', because the column identifier 'B35' exists in the input file 'zx_ida.txt'.

'FaB35' and its associated data including the infiltration rate '0.9211E-03 (kg/s)' in the output file 'gener.ext2a' are picked up from the input file 'qb.inf', because the column identifier 'B35' exists in the input file 'zx_ida.txt'.

(5) Range of Validation:

This software routine is valid for extracting 2D cross-sectional or 1D column models from any 3D TOUGH2 MESH or GENER files.

ATTACHMENT II

SOFTWARE ROUTINE 'va_ini_ext.f'.

ATTACHMENT II

Software routine 'va_ini_ext.f V.1'

This routine is used for preparing the INCON section of the TOUGH2 input by extracting data from a previously converged TOUGH2 output file (e.g., an output from TSPA-VA), for a given grid. The code listing given below and files referred to in this Attachment may be found in the technical data base under the data tracking number MO9909MWDUZT20.000.

(1) Code listing:

```
c
c     To get INCON by using a VA TOUGH2 output file.
c
      parameter(por_tp=0.20,por_bt=0.28)
      character*20 file_va,file_ini,file_mesh,file_va_trx
      character ele_name*5, ele_dum*6, dum*1, dum_char*80, ele_namex*5
      logical file13

      write(*,*) 'kode=3, 3D model, no truncation'
      write(*,*) 'kode=1 or 2, 1D or 2D model, need truncation'
      read(*,*) kode
      if(kode.ne.3) then
        write(*,*) 'MESH file for the truncated model: file_mesh'
        read(*,'(a20)') file_mesh
        open(14,file=file_mesh)
        write(*,*) 'truncated INCON: file_va_trx'
        read(*,'(a20)') file_va_trx
        open(15,file=file_va_trx)
      endif
      write(*,*) '3D INCON file to be generated: file_ini'
      write(*,*) '(if already exist, still input the file name)'
      read(*,'(a20)') file_ini
      inquire(file=file_ini,exist=file13)
      if(file13.and.kode.ne.3) then
         open(13,file=file_ini,status='old')
         goto 400
      endif
      if(file13.and.kode.eq.3) stop
c
c generate INCON for the 3D model using VA TOUGH2 output:
c
      open(13,file=file_ini)
      write(13,'(a5)') 'INCON'
      write(*,*) 'VA TOUGH2 output file: file_va'
      read(*,'(a20)') file_va
      open(12,file=file_va,status='old')
      100   read(12,'(a6)') ele_dum
      if(ele_dum.ne.' ELEM.') goto 100
      read(12,*)
      read(12,*)
150   read(12,'(a6)') ele_dum
      if(ele_dum.eq.' @@@@@') then
        write(13,*)
        close(12)
```

```
          if(kode.ne.3) goto 400
          stop
        endif
        if(ele_dum(2:6).eq.'ELEM.') then
          read(12,*)
          read(12,*)
          read(12,180) dum,ele_name,ind,pre,sat
        else
          backspace(12)
          read(12,180) dum,ele_name,ind,pre,sat
        endif
180     format(A1,A5,I6,2E12.5)
        por=0.
        if(ele_name(1:2).eq.'TP') por=por_tp
        if(ele_name(1:2).eq.'BT') por=por_bt
        if(abs(sat-1.0).le.1e-05) sat=0.999
        if(ele_name.ne.'     ') write(13,200) ele_name,por,sat,0,0,0
200     FORMAT(A5,10X,E15.8/(5E20.13))
        goto 150
c
c truncation:
c
400     read(14,*)
        write(15,'(a5)') 'INCON'
450     read(14,'(a5)') ele_name
        if(ele_name.eq.'     ') then
          write(15,*)
          close(13)
          close(14)
          close(15)
          stop
        endif
        rewind(13)
        read(13,*)
500     read(13,'(a5)') ele_namex
        if(ele_namex.eq.'     ') goto 450
        if(ele_namex.eq.ele_name) then
          backspace(13)
          read(13,'(a80)') dum_char
          write(15,'(a80)') dum_char
          read(13,'(a80)') dum_char
          write(15,'(a80)') dum_char
          goto 450
        else
          read(13,*)
        goto 500
        endif
        end
```

(2) Example Input Files:

(a) mnaqb_p.out

A TSPA-VA TOUGH2 output file for the present-day climate 3-D UZ model.

```
# input file for mean alpha, fitted fmx, present day q, ysw # AR 11/19/97
```

```
        OUTPUT DATA AFTER ( 200,  2)-2-TIME STEPS
THE TIME IS  0.73116E+10 DAYS

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M
MAX. RES.       NER    KER        DELTEX
  0.63172E+15    200      2    790     2       0.48677E+03  0.00000E+00  0.00000E+00
0.55870E-01     ****     1      0.50065E+06

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM.  INDEX   PRES         S(liq)       PCAP         K(rel)       DIFFUS.      Sf
Sm
                (PA)                      (PA)                      (m^2/s)

 Fi  1      1 0.92000E+05 0.18210E+00 -.16368E+06 0.67744E-04 0.80184E-07 0.18210E+00
0.18210E+00
 Mi  1      2 0.92000E+05 0.78032E+00 -.18936E+06 0.57954E-02 0.98985E-08 0.78032E+00
0.78032E+00
 Fj  1      3 0.92000E+05 0.48700E-01 -.25306E+05 0.80731E-07 0.44038E-10 0.48700E-01
0.48700E-01
...
FjB35 14247 0.92000E+05 0.71545E-01 -.15546E+05 0.68155E-06 0.14391E-09 0.71545E-01
0.71545E-01
MjB35 14248 0.92000E+05 0.58430E+00 -.17889E+06 0.97586E-03 0.20648E-08 0.58430E+00
0.58430E+00
...
```

(c) mesh.ext2a

A TOUGH2 MESH file for the extracted 2-D model.

See the listing in Appendix I.

(3) Example Output Files:

(a) INCON.va

A TOUGH2 INCON file for the 3-D grid, generated from 'mnaqb_p.out'.

```
INCON
Fi  1            0.00000000E+00
 0.1820999979973E+00 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
Mi  1            0.00000000E+00
 0.7803199887276E+00 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
Fj  1            0.00000000E+00
 0.4870000109076E-01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
...
FjB35            0.00000000E+00
 0.7154499739408E-01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
MjB35            0.00000000E+00
 0.5842999815941E+00 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
...
```

(b) INCON.va_tr2a

A TOUGH2 INCON file generated for the extracted 2-D model.

```
INCON
Fa   4             0.00000000E+00
 0.6924600154161E-01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
Ma   4             0.00000000E+00
 0.8419399857521E+00 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
Fb   4             0.00000000E+00
 0.7574599981308E-01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
...
FjB35              0.00000000E+00
 0.7154499739408E-01 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
MjB35              0.00000000E+00
 0.5842999815941E+00 0.0000000000000E+00 0.0000000000000E+00 0.0000000000000E+00
...
```

(4) Verification:

'FjB35' and its associated data including the water saturation '0.7154E-01' in the output file 'INCON.va' are correctly picked up from the input file 'mnaqb_p.out'.

'FjB35' and its associated data including the water saturation '0.7154E-01' in the output file 'INCON.va_tr2a' are picked up from 'INCON.va', because 'FjB35' exists in the input file 'mesh.ext2a'.

(5) Range of Validation:

This software routine is valid for preparing a TOUGH2 INCON file in 1D, 2D, or 3D from any TOUGH2 - EOS 9 3D output files.

ATTACHMENT III

SOFTWARE ROUTINE 'alt_tough2_aper.f'.

ATTACHMENT III

Software routine 'alt_tough2_aper.f v.1'

This routine is used for altering seismically affected parameters in a TOUGH2 input file, using the factor of change in fracture aperture as the primary parameter. For each selected factor, fracture porosity, permeability, and van Genuchten air-entry scaling parameters are changed in accordance with equations (4) to (6) in Section 6.2.1.6. As a practice of preserving the computational setups for dual-permeability models in TOUGH2, the pure fracture volumes used in the TOUGH2 MESH section are also changed. The code listing given below and files referred to in this Attachment may be found in the technical data base under the data tracking number MO9909MWDUZT20.000.

(1) Code Listing:

```
c
c     To alter hydrologic parameters for TOUGH2,
c     due to changes in fracture aperatures.
c
c     input files: --- tough2.inp containing 'ROCKS' section of data.
c                  --- altmat_aper.dat, containing material names for which
c                      the fracture apertures are to be altered.

c                 --- MESH.org, MESH file.
c
c     output files: --- tough2.inp_alt, containing altered 'ROCKS' section.
c                 --- MESH.alt, MESH file containing altered fracture volumes.
c
c     kode =1, do not alter fracture volume, but alter fracture porosity;
c          =2, do not alter fracture porosity, but alter fracture volume.
c
      parameter (mxmat_alt=200,mrock=200)
      double precision VOLX
      character dumele*5,EL*3,MATR*5,EL1*3,EL2*3
      character*5 rmat(mxmat_alt),MAT(mrock)
      character*80 dum_char
      character*40 file_in,file_out,file_alt,file_mesh,file_mesh_alt
      dimension DM(mrock),POR(mrock),PER(3,mrock),
     +      CWET(mrock),SH(mrock)
      dimension COM(mrock),EXPAN(mrock),CDRY(mrock),
     +      TORT(mrock),GK(mrock),perf(3,mrock)
      dimension RP(7,mrock),CP(7,mrock),IRP(mrock),ICP(mrock)
      dimension factor(mxmat_alt)

      write(6,*) 'input: kode'
      write(6,*) 'kode =1, do not alter fracture volume,'
      write(6,*) '         but alter apparent fracture porosity;'
      write(6,*) 'kode =2, do not alter apparent fracture porosity,'
      write(6,*) '         but alter fracture volume.'
      read(6,'(I1)') kode
      write(6,*) 'TOUGH2 input file containing ROCKS: file_in:'
      read(6,'(a40)') file_in
      write(6,*) 'Altered TOUGH2 input file: file_out:'
      read(6,'(a40)') file_out
```

```
      write(6,*) 'Altered parameter file: file_alt:'
      read(6,'(a40)') file_alt
      if(kode.eq.2) then
        write(6,*) 'Unaltered MESH file for the model: file_mesh'
        read(6,'(a40)') file_mesh
        write(6,*) 'Altered MESH file: file_mesh_alt'
        read(6,'(a40)') file_mesh_alt
      endif

      open(11,file=file_in, status='old')
      open(12,file=file_alt, status='old')
      open(13,file=file_out)
      if(kode.eq.2) then
        open(14,file=file_mesh, status='old')
        open(15,file=file_mesh_alt)
      endif
      read(12,*)
      read(12,*) nmat_alt
      do i=1,nmat_alt
        read(12,*) rmat(i),factor(i)
cc      Write(*,*) rmat(i),factor(i)
      enddo
      read(11,'(a80)') dum_char
      write(13,'(a80)') dum_char
      read(11,'(a80)') dum_char
      write(13,'(a80)') dum_char
C*****READ ROCK PROPERTIES.*********************************************
      NM=1
300   READ(11,200) MAT(NM),NAD,DM(NM),POR(NM),(PER(I,NM),I=1,3),
     +     CWET(NM),SH(NM)
200   FORMAT(A5,I5,7E10.3)
      if(MAT(NM).eq.'REFCO') write(13,200) MAT(NM),NAD,DM(NM),
     +     POR(NM),(PER(I,NM),I=1,3),CWET(NM),SH(NM)
      IF(MAT(NM).EQ.'     ') GOTO 450

      COM(NM)=0.D0
      EXPAN(NM)=0.D0
      CDRY(NM)=0.D0
      TORT(NM)=0.D0
      GK(NM)=0.D0
      IRP(NM)=0
      ICP(NM)=0
      perf(1,nm)=0.0
      perf(2,nm)=0.0
      perf(3,nm)=0.0
      IF(NAD.GE.1) then
      READ(11,220) COM(NM),EXPAN(NM),CDRY(NM),TORT(NM),GK(NM),
     + (perf(i,nm),i=1,3)
      ENDIF
220   FORMAT(8E10.3)
c
      IF(NAD.LE.1) GOTO 280
C-----READ PARAMETERS FOR RELATIVE PERMEABILITY AND CAPILLARY PRESSURE.
      READ(11,260) IRP(NM),(RP(I,NM),I=1,7)
      READ(11,260) ICP(NM),(CP(I,NM),I=1,7)
260   FORMAT(I5,5X,7E10.3)
C
```

```
      do i=1, nmat_alt
        if(MAT(NM).eq.rmat(i)) then
          if(kode.eq.1) POR(NM)=POR(NM)*factor(i)
          perf(3,NM)=perf(3,NM)*factor(i)
          CP(3,NM)=CP(3,NM)*factor(i)
          do j=1,3
            PER(j,NM)=PER(j,NM)*(factor(i)*factor(i)*factor(i))
          enddo
          goto 270
        endif
      enddo

270   write(13,200) MAT(NM),NAD,DM(NM),POR(NM),(PER(I,NM),I=1,3),
     +      CWET(NM),SH(NM)
      WRITE(13,220) COM(NM),EXPAN(NM),CDRY(NM),TORT(NM),GK(NM),
     +       (perf(i,nm),i=1,3)
      write(13,260) IRP(NM),(RP(I,NM),I=1,7)
      write(13,260) ICP(NM),(CP(I,NM),I=1,7)
C
280   NM=NM+1
      GOTO 300
450   NM=NM-1
      write(13,*)
500   read(11,'(a80)') dum_char
      write(13,'(a80)') dum_char
      if (dum_char(1:5).eq.'ENDCY') then
        write(13,*)
        close(11)
        close(12)
        close(13)
        if(kode.eq.2) goto 600
        stop
      endif
      goto 500
600   read(14,'(a5)') dumele
      write(15,'(a5)') dumele
50    read(14,'(a5)') dumele
      if(dumele.eq.'CONNE') then
        backspace(15)
        write(15,*)
        goto 120
      endif
      backspace(14)
      read(14,100) EL,NE,NSEQ,NADD,MATR,VOLX,AHTX,X,Y,Z
100   FORMAT(A3,I2,2I5,A5,2E10.4,10X,3f10.3)
      do i=1, nmat_alt
        if(MATR.eq.rmat(i)) then
          do k=1,NM
            if(MATR.eq.MAT(k)) then
              kk=k
              goto 103
            endif
          enddo
103       VOLX=VOLX*factor(i)
          goto 110
        endif
      enddo
```

```
110   write(15,100) EL,NE,NSEQ,NADD,MATR,VOLX,AHTX,X,Y,Z
      goto 50
120   write(15,'(a5)') dumele
150   read(14,700) EL1,NE1,EL2,NE2,NSEQ,NAD1,NAD2,ISOT,D1,D2,
     +      AREAX,BETAX,ifm
700   FORMAT(A3,I2,A3,I2,4I5,4E10.4,I5)
      write(15,700) EL1,NE1,EL2,NE2,NSEQ,NAD1,NAD2,ISOT,D1,D2,
     +      AREAX,BETAX,ifm
      if(EL1.eq.'+++'.or.EL1.eq.'    ') then
        backspace(15)
        write(15,*)
        close(14)
        close(15)
        stop
      endif
      goto 150
      end
```

(2) Example Input Files:

(a) tough2.inp2a
A TOUGH2 input file for the base case 2-D model.

```
# input file for mean alpha, fitted fmx, present day q, ysw # AR 11/19/97
ROCKS from inversion "itough2 p9mnmni p9mnmn  9"  Date: 19-Nov-97  09:17
tcwM1   2 2480.  0.6600E-010.5370E-170.5370E-170.5370E-17 1.660    847.0
              0.7200  0.7000
   7   0.2317   0.1300   1.000   0.2000E-01       0.8001E-02
   7   0.2317   0.1300   0.1175E-050.1000E+11 1.000
tcwM2   2 2480.  0.6600E-010.5370E-170.5370E-170.5370E-17 1.880    837.0
              1.2800  0.7000
   7   0.2362   0.1300   1.000   0.2000E-01       0.8001E-02
   7   0.2362   0.1300   0.1318E-050.1000E+11 1.000
tcwM3   2 2480.  0.1400   0.4898E-160.4898E-160.4898E-160.9800    857.0
              0.5400  0.7000
   7   0.4269   0.3300   1.000   0.2000E-01       0.8001E-02
   7   0.4269   0.3300   0.6456E-060.1000E+11 1.000
...
tcwF3   2 2480.   1.000   0.2399E-120.2399E-120.2818E-110.9800    857.0
              0.5400  0.7000                  7.0500e-05
   7   0.4920   0.1000E-01 1.000   0.2000E-01       0.8001E-02
   7   0.4920   0.1000E-010.8100E-030.1000E+11 1.000
ptnF1   2 2300.   1.000   0.5248E-120.5248E-120.5248E-120.5000    1080.
              0.3500  0.7000                  4.8400e-05
   7   0.4920   0.1000E-01 1.000   0.2000E-01       0.8358
   7   0.4920   0.1000E-010.1310E-020.1000E+11 1.000
...
```

(b) mesh.ext2a
A TOUGH2 MESH file for the base case 2-D model.
See the listing in Appendix I.

(c) alt_aper.dat
Factors of change in fracture apertures prescribed for various units of the UZ model.

```
altered units and the altered factors:
44
tcwFg       5.0
ptnFg       5.0
tswFg       5.0
chnFg       5.0
tcwFi       5.0
ptnFi       5.0
tswFi       5.0
chnFi       5.0
tcwFd       5.0
ptnFd       5.0
tswFd       5.0
chnFd       5.0
tcwFs       5.0
ptnFs       5.0
tswFs       5.0
chnFs       5.0
tcwF1          5.0
tcwF2          5.0
tcwF3          5.0
ptnF1          5.0
ptnF2          5.0
ptnF3          5.0
ptnF4          5.0
ptnF5          5.0
tswF1          5.0
tswF2          5.0
tswF3          5.0
tswF4          5.0
tswF5          5.0
tswF6          5.0
tswF7          5.0
ch1Fv          5.0
ch2Fv          5.0
ch3Fv          5.0
ch4Fv          5.0
ch1Fz          5.0
ch2Fz          5.0
ch3Fz          5.0
ch4Fz          5.0
pp3Fv          5.0
pp2Fz          5.0
bf3Fv          5.0
bf2Fz          5.0
tm3Fv          5.0
```

(3) Example Output Files:

(a) tough2.inp2a_5
The TOUGH2 input file with its fracture hydrological parameters being altered in accordance with equation (2) when fracture apertures are multiplied by a factor of 5.

```
# input file for mean alpha, fitted fmx, present day q, ysw # AR 11/19/97
ROCKS from inversion "itough2 p9mnmni p9mnmn 9" Date: 19-Nov-97 09:17
tcwM1    2 0.248E+04 0.660E-01 0.537E-17 0.537E-17 0.537E-17 0.166E+01 0.847E+03
 0.000E+00 0.000E+00 0.720E+00 0.700E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   7     0.232E+00 0.130E+00 0.100E+01 0.200E-01 0.000E+00 0.800E-02 0.000E+00
   7     0.232E+00 0.130E+00 0.117E-05 0.100E+11 0.100E+01 0.000E+00 0.000E+00
```

```
tcwM2   2 0.248E+04 0.660E-01 0.537E-17 0.537E-17 0.537E-17 0.188E+01 0.837E+03
 0.000E+00 0.000E+00 0.128E+01 0.700E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   7     0.236E+00 0.130E+00 0.100E+01 0.200E-01 0.000E+00 0.800E-02 0.000E+00
   7     0.236E+00 0.130E+00 0.132E-05 0.100E+11 0.100E+01 0.000E+00 0.000E+00
tcwM3   2 0.248E+04 0.140E+00 0.490E-16 0.490E-16 0.490E-16 0.980E+00 0.857E+03
 0.000E+00 0.000E+00 0.540E+00 0.700E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   7     0.427E+00 0.330E+00 0.100E+01 0.200E-01 0.000E+00 0.800E-02 0.000E+00
   7     0.427E+00 0.330E+00 0.646E-06 0.100E+11 0.100E+01 0.000E+00 0.000E+00
...
tcwF3   2 0.248E+04 0.100E+01 0.300E-10 0.300E-10 0.352E-09 0.980E+00 0.857E+03
 0.000E+00 0.000E+00 0.540E+00 0.700E+00 0.000E+00 0.000E+00 0.000E+00 0.353E-03
   7     0.492E+00 0.100E-01 0.100E+01 0.200E-01 0.000E+00 0.800E-02 0.000E+00
   7     0.492E+00 0.100E-01 0.405E-02 0.100E+11 0.100E+01 0.000E+00 0.000E+00
ptnF1   2 0.230E+04 0.100E+01 0.656E-10 0.656E-10 0.656E-10 0.500E+00 0.108E+04
 0.000E+00 0.000E+00 0.350E+00 0.700E+00 0.000E+00 0.000E+00 0.000E+00 0.242E-03
   7     0.492E+00 0.100E-01 0.100E+01 0.200E-01 0.000E+00 0.836E+00 0.000E+00
   7     0.492E+00 0.100E-01 0.655E-02 0.100E+11 0.100E+01 0.000E+00 0.000E+00
...
```

(b) mesh.ext2a_5
The TOUGH2 MESH file corresponding to the case when fracture apertures are multiplied by a factor of 5.

```
ELEME
Fa   4     0     0tcwF10.1484E+050.1000E+01          168600.500231800.000   1344.840
Ma   4     0     0tcwM10.1274E+080.0000E+00          168600.000231800.000   1344.840
Fb   4     0     0tcwF20.1905E+050.1000E+01          168600.500231800.000   1285.550
...
FjB35      0     0tswF20.2248E+030.1000E+01          171238.672231752.797   1199.370
MjB35      0     0tswM20.3485E+060.0000E+00          171238.172231752.797   1199.370
...
```

(4) Verification:

The data associated with the material identifier 'tcwF3' in the output file 'tough2.inp2a_5' are taken or modified from the input file 'tough2.inp2a'. The modifications are performed in accordance with equations (4) to (6) in Section 6.2.1.6 using the factor of 5 as given in the input file 'alt_aper.dat' for 'tcwF3'. For example, the porosity is changed from '7.05E05' in 'tough2.inp2a' to '0.353E03' in 'tough2.inp2a_5', and the permeability in the vertical direction is changed from '0.2818E-11 (m^2)' in 'tough2.inp2a' to '0.352E-09 (m^2)' in 'tough2.inp2a_5'.

The data in the output file 'mesh.ext2a_5' are taken or modified from the input file 'mesh.ext2a'. The modification concerns the element volume in the 'ELEME' section: for element 'FjB35', '0.2248E03' in the output file 'mesh.ext2a_5' is obtained by multiplying '0.4496E02' in the input file ''mesh.ext2a' by a factor of 5 as given in the input file 'alt_aper.dat' for the material identifier 'tswF2'. Since the volume for the corresponding matrix element 'MjB35' is several orders of magnitude larger, the effect due to fracture aperture change is ignored.

(5) Range of Validation:

This software routine is valid for modifying any TOUGH2 input file using the dual-permeability model with the van Genuchten capillary pressure and relative permeability functions to account for a change fracture aperture by some multiplicative scaling factor.

ATTACHMENT IV

SOFTWARE ROUTINE 'fehm_post.f'

ATTACHMENT IV

Software routine 'fehm_post.f v.1'

This routine is used for processing FEHM particle-tracking results into cumulative breakthrough histories synthesized for the entire system outlet. Modifications were made mainly to make the program capable of handling multiple species with variable number of input particles (irrelevant to this study). The code listing given below and files referred to in this Attachment may be found in the technical data base under the data tracking number MO9909MWDUZT20.000.

(1) Code Listing:

```
      parameter(cmin=1.e-10,max_spec=10)
      character*80 line,prx*5,cidx*5,title*31
      character*60 outfile,fout*10,dfile*30,ctmp
      real*8 time,time_old(max_spec)
      double precision total(max_spec),conc,rate_const(max_spec)
      integer entered,cur_in,left,tot_entered,decayed
      integer left_old(max_spec)
      character*6 spacer2
      do i=1,max_spec
      time_old(i)=0.
      left_old(i)=0.
      rate_const(i)=0.
      enddo
      ifehm=2
      prx='spec_'
      title='Particle Tracking ==> Species: '
      dfile='fehmn.files'
      open(ifehm,file=dfile,status='old',iostat=iofehm)
      if(iofehm.eq.0)then
        do ip=1,4
          read(ifehm,*)outfile
        end do
      else
        write(*,*) 'name of FEHM output file: '
        read(*,'(a60)') outfile
      endif
9     write(*,*)'decay (1) or conservative (2)? '
      read(*,*) iflag
      if(abs(iflag).gt. 2 ) then
        write(*,*) 'Bad input, Try again'
        goto 9
      endif
      write(*,*) 'total mass (in mass unit): '
      read(*,*) totmass
      write(*,*) 'time_sim (in years):'
      read(*,*) time_sim

      call prefix(outfile,leng)
      open(7,file=outfile)

c determine number of particles in problem
 1    read(7,'(a80)') line
```

```
      if (line(12:16).eq.'Years') read(7,*) time
      if(abs(time-time_sim).le.1.0) then
        numspec=0
901     read(7,'(a80)',end=99) line
        if (line(16:22).eq.'Entered') then
          numspec=numspec+1
          read(line,72) spacer2,total(numspec)
 72       format(1a30,i11)
        endif
        goto 901
      endif
      goto 1
 99   write(6,*) 'total number of particles: '
      write(6,*) (i,total(i),i=1,numspec)
      if(iflag.eq.1) then
      write(*,*) 'rate_const (in 1/year):'
      read(*,*) (rate_const(i),i=1,numspec)
      endif
c
      rewind(7)
      write(6,*)''
      ist=0
 2    read(7,'(a80)',end=999) line
      if (line(12:16).eq.'Years') then
        read(7,*) time
        ist=ist+1
        iout=20
        idx=0
      else
        if(line(24:54).eq.title)then
          read(line,59) ctmp,cidx
59        format(A54,a5)
          iout=iout+1
          idx=idx+1
          if(ist.eq.1)then
             do i=1,5
               if(cidx(i:i).ne.' ') then
                 jj=i
                 goto 777
               endif
             enddo
777          fout=prx//cidx(jj:5)
             open(iout,file=fout)
             write(6,*) 'Output Data Stored in File: ',fout
           endif
           read(7,'(a80)') line
           if (line(16:22).eq.'Entered') then
             read(line,72) spacer2,entered
             read(7,'(a80)') line
             read(line,72) spacer2,cur_in
             read(7,'(a80)') line
             read(line,72) spacer2,left
             read(7,'(a80)') line
             read(line,72) spacer2,decayed
             left_this = left - left_old(idx)
             delta_time = time - time_old(idx)
             if(delta_time.ne.0.)then
```

```
                if(iflag.eq.1) then
                  conc = exp(-rate_const(iout-20)*time)*real(left_this)
                else
                  conc = real(left_this)
                end if
                cnorm=conc/total(iout-20)
                conc = (totmass/total(iout-20))*conc/delta_time
                if(conc.le.cmin) conc=cmin
                left_old(idx) = left
                time_old(idx) = time
                write(iout,100) time,conc,cnorm,left/total(iout-20)
              endif
           endif
         endif
       endif
       goto 2

999    write(6,*) '  '
       write(6,*)'Finished'

100    format(1x,g13.3,3x,g13.6,2(3x,f7.4))
       end
       subroutine prefix(fname,length)
       character*60 fname
       do length=1,60
         if(fname(length:length).eq.'.')goto 100
       end do
100    length=length-1
       return
       end
```

(2) Example Input File:

fout2a.out

A FEHM output file for the base-case present-day climate 2-D model.

FEHMN 97-10-01p   09/20/99   16:22:28

File purpose - Variable - Unit number - File name

```
  control      - iocntl -  1 - ra.files
  input        - inpt   - 11 - ra.dat
  geometry     - incoor - 12 - ra.grid
  zone         - inzone - 13 - ra.zone
  output       - iout   - 14 - ra.out
  initial state - iread - 15 - ra.ini
  final state  - isave  - 16 - ra.fin
  time history - ishis  - 17 - ra.his
  time his.(tr) - istrc - 18 - ra.trc
  contour plot - iscon  - 19 - ra.con
  con plot (dp) - iscon1 -  0 - not using
  fe coef stor - isstor - 21 - ra.stor
  input check  - ischk  - 22 - ra.chk
Value provided to subroutine user: not using
```

ptrk read from optional input file: ra.ptrk

```
# input file for mean alpha, fitted fmx, present day q, ysw # AR 11/19/97

File purpose - Variable - Unit number - File name

  control      - iocntl -  1 - ra.files
  input        - inpt   - 11 - ra.dat
  geometry     - incoor - 12 - ra.grid
  zone         - inzone - 13 - ra.zone
  output       - iout   - 14 - ra.out
  initial state - iread  - 15 - ra.ini
  final state  - isave  - 16 - ra.fin
  time history - ishis  - 17 - ra.his
  time his.(tr) - istrc  - 18 - ra.trc
  contour plot - iscon  - 19 - ra.con
  con plot (dp) - iscon1 -  0 - not using
  fe coef stor - isstor - 21 - ra.stor
  input check  - ischk  - 22 - ra.chk
Value provided to subroutine user: not using

**** input title : coor **** incoor =  12 ****
**** input title : elem **** incoor =  12 ****
**** input title : stop **** incoor =  12 ****
**** input title : zone **** inzone =  13 ****
**** input title : stop **** inzone =  13 ****
**** input title : dpdp **** inpt =  11 ****
dpdp read from optional input file: ra.dpdp
**** input title : perm **** inpt =  11 ****
**** input title : rlp  **** inpt =  11 ****
**** input title : rock **** inpt =  11 ****
rock read from optional input file: ra.rock
**** input title : flow **** inpt =  11 ****
**** input title : time **** inpt =  11 ****
**** input title : ctrl **** inpt =  11 ****
**** input title : iter **** inpt =  11 ****
**** input title : sol  **** inpt =  11 ****
**** input title : rflo **** inpt =  11 ****
**** input title : air  **** inpt =  11 ****
**** input title : node **** inpt =  11 ****
**** input title : zone **** inpt =  11 ****
zone read from optional input file: ra.zone2
**** input title : ptrk **** inpt =  11 ****
ptrk read from optional input file: ra.ptrk
**** input title : stop **** inpt =  11 ****
 !!!!!!!!!!!!!!!!!!!!!!!!!!
Coefficients read from *.stor file
 !!!!!!!!!!!!!!!!!!!!!!!!!!

storage for geometric coefficients      4611 in common(nr)      4611

no particle tracking on restart file

storage needed for ncon        5483 available      69760
storage needed for nop         5483 available      6105
storage needed for a matrix    73760 available     73760
storage needed for b matrix    73760 available     97680
storage needed for gmres      143008 available    143008
storage available for b matrix resized to          1<<<<<<
```

```
time for reading input, forming coefficients  4.69


**** analysis of input data on file ra.chk                    ****


note>>h.t. solution stopped after time step    1

note>>tracer solution started on time step    1
Species:  1
at time:  1.0
rest:  0.0 0.0
********************************************************************
Time Step        1

          Timing Information
     Years          Days        Step Size (Days)
   0.100000E+01    0.365250E+03    0.365250E+03
Heat and Mass Solution Disabled

          *************************
            Particle Tracking ==> Species:  1
Number Having Entered System:     9990
Number Currently In System  :     9990
Number Having Left System   :        0
Number Having Decayed       :        0

 Node   Concentration   # of Particles
   1    0.000000E+00          0
 873    0.000000E+00          0
Species:  1
at time:  2.2
rest:  0.0 0.0
********************************************************************

...

********************************************************************
Time Step       50

          Timing Information
     Years          Days        Step Size (Days)
   0.454972E+05    0.166178E+08    0.276995E+07
Heat and Mass Solution Disabled

          *************************
            Particle Tracking ==> Species:  1
Number Having Entered System:     9990
Number Currently In System  :      248
Number Having Left System   :     9742
Number Having Decayed       :        0

 Node   Concentration   # of Particles
   1    0.000000E+00          0
 873    0.000000E+00          0
Species:  1
at time:  54597.62890001281
rest:  0.0 94.0
********************************************************************
...

********************************************************************
```

Time Step 65

Timing Information
Years Days Step Size (Days)
0.701048E+06 0.256058E+09 0.426766E+08
Heat and Mass Solution Disabled

****

Particle Tracking ==> Species: 1
Number Having Entered System: 9990
Number Currently In System : 0
Number Having Left System : 9990
Number Having Decayed : 0

Node	Concentration	# of Particles
1	0.000000E+00	0
873	0.000000E+00	0

Species: 1
at time: 841258.8814916301
rest: 0.0 0.0
****
Time Step 66

Timing Information
Years Days Step Size (Days)
0.841259E+06 0.307270E+09 0.512119E+08
Heat and Mass Solution Disabled

****

Particle Tracking ==> Species: 1
Number Having Entered System: 9990
Number Currently In System : 0
Number Having Left System : 9990
Number Having Decayed : 0

Node	Concentration	# of Particles
1	0.000000E+00	0
873	0.000000E+00	0

Species: 1
at time: 1000000.0
rest: 0.0 0.0
****
Time Step 67

Timing Information
Years Days Step Size (Days)
0.100000E+07 0.365250E+09 0.579802E+08
Heat and Mass Solution Disabled

****

Particle Tracking ==> Species: 1
Number Having Entered System: 9990
Number Currently In System : 0
Number Having Left System : 9990
Number Having Decayed : 0

Node	Concentration	# of Particles
1	0.000000E+00	0
873	0.000000E+00	0

simulation ended: days 3.653E+08 timesteps 67

```
total newton-raphson iterations =        0

total code time(timesteps) =     4.730469

****-----------------------------------------------------****
**** This program for                                 ****
****  Finite Element Heat and Mass Transfer in porous media ****
****-----------------------------------------------------****
****                 Version  : FEHMN 97-10-01p     ****
****                 End Date : 09/20/99          ****
****                   Time : 16:22:38           ****
****-----------------------------------------------------****
```

(3) Example Output File:

out2a.plt
Histories of concentration, normalized concentration, and accumulative normalized concentration for the base-case present-day climate 2-D model.

1.00	0.100000E-09	0.0000	0.0000
2.20	0.100000E-09	0.0000	0.0000
3.64	0.100000E-09	0.0000	0.0000
5.37	0.100000E-09	0.0000	0.0000
7.44	0.100000E-09	0.0000	0.0000
9.93	0.100000E-09	0.0000	0.0000
12.9	0.100000E-09	0.0000	0.0000
16.5	0.100000E-09	0.0000	0.0000
20.8	0.100000E-09	0.0000	0.0000
26.0	0.100000E-09	0.0000	0.0000
32.2	0.100000E-09	0.0000	0.0000
39.6	0.100000E-09	0.0000	0.0000
48.5	0.100000E-09	0.0000	0.0000
59.2	0.100000E-09	0.0000	0.0000
72.0	0.100000E-09	0.0000	0.0000
87.4	0.100000E-09	0.0000	0.0000
106.	0.100000E-09	0.0000	0.0000
128.	0.100000E-09	0.0000	0.0000
155.	0.100000E-09	0.0000	0.0000
187.	0.100000E-09	0.0000	0.0000
225.	0.100000E-09	0.0000	0.0000
271.	0.100000E-09	0.0000	0.0000
326.	0.100000E-09	0.0000	0.0000
392.	0.100000E-09	0.0000	0.0000
472.	0.100000E-09	0.0000	0.0000
567.	0.100000E-09	0.0000	0.0000
682.	0.100000E-09	0.0000	0.0000
819.	0.100000E-09	0.0000	0.0000
984.	0.121448E-05	0.0002	0.0002
0.118E+04	0.506037E-06	0.0001	0.0003
0.142E+04	0.421687E-06	0.0001	0.0004
0.170E+04	0.421696E-05	0.0012	0.0016
0.205E+04	0.122995E-04	0.0042	0.0058
0.246E+04	0.195227E-04	0.0080	0.0138
0.295E+04	0.392494E-04	0.0193	0.0331
0.354E+04	0.576194E-04	0.0340	0.0672

0.425E+04	0.766850E-04	0.0544	0.1215
0.510E+04	0.854410E-04	0.0727	0.1942
0.612E+04	0.888532E-04	0.0907	0.2849
0.734E+04	0.795204E-04	0.0974	0.3823
0.881E+04	0.719199E-04	0.1057	0.4880
0.106E+05	0.610100E-04	0.1076	0.5956
0.127E+05	0.472973E-04	0.1001	0.6957
0.152E+05	0.333036E-04	0.0846	0.7803
0.183E+05	0.202979E-04	0.0619	0.8421
0.219E+05	0.126449E-04	0.0462	0.8884
0.263E+05	0.713909E-05	0.0313	0.9197
0.316E+05	0.469481E-05	0.0247	0.9444
0.379E+05	0.293024E-05	0.0185	0.9630
0.455E+05	0.161032E-05	0.0122	0.9752
0.546E+05	0.103396E-05	0.0094	0.9846
0.655E+05	0.659964E-06	0.0072	0.9918
0.786E+05	0.336096E-06	0.0044	0.9962
0.943E+05	0.146406E-06	0.0023	0.9985
0.113E+06	0.477407E-07	0.0009	0.9994
0.136E+06	0.176816E-07	0.0004	0.9998
0.163E+06	0.736734E-08	0.0002	1.0000
0.196E+06	0.100000E-09	0.0000	1.0000
0.235E+06	0.100000E-09	0.0000	1.0000
0.282E+06	0.100000E-09	0.0000	1.0000
0.338E+06	0.100000E-09	0.0000	1.0000
0.406E+06	0.100000E-09	0.0000	1.0000
0.487E+06	0.100000E-09	0.0000	1.0000
0.584E+06	0.100000E-09	0.0000	1.0000
0.701E+06	0.100000E-09	0.0000	1.0000
0.841E+06	0.100000E-09	0.0000	1.0000
0.100E+07	0.100000E-09	0.0000	1.0000

(4) Verification

The synthetic cumulative breakthrough at the water table is '0.9752' at the time of '0.455E05' years, as in the output file 'out2a.plt'. This value is calculated by dividing the 'Number Having Left System: 9742' with 'Number Having Entered System: 9990' the input file 'fout2a.out'.

(5) Range of Validation:

This software routine is valid for constructing cumulative breakthrough histories from FEHM output at any given downstream boundary given a pulse input of any solute.

ATTACHMENT V

SOFTWARE ROUTINE 'T2FEHM2'

ATTACHMENT V

The most of the following attachment is taken from Ho (1997).

MOL.19980218.0246

Sandia National Laboratories

T2FEHM2

Post-Processor to Convert TOUGH2 Files to FEHM-Readable Files for Particle Tracking

User's Manual

November 1997

Clifford K. Ho
Sandia National Laboratories
Albuquerque, NM 87185
(505) 848-0712
ckho@sandia.gov

Abstract

This document describes a post-processor that is used to reformat TOUGH2 input and output files into FEHM-readable files for particle tracking. Specifically, this post-processor was written as a means to use TOUGH2 simulations of unsaturated-zone flow fields at Yucca Mountain with the particle tracking capabilities of FEHM for TSPA-VA calculations. A description of the required input files for the post-processor, T2FEHM2, and the FEHM-formatted output files are provided. A sample run is also provided as a verification of the post-processor, and a complete listing of the program is included in Appendix C.

The executable for T2FEHM2 (t2fehm2) can be obtained on the Sandia NWER network from the following directory: /home/ckho/bin. The executable can also be obtained from Cliff Ho at ckho@sandia.gov.

Table of Contents

Introduction

Simulations of unsaturated groundwater flow and radionuclide transport at Yucca Mountain, Nevada, are being performed as part of a Total Systems Performance Assessment—Viability Assessment (TSPA-VA). The TSPA-VA evaluates the suitability of Yucca Mountain as a potential repository site for high-level radioactive nuclear waste. Two numerical simulators are being used to perform the flow and transport simulations: 1) TOUGH2 (Pruess, 1991, 1987) and 2) FEHM (Zyvoloski et al., 1995). To facilitate the flow and transport simulation methodology, a post-processor has been written to reformat TOUGH2 files, which consist of information pertaining to unsaturated flow, to FEHM-readable files that can be used for radionuclide particle tracking. This method maintains consistency with the three-dimensional unsaturated-zone (UZ) site-scale model and data set that have been calibrated using TOUGH2 (Bodvarsson et al., 1997).

FEHM uses a cell-based particle tracking model that preserves the overall residence time through any portion of the model and probabilistically reproduces the migration of a solute through the domain. The requirement for the method is that the flow calculation be based on a control volume in which fluid flow rates into and out of each cell are computed. Since TOUGH2 is an integrated finite difference code and FEHM employs a control volume finite element technique, the two codes are compatible from the standpoint of implementation of the particle tracking technique. The required inputs for FEHM to use an externally developed flow field are: 1) grid connectivity information and cell volumes; 2) properties and state variables (rock grain density, fluid saturation, and rock porosity at each grid point); 3) inter-nodal fluid mass flow rate for every connection in the numerical grid; and 4) fluid source and sink flow rates for each grid block. The post-processor, T2FEHM2, was written to generate these required data from existing TOUGH2 files.

The remainder of this paper describes the required inputs to T2FEHM2 and the corresponding output files. A sample run is included for illustration and verification, and a complete program listing of T2FEHM2 is included in Appendix C.

Description of Required Input Files

When executed, T2FEHM2 will prompt the user for the names of three required files: 1) TOUGH2 input file; 2) TOUGH2 output file; and 3) TOUGH2 mesh file. T2FEHM2 will also prompt the user for the name of a fourth file containing the names of repository elements, but this file is optional.

TOUGH2 Input File

The TOUGH2 input file must contain the ROCKS and GENER cards. ROCKS contains material property information for fracture and matrix materials corresponding to a dual-permeability model. Fracture and matrix materials must have an 'F' or 'M', respectively, in the third or fourth character of the material name. Each material must have four lines associated with its entry. The GENER card should contain information on the infiltration source terms for prescribed elements. The generation rate is specified in units of kg/s.

TOUGH2 Output File

The TOUGH2 output file contains all simulated state variables (pressure, saturation) for each element and flux variables (mass flow rate) for each connection pair at user-specified print-out times. T2FEHM2 reads in these state and flux variables and puts them in a format that is compatible with FEHM.

TOUGH2 Mesh File

The TOUGH2 mesh file contains the ELEME and CONNE cards. ELEME contains the element names, material names, volumes, and coordinates of each element in the TOUGH2 model. The fracture and matrix elements should be listed alternately with a fracture element listed first. Also, all boundary elements must be listed at the end of the ELEME card. The material names associated with each element should be five-character names (not integers) that correspond identically to the name of one of the materials in the ROCKS card. The CONNE card contains all connection pairs and associated connection information for each element in the TOUGH2 model. T2FEHM2 stores these connection pairs to create connectivity arrays (ncon, istrw, nelmdg) for FEHM.

File Containing Repository Elements

A file containing the names of repository elements is optional. If present, T2FEHM2 will read the number of repository elements in the first line of the file. All repository element names will then be read from the file. These elements will be used to create special fracture and matrix zones in a FEHM file that will used to define the location of radionuclide release for particle tracking.

Description of Output Files

After reading the required information from the input files, T2FEHM2 prints out nine (9) files that are used by FEHM. The user specifies a reference file name, and the code appends the following nine suffixes to the reference file name to create nine output files:

.dat
.dpdp
.files
.grid
.ini
.rock
.stor
.zone
.zone2

A tenth file, file_name.check, is also printed but it is not used by FEHM. This file contains the node numbers and number of connections for each node. More detailed information on the contents of the FEHM macros can be found in Zyvoloski et al. (1995).

.dat

This file contains the required macros used by FEHM: dpdp, perm, rlp, rock, flow, time, ctrl, iter, sol, rflo, air, node, zone, ptrk. If the macros are not explicitly defined in this file, the names of macro files containing the actual information is listed here. Macros perm and rlp are not required by the particle tracking solution, so dummy values are inserted here.

.dpdp

This file contains a list of the zones corresponding to the fracture materials and lists the fracture porosities. It also contains dummy information regarding the length scale for matrix nodes that is not required for the TOUGH2-FEHM coupling.

.files

This control file contains a list of files that FEHM reads for necessary information.

.grid

This file contains the coor and elem macros. The first line of the coor macro gives the total number of fracture elements, followed by a list of all the nodes in the fracture domain and their respective x, y, and z coordinates. The elem macro contains dummy information regarding the nodes associated with each element, but this is not required for the TOUGH2-FEHM coupling.

.ini

This file contains re-start information for FEHM. The saturations of all fracture and matrix nodes are listed following two header lines. Then, mass flux values (kg/s) are listed for each connection of each node, starting with node 1 (same as ncon array in .stor without pointer information). The mass flux values include sources (infiltration) and sinks (connection to water table) for each node. Flow into a node is negative, and flow out of a node is positive. The mass flux values for the fracture domain are listed first followed by the mass flux values in the matrix domain. The mass flux between fracture and matrix elements are listed last. Flow from the fracture to the matrix is denoted as positive.

.rock

This file lists the zones of all fracture and matrix materials. For each zone, the rock grain density (kg/m3), specific heat (J/kg-K), matrix porosity, and intrinsic fracture porosity (1) are listed.

.stor

The file contains connectivity arrays and control volumes for the grid. Following two header lines, four integers are listed:

iwtotl: Total number of connections in a continuum (either fracture or matrix) for which inter-node fluxes and areas are assigned. This includes connections for a node to itself for sources and sinks. Equal to ncont-(neq+1).

neq: Number of nodes in either the fracture or matrix continuum.

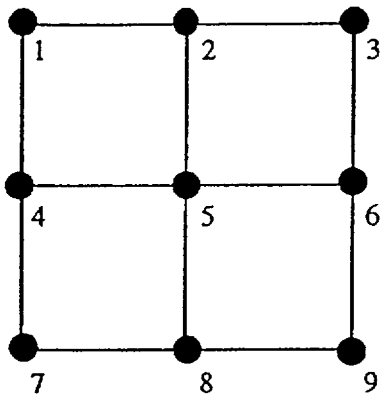
ncont: Number of values in the ncon array (see below)

sehtemp: Flag that is equal to 1 for particle tracking

The following arrays are then read from .stor:

sx1(i), i=1,neq: Primary volume of each node in a continuum

ncon(i), i=1,ncont: Node connectivity array that contains the node numbers for each connection to a specified node in one continuum, starting with node 1. The node numbers in ncon associated with connections to a given node include the node of interest. All nodes connected to a given node are listed in ascending order. In the beginning of this array is pointer information with neq+1 entries. The entries identify the index of the array (i=1,ncont) that precedes the node denoted by the index of the pointer information. See Figure 1 for an example of a 9-node network.



index i	ncon(i)	
1	10	Pointer Information
2	13	
3	17	
4	20	
5	24	
6	29	
7	33	
8	36	
9	40	
10	43	
11	1	Node 1
12	2	
13	4	
14	1	Node 2
15	2	
16	3	
17	5	
18	2	Node 3
19	3	
20	6	
21	1	Node 4
22	4	
23	5	
24	7	
25	2	Node 5
26	4	
27	5	
28	6	
29	8	
30	3	Node 6
31	5	
32	6	
33	9	
34	4	Node 7
35	7	
36	8	
37	5	Node 8
38	7	
39	8	
40	9	
41	6	Node 9
42	8	
43	9	

Figure 1. 9-node example of the ncon array used in FEHM.

istrw(i), i=1,ncont: Not used in this application. The array is filled using following algorithm:

```
do i = 1, ncont
      if(i.le.iwtotl) then
            istrw(i) = i
      else
            istrw(i) = 0
      end if
end do
```

nelmdg(i), i=1,neq: Position (index) of node i in the ncon array:

```
do i = 1, neq
      do j = ncon(i) + 1, ncon(i+1)
            if(ncon(j).eq.i) nelmdg(i) = j
      end do
end do
```

iwtotl numbers: Three groups of iwtotl numbers signifying the x, y, and z components of the are divided by distance terms for all internode connections. Only place-holders are required:

```
do i = 1, 3
      write(15,'(5(1pe16.8))') (-1.0, j = 1, iwtotl)
end do
```

.zone

This file contains definitions of zones that correspond to ROCKS materials in TOUGH2. The materials are listed sequentially in the same order as they appear in the ROCKS card. A comment (#) is added to identify the name of the material as it appears in ROCKS. The number of nodes within each zone is listed after the header 'nnum'. Following that line, the nodes are listed in the order that they appear in the ELEME card in TOUGH2. Note that the fracture AND matrix nodes are listed here. In the standard version of FEHM, only the fracture nodes are listed, and additional zones are created to accommodate the matrix nodes. Due to the non-symmetric nature of fracture and matrix materials in the LBNL site-scale model, modifications were required to FEHM. The number of fracture nodes are read in macro coord. If the number of nodes that are listed in the zone macro accounts for twice the total number of fracture nodes, then additional zones are not created. Additional comments are added after the 'stop' line of the file.

.zone2

This file is identical to the .zone file except that it also contains two additional zones that define the repository nodes for the fractures and matrix. The repository elements are listed in another file that is specified by the user during one of the prompts by T2FEHM2. This external file should contain the total number of repository elements in the file followed by a line-by-line listing of all the repository elements. This zone (.zone2) is read at the end of the .dat file to identify nodes where particles will be released in the ptrk macro (note that ptrk is not created by this post-processor). The nodes that are defined in .zone2 will retain the porosities and densities assigned to them previously in .rock and .dpdp.

Sample Run

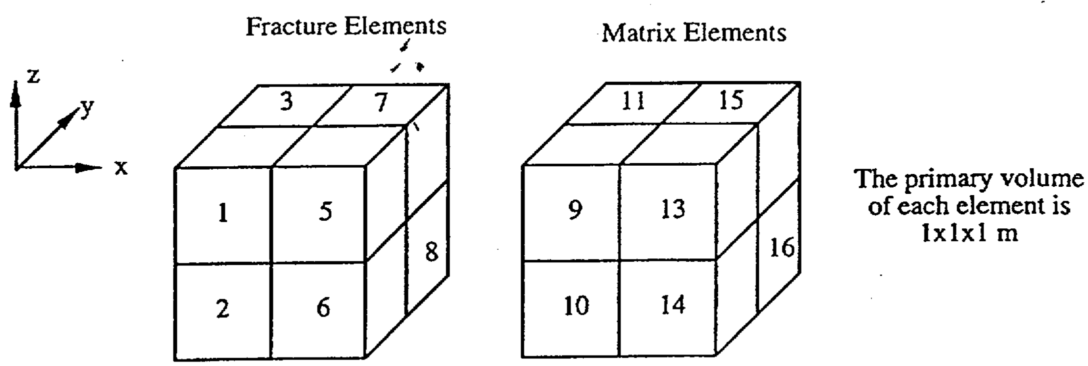
A sample TOUGH2 run has been created to test and illustrate the use of T2FEHM2. A sketch of the 2x2x2-element domain is shown in Figure 2. Both the fracture and matrix continua are shown and numbered according to FEHM convention. The corresponding name and material for each TOUGH2 element is also tabulated in Figure 2. Not shown in Figure 2 are the top and bottom boundary elements. The four top boundary elements are connected to the four top matrix elements, and the four bottom boundary elements are connected to the four bottom fracture elements. The bottom boundary is fixed at a constant liquid saturation of 0.85, and the top boundaries remain active.

The Richards' equation module of TOUGH2 (EOS9) is used to simulate a steady-state condition for this system. The TOUGH2 input and output files for this sample run are included in Appendix A. The output includes liquid saturations for each element and mass flow rates for each connection pair, including fracture-matrix connections. Appendix A also includes a file called 'mesh.dat', which contains the ELEME and CONNE cards in the TOUGH2 input file. In the LBNL 3-D site-scale model, the mesh file containing ELEME and CONNE is not included in the TOUGH2 input file (in contrast to this sample run), so the mesh file is read as an external file. Another file included in Appendix A that is optionally used by T2FEHM2, called 'rep.names', contains the names of two elements that are arbitrarily denoted as repository elements to test the proper creation of .zone2.

T2FEHM2 is used to post-process the input and output files to create FEHM readable files as described in the previous section. Appendix B contains the screen input and all the T2FEHM2 output files for this sample run. The output files are described in detail in the previous section. All of the output files are hand-checked, and the data are compared to the TOUGH2 output file to verify T2FEHM2. All of the output for this sample 3-D run were verified as being correct.

Range of Validation

T2FEHM2 is valid for any consistent set of TOUGH2 input/output/mesh files for conversion to FEHM-readable files for the cell volumes and connectivity, rock properties and state variables, mass flux for each cell connection, and source/sink flow rate information.



FEHM Node Number	TOUGH2 Element Name	TOUGH2 Material Name
1	F11_1	tcwF1
2	F21_1	ptnF1
3	F12_1	tswF5
4	F22_1	tswF7
5	F11_2	ch3Fv
6	F21_2	ch3Fz
7	F12_2	ptnF3
8	F22_2	pwF37
9	M11_1	tcwM1
10	M21_1	ptnM1
11	M12_1	tswM5
12	M22_1	tswM7
13	M11_2	ch3Mv
14	M21_2	ch3Mz
15	M12_2	ptnM3
16	M22_2	pcM37

Figure 2. Three-dimensional model used in the verification run of the TOUGH2 post-processor used to create FEHM readable files for particle tracking.

Acknowledgments

The author gratefully acknowledges Bruce Robinson for his assistance with the development of T2FEHM2.

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Appendix A
TOUGH2 Input and Output Files

```
*************************
File name:  TOUGH2.INP
*************************

START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97
START  The option 1 method uses TOUGH2 flow fields and FEHM particle tracking.
START  A post-processor has been written to reformat the TOUGH2 files for use
START  with FEHM.  The domain considered here is a 3-D 3x3x3 cube.  Each of
START  the 27 elements are assigned arbitrary material properties from the LBL
START  (7/97) property set. A top and bottom boundary are added to the domain
START  to replicate the conditions of the site-scale model. The flow field
START  will be post-processed and the reformatted FEHM files will be hand-
START  checked for accuracy.
START  *** t2v3.1.1 is used here (EOS9) to generate steady-state conditions ***
START      The initial saturation is a uniform 0.85
START  ROCKS from inversion "itough2 97dkfxk1i 97dkfxk1  3"
START  *** Note that in ROCKS, fracture materials that were created to account
START      for perched water do not have a porosity in columns 71-80, but they
START      should have a fracture porosity of 1.1e-5 (per Yu-Shu Wu)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
tcwM1    2 2480.    0.6600E-010.5370E-170.5370E-170.5370E-17 1.660    847.0
                        0.7200    0.7000
    7     0.2317    0.1300     1.000     0.2000E-01          0.4898E-03
    7     0.2317    0.1300     0.1175E-050.1000E+11 1.000
ptnM1    2 2300.    0.3690     0.3090E-130.3090E-130.3090E-13 0.500    1080.
                        0.3500    0.7000
    7     0.2307    0.1000     1.000     0.2000E-01          0.1096
    7     0.2307    0.1000     0.3802E-040.1000E+11 1.000
ptnM3    2 2300.    0.3530     0.8318E-130.8318E-130.8318E-13 1.020    1020.
                        0.4600    0.7000
    7     0.2869    0.1700     1.000     0.2000E-01          0.6918
    7     0.2869    0.1700     0.4571E-040.1000E+11 1.000
tswM5    2 2480.    0.1150     0.1549E-160.1549E-160.1549E-16 1.800    900.0
                        0.6500    0.7000
    7     0.2294    0.8000E-01 1.000     0.2000E-01          0.7762E-01
    7     0.2294    0.8000E-010.3311E-050.1000E+11 1.000
tswM7    2 2480.    0.2000E-010.1288E-160.1288E-160.1288E-16 2.080    984.0
                        1.6900    0.7000
    7     0.3874    0.5000     1.000     0.2000E-01          0.4898E-03
    7     0.3874    0.5000     0.1549E-050.1000E+11 1.000
ch3Mv    2 2300.    0.3210     0.2570E-120.2570E-120.2570E-12 1.170    1200.
                        0.5800    0.7000
    7     0.2242    0.6000E-01 1.000     0.2000E-01          0.4898
    7     0.2242    0.6000E-010.7413E-040.1000E+11 1.000
ch3Mz    2 2300.    0.2400     0.9120E-170.9120E-170.9120E-17 1.200    1150.
                        0.6100    0.7000
    7     0.2204    0.2000     1.000     0.2000E-01          1.000
    7     0.2204    0.2000     0.1950E-050.1000E+11 1.000
pcM37    2 2480.    0.3600E-010.6081E-170.6081E-170.6081E-17 1.280     782.8
                        1.2800
    7     0.3720    0.2000     1.000     0.02                1.00
    7     0.3720    0.2000     0.3366E-060.1000E+13 0.98
tcwF1    2 2480.    1.000      0.6206E-110.6206E-112.2910E-11 1.660    847.0
                        0.7200    0.7000                             2.3300e-04
    7     0.4920    0.1000E-01 1.000     0.2000E-01          0.4898E-03
    7     0.4920    0.1000E-010.2951E-030.1000E+11 1.000
ptnF1    2 2300.    1.000      5.2480E-135.2480E-135.2480E-13 0.500    1080.
                        0.3500    0.7000                             4.8400e-05
```

```
    7      0.4920    0.1000E-01 1.000    0.2000E-01          0.1096
    7      0.4920    0.1000E-010.1096E-020.1000E+11 1.000
ptnF3    2 2300.    1.000    0.2570E-120.2570E-120.2570E-12 1.020    1020.
                       0.4600    0.7000                                1.3000e-04
    7      0.4920    0.1000E-01 1.000    0.2000E-01          0.6918
    7      0.4920    0.1000E-010.3388E-020.1000E+11 1.000
tswF5    2 2480.    1.000    0.9120E-120.9120E-120.3802E-11 1.800    900.0
                       0.6500    0.7000                                3.2900e-04
    7      0.4917    0.1000E-01 1.000    0.2000E-01          0.7762E-01
    7      0.4917    0.1000E-010.1096E-030.1000E+11 1.000
tswF7    2 2480.    1.000    0.1202E-110.1202E-110.1202E-11 2.080    984.0
                       1.6900    0.7000                                4.9200e-04
    7      0.4920    0.1000E-01 1.000    0.2000E-01          0.4898E-03
    7      0.4920    0.1000E-010.1175E-030.1000E+11 1.000
ch3Fv    2 2300.    1.000    0.2884E-120.2884E-120.2884E-12 1.170    1200.
                       0.5800    0.7000                                7.1400e-05
    7      0.4920    0.1000E-01 1.000    0.2000E-01          0.4898
    7      0.4920    0.1000E-010.1175E-020.1000E+11 1.000
ch3Fz    2 2300.    1.000    0.1175E-130.1175E-130.1175E-13 1.200    1150.
                       0.6100    0.7000                                1.1000e-05
    7      0.4918    0.1000E-01 1.000    0.2000E-01          1.000
    7      0.4918    0.1000E-010.1230E-020.1000E+11 1.000
pwF37    2 2480.    1.000    0.1500E-12 .3040E-17 .3040E-17 1.280     782.8
                       1.2800
    7      0.3720    0.2000     1.00       0.98              1.00
    7      0.3720    0.2000     0.3366E-060.1000E+13 0.98
topbd    2    0.995     1.0     0.747E-10 0.747E-10 0.747E-10    0.03      1009.
                                   1.0
    2        500.
    1          0.       0.       1.0
botbd    2 2300.    0.2800    0.5370E-170.5370E-170.5370E-17 1.350    0.1000E+31
                       1.5600
    7      0.3900                1.000
    7      0.3900             0.5800E-060.1000E+13 1.000
REFCO      0.920E+05      25.00

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   29000    45000000000000000003000 39      2.13E-5
        0.  3.1536e13      .1                          -9.81
     1.E-5     1.E00                                          1.E-7
               0.85
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    0
      0.1  7.884e8   1.5768e9   3.1536e9   7.884e9   1.5768e10
ELEME
F11 1          tcwF1 2.330E-04                         0.5       0.5      -0.5
M11 1          tcwM1 0.100E+01                         0.5       0.5      -0.5
F21 1          ptnF1 4.840E-05                         0.5       0.5      -1.5
M21 1          ptnM1 0.100E+01                         0.5       0.5      -1.5
F12 1          tswF5 3.290E-04                         0.5       1.5      -0.5
M12 1          tswM5 0.100E+01                         0.5       1.5      -0.5
F22 1          tswF7 4.920E-04                         0.5       1.5      -1.5
M22 1          tswM7 0.100E+01                         0.5       1.5      -1.5
F11 2          ch3Fv 7.140E-05                         1.5       0.5      -0.5
M11 2          ch3Mv 0.100E+01                         1.5       0.5      -0.5
F21 2          ch3Fz 1.100E-05                         1.5       0.5      -1.5
M21 2          ch3Mz 0.100E+01                         1.5       0.5      -1.5
```

```
F12 2          ptnF3 1.300E+04                          1.5        1.5       -0.5
M12 2          ptnM3 0.100E+01                          1.5        1.5       -0.5
F22 2          pwF37 1.100E-05                          1.5        1.5       -1.5
M22 2          pcM37 0.100E+01                          1.5        1.5       -1.5
TP  1          topbd     .001                           0.         0.        0.
TP  2          topbd     .001                           0.         0.        0.
TP  3          topbd     .001                           0.         0.        0.
TP  4          topbd     .001                           0.         0.        0.
BT  1          botbd    0.000                           0.         0.        0.
BT  2          botbd    0.000                           0.         0.        0.
BT  3          botbd    0.000                           0.         0.        0.
BT  4          botbd    0.000                           0.         0.        0.

CONNE
F11 1F11 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M11 1M11 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F11 1F12 1                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M11 1M12 1                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F11 1F21 1                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
M11 1M21 1                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
F21 1F21 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M21 1M21 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F21 1F22 1                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M21 1M22 1                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F12 1F12 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M12 1M12 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F12 1F22 1                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
M12 1M22 1                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
F22 1F22 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M22 1M22 2                    1 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F11 2F12 2                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M11 2M12 2                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F11 2F21 2                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
M11 2M21 2                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
F21 2F22 2                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
M21 2M22 2                    2 0.500E+00 0.500E+00 0.100E+01 0.000E+00
F12 2F22 2                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
M12 2M22 2                    3 0.500E+00 0.500E+00 0.100E+01 0.100E+01
F11 1M11 1                    1 0.000E+00 0.163E+00 0.204E+01 0.000E+00 0.490E-03
F21 1M21 1                    1 0.000E+00 0.192E+00 0.174E+01 0.000E+00 0.110E+00
F12 1M12 1                    1 0.000E+00 0.917E-01 0.364E+01 0.000E+00 0.776E-01
F22 1M22 1                    1 0.000E+00 0.583E-01 0.571E+01 0.000E+00 0.490E-03
F11 2M11 2                    1 0.000E+00 0.583E-01 0.571E+01 0.000E+00 0.000E+00
F21 2M21 2                    1 0.000E+00 0.583E-01 0.571E+01 0.000E+00 0.000E+00
F12 2M12 2                    1 0.000E+00 0.575E+00 0.580E+00 0.000E+00 0.692E+00
F22 2M22 2                    1 0.000E+00 0.132E+00 0.253E+01 0.000E+00 0.490E-03
TP  1M11 1                    3   0.         0.5       1.        -1.
TP  2M11 2                    3   0.         0.5       1.        -1.
TP  3M12 1                    3   0.         0.5       1.        -1.
TP  4M12 2                    3   0.         0.5       1.        -1.
BT  1F21 1                    3   0.         0.5       1.        -1.
BT  2F21 2                    3   0.         0.5       1.        -1.
BT  3F22 1                    3   0.         0.5       1.        -1.
BT  4F22 2                    3   0.         0.5       1.        -1.

GENER
F11 1                              WATE   3.16e-8
F11 2                              WATE   2.16e-8
```

```
F12 1                                WATE   4.16e-8
F12 2                                WATE   1.16e-8

INCON
BT  1    3    1
0.85

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

The code ignores everything that follows:


MESHMAKER
XYZ
0.
NX       2    1.
NY       2    1.
NZ       2    1.

ENDCY
```

```
************************
File name:  TOUGH2.OUT
************************

     @@@@@  @@  @ @  @@@ @ @  @@     @@@ @ @  @ @ @ @    @@  @@@@@ @  @@  @  @    @@@  @ @ @  @
       @   @ @ @ @ @     @ @ @ @    @     @ @@ @@ @ @ @   @ @    @    @ @ @ @@ @    @ @ @ @ @@ @
       @   @ @ @ @ @ @@ @@@@    @     @@   @ @ @ @ @ @ @   @@@@   @    @ @ @ @ @ @   @@@  @ @ @ @ @
       @   @ @ @ @ @ @ @ @ @   @        @ @ @  @ @ @ @   @ @    @    @ @ @ @ @@    @ @  @ @ @ @@
       @    @@   @@   @@@ @ @ @@@@   @@@  @ @  @  @@  @@@@ @ @    @    @  @@  @  @    @ @  @@  @  @

              TOUGH2 IS A PROGRAM FOR MULTIPHASE MULTICOMPONENT FLOW IN PERMEABLE MEDIA, INCLUDING HEAT FLOW.
         IT IS A MEMBER OF THE MULKOM FAMILY OF CODES, DEVELOPED BY KARSTEN PRUESS AT LAWRENCE BERKELEY LABORATORY.
                                 WIPP VERSION BY STEPHEN W. WEBB - MAY 27, 1993.

                    ****************************************************************************
                    ********************   TOUGH2 - VERSION 3.1.1  (June 1997)   ********************
                    **************   includes a choice of conjugate gradient solvers   *************
                    **************   AND A CAPABILITY FOR FRACTURE-MATRIX INTERACTION   *************
   ***   AND LINEARLIZED V.G. CAPILLARY PRESSURE FUNCTIONS(ICP=7) for Sl<(Sr+CP(4)) with CP(4)<1 (No change if CP(4)>1)   ***
 ***************************************************************************************************************************
   To engage fracture-matrix interchange, enter a factor "FMX" in the last field (columns 71-80) of a connection record.
   If MOP(22)=9, fracture-matrix fluxes are multiplied by ABS(FMX).
   If MOP(22)=8, then upstream saturation is used if FMX is positive, and upstream relative permeability is used
   if FMX is negative. ABS(FMX) is also used as a multiplier for liquid flux.


PARAMETERS FOR FLEXIBLE DIMENSIONING OF MAJOR ARRAYS (MAIN PROGRAM) ARE AS FOLLOWS

MNEL =15003   MNCON = 45003   MNEQ =  3   MNK =  2   MNPH =  2   MNB =  6   MNOGN = 500   MGTAB = 2000
==========================================================================================================

MAXIMUM NUMBER OF VOLUME ELEMENTS (GRID BLOCKS):               MNEL  =  15003
MAXIMUM NUMBER OF CONNECTIONS (INTERFACES):                    MNCON =  45003
MAXIMUM LENGTH OF PRIMARY VARIABLE ARRAYS:                     MPRIM =  45009
MAXIMUM NUMBER OF GENERATION ITEMS (SINKS/SOURCES):            MNOGN =    500
MAXIMUM NUMBER OF TABULAR (TIME-DEPENDENT) GENERATION DATA:    MGTAB =   2000
LENGTH OF SECONDARY PARAMETER ARRAY:                           MSEC  =1080216
MAXIMUM NUMBER OF JACOBIAN MATRIX ELEMENTS:                    MNZ   = 945081

LARGE LINEAR EQUATION ARRAYS: LENGTH OF IRN IS                 LIRN  =  945081
                              LENGTH OF ICN AND CO IS          LICN  =  945081

==========================================================================================================

======== CHOICE OF FRACTURE-MATRIX MULTIPLIERS IF FMX (COLUMNS 71-80 IN CONNE CARD) IS NON-ZERO (C. K. Ho) ========

      MOP(22) = 9: F-M LIQUID FLUX MULTIPLIER IS ABS(FMX) ONLY
      MOP(22) = 8: F-M GAS AND LIQUID FLUX MULTIPLIER IS UPSTREAM SATURATION IF FMX IS POSITIVE AND
                   IS UPSTREAM RELATIVE PERMEABILITY IF FMX IS NEGATIVE. ABS(FMX) IS ALSO MULTIPLIED BY LIQUID FLUX


==================================== CHOICE OF LINEAR EQUATION SOLVERS ====================================

      MOP(21) = 1: DIRECT SOLVER - MA28
      MOP(21) = 2: SUBROUTINE DSLUBC: BI-CONJUGATE GRADIENT SOLVER WITH INCOMPLETE LU FACTORIZATION
      MOP(21) = 3: SUBROUTINE DSLUCS: BI-CONJUGATE GRADIENT SOLVER - LANCZOS TYPE WITH INCOMPLETE LU FACTORIZATION
      MOP(21) = 4: SUBROUTINE DSLUGM: GENERALIZED MINIMUM RESIDUAL CONJUGATE GRADIENTS WITH INCOMPLETE LU FACTORIZATION

array dimensioning is made according to the needs of the conjugate gradient solvers
when using MA28, only a smaller-size problem can be accommodated
restriction with MA28 is: (number of elements) + 2 * (number of connections) < (MNEL + 2* MNCON)/4
```

```
SUMMARY OF DISK FILES

FILE *VERS* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *MESH* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *INCON* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *GENER* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *SAVE* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *LINEQ* DOES NOT EXIST --- OPEN AS A NEW FILE
FILE *TABLE* DOES NOT EXIST --- OPEN AS A NEW FILE

   PROBLEM TITLE:  START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97

DOMAIN NO.  1     MATERIAL NAME -- tcwM1
DOMAIN NO.  2     MATERIAL NAME -- ptnM1
DOMAIN NO.  3     MATERIAL NAME -- ptnM3
DOMAIN NO.  4     MATERIAL NAME -- tswM5
DOMAIN NO.  5     MATERIAL NAME -- tswM7
DOMAIN NO.  6     MATERIAL NAME -- ch3Mv
DOMAIN NO.  7     MATERIAL NAME -- ch3Mz
DOMAIN NO.  8     MATERIAL NAME -- pcM37
DOMAIN NO.  9     MATERIAL NAME -- tcwF1
DOMAIN NO. 10     MATERIAL NAME -- ptnF1
DOMAIN NO. 11     MATERIAL NAME -- ptnF3
DOMAIN NO. 12     MATERIAL NAME -- tswF5
DOMAIN NO. 13     MATERIAL NAME -- tswF7
DOMAIN NO. 14     MATERIAL NAME -- ch3Fv
DOMAIN NO. 15     MATERIAL NAME -- ch3Fz
DOMAIN NO. 16     MATERIAL NAME -- pwF37
DOMAIN NO. 17     MATERIAL NAME -- tcpbd
DOMAIN NO. 18     MATERIAL NAME -- botbd
DOMAIN NO. 19     MATERIAL NAME -- REFCO
WRITE FILE *MESH* FROM INPUT DATA
WRITE FILE *GENER* FROM INPUT DATA
WRITE FILE *INCON* FROM INPUT DATA
```

```
***************************************************************************
*                    EVALUATE FLOATING POINT ARITHMETIC                   *
***************************************************************************
*                                                                         *
* FLOATING POINT PROCESSOR HAS APPROXIMATELY 15 SIGNIFICANT DIGITS        *
*                                                                         *
* DEFAULT VALUE OF INCREMENT FACTOR FOR NUMERICAL DERIVATIVES IS DFAC = 0.1051E-07 *
* USER-SPECIFIED VALUE DFAC = 0.1000E-06 WILL BE USED                     *
*                                                                         *
***************************************************************************


MESH HAS   24 ELEMENTS (   20 ACTIVE) AND   40 CONNECTIONS (INTERFACES) BETWEEN THEM
GENER HAS   4 SINKS/SOURCES

END OF TOUGH2 INPUT JOB --- ELAPSED TIME =    0.0240 SECONDS

****************************************************************************************************************
*          ARRAY "MOP" ALLOWS TO GENERATE MORE PRINTOUT IN VARIOUS SUBROUTINES, AND TO MAKE SOME CALCULATIONAL CHOICES.  *
****************************************************************************************************************

  MOP(1)  = 0 *** ALLOWS TO GENERATE A SHORT PRINTOUT FOR EACH NEWTON-RAPHSON ITERATION
          = 0, 1, OR 2: GENERATE 0, 1, OR 2 LINES OF PRINTOUT

          MORE PRINTOUT IS GENERATED FOR MOP(I) > 0 IN THE FOLLOWING SUBROUTINES (THE LARGER MOP IS, THE MORE WILL BE PRINTED).

  MOP(2)  = 0 *** CYCIT       MOP(3) = 0 *** MULTI       MOP(4) = 0 *** QU        MOP(5) = 0 *** EOS        MOP(6) = 0 *** LINEQ

  MOP(7)  = 0 *** IF UNEQUAL ZERO, WILL GENERATE A PRINTOUT OF INPUT DATA

          CALCULATIONAL CHOICES OFFERED BY MOP ARE AS FOLLOWS:

  MOP(9)  = 0 *** CHOOSES FLUID COMPOSITION ON WITHDRAWAL (PRODUCTION).
          = 0: ACCORDING TO RELATIVE MOBILITIES.
          = 1: ACCORDING TO COMPOSITION IN PRODUCING ELEMENT.

  MOP(10) = 0 *** CHOOSES INTERPOLATION FORMULA FOR DEPENDENCE OF THERMAL CONDUCTIVITY ON LIQUID SATURATION (SL).
          = 0: K = KDRY + SQRT(SL)*(KWET-KDRY)
          = 1: K = KDRY + SL*(KWET-KDRY)

  MOP(11) = 0 *** CHOOSES EVALUATION OF MOBILITY AND ABSOLUTE PERMEABILITY AT INTERFACES.
          = 0: MOBILITIES ARE UPSTREAM WEIGHTED WITH WUP. (DEFAULT IS WUP = 1.0). PERMEABILITY IS UPSTREAM WEIGHTED.
          = 1: MOBILITIES ARE AVERAGED BETWEEN ADJACENT ELEMENTS. PERMEABILITY IS UPSTREAM WEIGHTED.
          = 2: MOBILITIES ARE UPSTREAM WEIGHTED WITH WUP. (DEFAULT IS WUP = 1.0). PERMEABILITY IS HARMONIC WEIGHTED.
          = 3: MOBILITIES ARE AVERAGED BETWEEN ADJACENT ELEMENTS. PERMEABILITY IS HARMONIC WEIGHTED.
          = 4: MOBILITY * PERMEABILITY PRODUCT IS HARMONIC WEIGHTED.

  MOP(12) = 0 *** CHOOSES PROCEDURE FOR INTERPOLATING GENERATION RATES FROM A TIME TABLE.
          = 0: TRIPLE LINEAR INTERPOLATION.
          = 1: "STEP FUNCTION" OPTION.

  MOP(14) = 0 *** SPECIFIES THE HANDLING OF PIVOT FAILURES IN THE LINEAR EQUATION SOLUTION
          = 0: PERFORM NEW MATRIX DECOMPOSITION AFTER PIVOT FAILURE
          > 0: IGNORE PIVOT FAILURE AND PROCEED

  MOP(15) = 0 *** ALLOWS TO SELECT A SEMI-ANALYTICAL HEAT EXCHANGE CALCULATION WITH CONFINING BEDS.
          = 0: NO SEMI-ANALYTICAL HEAT EXCHANGE
          > 0: SEMI-ANALYTICAL HEAT EXCHANGE ENGAGED (WHEN A SPECIAL SUBROUTINE MODULE "QLOSS" IS PRESENT)

  MOP(16) = 3 *** PERMITS TO CHOOSE TIME STEP SELECTION OPTION
          = 0: USE TIME STEPS EXPLICITLY PROVIDED AS INPUT.
```

```
        > 0: INCREASE TIME STEP BY AT LEAST A FACTOR 2, IF CONVERGENCE OCCURS IN .LE. MOP(16) ITERATIONS.

MOP(17) = 0 *** HANDLES SCALING OPTIONS.
        = 0: NO SCALING.
        = 7: SCALING.

MOP(18) = 0 *** ALLOWS TO SELECT HANDLING OF INTERFACE DENSITY.
        = 0: PERFORM UPSTREAM WEIGHTING FOR INTERFACE DENSITY.
        > 0: COMPUTE INTERFACE DENSITY AS AVERAGE OF THE TWO GRID BLOCK DENSITIES.
             HOWEVER, WHEN ONE OF THE TWO PHASE SATURATIONS IS ZERO, DO UPSTREAM WEIGHTING.

MOP(21) = 3 *** PERMITS TO SELECT LINEAR EQUATION SOLVER
        = 0: DEFAULTS TO MOP(21) = 4
        = 1: DIRECT SOLVER - MA28
        = 2: SUBROUTINE DSLUBC: BI-CONJUGATE GRADIENT SOLVER; PRECONDITIONER: INCOMPLETE LU FACTORIZATION
        = 3: SUBROUTINE DSLUCS: BI-CONJUGATE GRADIENT SOLVER - LANCZOS TYPE; PRECONDITIONER: INCOMPLETE LU FACTORIZATION
        = 4: SUBROUTINE DSLUGM: GENERALIZED MINIMUM RESIDUAL CONJUGATE GRADIENTS; PRECONDITIONER: INCOMPLETE LU FACTORIZATION

*****************************************************************************************************************

*****************************************************************************************************************
*                        EOS9: EQUATION OF STATE FOR SATURATED/UNSATURATED FLOW (RICHARDS EQUATION)           *
*****************************************************************************************************************

  OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (1,1,1, 6)

                      NK  = 1   - NUMBER OF FLUID COMPONENTS
                      NEQ = 1   - NUMBER OF EQUATIONS PER GRID BLOCK
                      NPH = 1   - NUMBER OF PHASES THAT CAN BE PRESENT
                      NB  = 6   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN COMPONENT MASS FRACTIONS)

  ONLY AVAILABLE OPTION IS: (NK,NEQ,NPH,NB) = (1,1,1,6)

*****************************************************************************************************************

DEFAULT REFERENCE CONDITIONS ARE (P,T) = ( .1013e6 Pascal, 15.0 deg-C)

USER-SPECIFIED CONDITIONS ARE USED:  (P,T) = (0.920000E+05 Pascal, 0.250000E+02 deg-C)
WATER DENSITY is d = 0.997156E+03 kg/m^3;      VISCOSITY is vis = 0.890433E-03 Pa-s;      COMPRESSIBILITY is cp = 0.449737E-09 1/Pa

THE PRIMARY VARIABLE X1 IS PRESSURE FOR (X1.GE.0.920000E+05); IT IS LIQUID SATURATION FOR (X1.LT. 1.)

*****************************************************************************************************************

********** VOLUME- AND MASS-BALANCES ****************************************************************************

********** [KCYC,ITER] = [    0,   0] *****                              THE TIME IS  0.00000E+00 SECONDS, OR  0.00000E+00 DAYS

PHASE VOLUMES IN PLACE
GAS  0.22880E+00 M**3;   LIQUID  0.12965E+01 M**3

LIQUID MASS IN PLACE  0.12928E+04 KG

*****************************************************************************************************************

+++++++++ REDUCE TIME STEP AT (   1,  9) +++++++++++++++   NEW DELT = 0.250000E-01
F22 2(   1,  6) ST = 0.250000E-01 DT = 0.250000E-01 DX1= 0.125808E+00 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.975808E+00
+++++++++ REDUCE TIME STEP AT (   2,  9) +++++++++++++++   NEW DELT = 0.625000E-02
+++++++++ REDUCE TIME STEP AT (   2,  9) +++++++++++++++   NEW DELT = 0.156250E-02
```

```
F22 2(   2,  4) ST = 0.265625E-01 DT = 0.156250E-02 DX1= 0.312705E-02 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.978935E+00
F22 2(   3,  4) ST = 0.281250E-01 DT = 0.156250E-02 DX1= 0.876988E-03 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.979812E+00
F22 2(   4,  4) ST = 0.296875E-01 DT = 0.156250E-02 DX1= 0.151112E-03 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.979963E+00
F22 2(   5,  3) ST = 0.312500E-01 DT = 0.156250E-02 DX1= 0.192079E-04 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.979982E+00
F22 2(   6,  3) ST = 0.343750E-01 DT = 0.312500E-02 DX1= 0.227069E-05 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.979985E+00
F21 1(   7,  3) ST = 0.406250E-01 DT = 0.625000E-02 DX1= -.142948E-01 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.732586E+00
F21 1(   8,  3) ST = 0.531250E-01 DT = 0.125000E-01 DX1= -.238158E-01 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.708770E+00
F21 1(   9,  3) ST = 0.781250E-01 DT = 0.250000E-01 DX1= -.359446E-01 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.672825E+00
F21 1(  10,  4) ST = 0.128125E+00 DT = 0.500000E-01 DX1= -.484749E-01 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.624350E+00

*** Lines deleted here for brevity ***

F11 2( 248,  2) ST = 0.889572E+12 DT = 0.439805E+12 DX1= -.335990E-11 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.289068E-01
F22 1( 249,  2) ST = 0.176918E+13 DT = 0.879609E+12 DX1= -.146115E-13 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.390151E-01
F12 1( 250,  2) ST = 0.352840E+13 DT = 0.175922E+13 DX1= -.892238E-15 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.553506E-01
F22 1( 251,  2) ST = 0.704684E+13 DT = 0.351844E+13 DX1= 0.202918E-14 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.390151E-01
F22 1( 252,  6) ST = 0.140837E+14 DT = 0.703687E+13 DX1= -.113391E-14 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.390151E-01
F22 2( 253,  2) ST = 0.211206E+14 DT = 0.703687E+13 DX1= -.174201E-16 DX2= 0.000000E+00 T =  25.000 P =        1. S = 0.927381E+00
F11 1( 254,  7) ST = 0.315360E+14 DT = 0.104154E+14 DX1= 0.102975E-14 DX2= 0.000000E+00 T =  25.000 P =        0. S = 0.428039E-01

START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97

       OUTPUT DATA AFTER ( 254,  7)-2-TIME STEPS                                        THE TIME IS  0.36500E+09 DAYS

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 TOTAL TIME     KCYC   ITER  ITERC   KON       DX1M          DX2M          DX3M        MAX. RES.     NER   KER      DELTEX
 0.31536E+14    254      7    998     2     0.24469E-14  0.00000E+00  0.24469E-14   0.89921E-05      1     1    0.10415E+14

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

ELEM.  INDEX  PRES       S(liq)       PCAP        K(rel)      DIFFUS.
              (PA)                    (PA)                    (m^2/s)

F11 1      1 0.92000E+05 0.42804E-01 -.11419E+06 0.42580E-07 0.10677E-08
M11 1      2 0.92000E+05 0.95895E+00 -.27693E+06 0.10049E+00 0.54027E-07
F21 1      3 0.92000E+05 0.18497E-01 -.12408E+06 0.89330E-10 0.79385E-12
M21 1      4 0.92000E+05 0.53349E+00 -.29078E+06 0.67816E-04 0.14894E-07
F12 1      5 0.92000E+05 0.55351E-01 -.22082E+06 0.18521E-06 0.95664E-09
M12 1      6 0.92000E+05 0.87371E+00 -.27930E+06 0.22934E-01 0.86397E-08
F22 1      7 0.92000E+05 0.39015E-01 -.32558E+06 0.24313E-07 0.38055E-09
M22 1      8 0.92000E+05 0.95512E+00 -.29261E+06 0.19161E+00 0.65359E-06
F11 2      9 0.92000E+05 0.28907E-01 -.50677E+05 0.34404E-08 0.30849E-11
M11 2     10 0.92000E+05 0.45117E+00 -.27591E+06 0.13213E-04 0.29590E-07
F21 2     11 0.92000E+05 0.22066E-01 -.77260E+05 0.43921E-09 0.38352E-13
M21 2     12 0.92000E+05 0.93434E+00 -.28694E+06 0.46808E-01 0.85756E-08
F12 2     13 0.92000E+05 0.40142E-01 -.10856E+05 0.28932E-07 0.31078E-11
M12 2     14 0.92000E+05 0.46551E+00 -.27937E+06 0.37428E-04 0.23928E-07
F22 2     15 0.92000E+05 0.92738E+00 -.11033E+07 0.17239E+00 0.43442E-03
M22 2     16 0.92000E+05 0.97286E+00 -.29309E+06 0.34690E+00 0.17260E-05
TP  1     17 0.92000E+05 0.85000E+00 0.00000E+00 0.51223E-35 0.00000E+00
TP  2     18 0.92000E+05 0.85000E+00 0.00000E+00 0.51223E-35 0.00000E+00
TP  3     19 0.92000E+05 0.85000E+00 0.00000E+00 0.51223E-35 0.00000E+00
TP  4     20 0.92000E+05 0.85000E+00 0.00000E+00 0.51223E-35 0.00000E+00
BT  1     21 0.92000E+05 0.85000E+00 -.11529E+07 0.10837E+00 0.14530E-07
BT  2     22 0.92000E+05 0.85000E+00 -.11529E+07 0.10837E+00 0.14530E-07
BT  3     23 0.92000E+05 0.85000E+00 -.11529E+07 0.10837E+00 0.14530E-07
BT  4     24 0.92000E+05 0.85000E+00 -.11529E+07 0.10837E+00 0.14530E-07

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

       START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97
```

KCYC = 254 - ITER = 7 - TIME = 0.31536E+14

ELEM1	ELEM2	INDEX	FLO(LIQ.) (KG/S)	VEL(LIQ.) (M/S)
F11 1	F11 2	1	0.70577E-10	0.24485E-11
M11 1	M11 2	2	0.38905E-08	0.26940E-10
F11 1	F12 1	3	-0.31552E-07	-0.73924E-09
M11 1	M12 1	4	-0.14320E-08	-0.22690E-10
F11 1	F21 1	5	-0.11833E-09	-0.27724E-11
M11 1	M21 1	6	-0.24584E-08	-0.38954E-10
F21 1	F21 2	7	0.27061E-12	0.12298E-13
M21 1	M21 2	8	0.18341E-08	0.82024E-11
F21 1	F22 1	9	-0.10578E-10	-0.57351E-12
M21 1	M22 1	10	-0.42930E-08	-0.21870E-10
F12 1	F12 2	11	0.17483E-08	0.43677E-10
M12 1	M12 2	12	-0.29099E-10	-0.29044E-12
F12 1	F22 1	13	-0.74900E-07	-0.13571E-08
M12 1	M22 1	14	-0.14035E-08	-0.14008E-10
F22 1	F22 2	15	-0.25453E-07	-0.65425E-09
M22 1	M22 2	16	-0.13234E-08	-0.69478E-10
F11 2	F12 2	17	0.33158E-09	0.82838E-11
M11 2	M12 2	18	-0.13180E-07	-0.91269E-10
F11 2	F21 2	19	-0.18668E-10	-0.64766E-12
M11 2	M21 2	20	-0.47716E-08	-0.33042E-10
F21 2	F22 2	21	-0.59297E-11	-0.26949E-12
M21 2	M22 2	22	-0.29376E-08	-0.13137E-10
F12 2	F22 2	23	-0.90150E-08	-0.22522E-09
M12 2	M22 2	24	-0.13715E-07	-0.83698E-10
F11 1	M11 1	25	-0.25554E-15	-0.59895E-14
F21 1	M21 1	26	-0.51366E-12	-0.14550E-12
F12 1	M12 1	27	-0.57876E-12	-0.37124E-13
F22 1	M22 1	28	0.43731E-08	0.82056E-07
F11 2	M11 2	29	-0.21842E-07	-0.13271E-09
F21 2	M21 2	30	-0.92120E-13	-0.73321E-15
F12 2	M12 2	31	-0.50512E-09	-0.31441E-10
F22 2	M22 2	32	0.17976E-07	0.41519E-06
TP 1	M11 1	33	-0.17362E-40	-0.20484E-43
TP 2	M11 2	34	-0.82790E-36	-0.97678E-39
TP 3	M12 1	35	-0.50503E-40	-0.59584E-43
TP 4	M12 2	36	-0.27126E-36	-0.32005E-39
BT 1	F21 1	37	0.10751E-09	0.58286E-11
BT 2	F21 2	38	0.12376E-10	0.56245E-12
BT 3	F22 1	39	0.53831E-07	0.13837E-08
BT 4	F22 2	40	0.52449E-07	0.56718E-10

@@@

START *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97

KCYC = 254 - ITER = 7 - TIME = 0.31536E+14

ELEMENT	SOURCE	INDEX	GENERATION RATE (KG/S) OR (W)	ENTHALPY (J/KG)	FF(GAS)	FF(LIQ.)	P(WB) (PA)
F11 1	0	1	0.31600E-07	0.00000E+00			
F11 2	0	2	0.21600E-07	0.00000E+00			
F12 1	0	3	0.41600E-07	0.00000E+00			
F12 2	0	4	0.11600E-07	0.00000E+00			

@@@

```
WRITE FILE *SAVE* AFTER  254 TIME STEPS  ---  THE TIME IS 0.315360E+14 SECONDS

********** VOLUME- AND MASS-BALANCES ****************************************************************

********** [KCYC,ITER] = [ 254,  7] *****                    THE TIME IS  0.31536E+14 SECONDS, OR  0.36500E+09 DAYS

PHASE VOLUMES IN PLACE
GAS  0.57372E+00 M**3;   LIQUID  0.95161E+00 M**3

LIQUID MASS IN PLACE  0.94890E+03 KG

*****************************************************************************************************


WRITE FILE *SAVE* AFTER  254 TIME STEPS  ---  THE TIME IS 0.315360E+14 SECONDS

*****************************************************************************************************
*                                                                                                   *
*                                   SUMMARY OF PROGRAM UNITS USED                                   *
*                                                                                                   *
*****************************************************************************************************

    UNIT    VERSION    DATE              COMMENTS
-----------------------------------------------------------------------------------------------------

    IO       1.0      15 APRIL     1991   OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*

    TOUGH2   1.1 CG   23 April     1993   MAIN PROGRAM
                                          special version for conjugate gradient package

    INPUT    1.02      7 FEBRUARY  1992   READ ALL DATA PROVIDED THROUGH FILE *INPUT*
    FLOP     1.0      11 APRIL     1991   CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC
    RFILE    1.02      7 FEBRUARY  1992   INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*

    CYCIT    1.11      7 FEBRUARY  1992   EXECUTIVE ROUTINE FOR MARCHING IN TIME

    EOS      0.9 X    18 August    1994   *EOS9* ... THERMOPHYSICAL PROPERTIES MODULE FOR SATURATED/UNSATURATED FLOW OF WATER
                                          includes capability for random modification of Pcap
                                          "finite" phase change window: remain single phase as long as P > PG*(1.-zero)
    SAT      1.1      10 JULY      1991   STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE
    VISW     1.1      10 JULY      1991   VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
    COWAT    1.1      10 JULY      1991   LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
    RELP     1.2      23 JANUARY   1992   LIQUID AND GAS PHASE RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION
    PCAP     1.2      23 JANUARY   1992   CAPILLARY PRESSURE AS FUNCTION OF SATURATION

    BALLA    1.0 S    15 JANUARY   1993   FOR EOS9: PERFORM SUMMARY BALANCES FOR VOLUME AND MASS

    MULTI    1.0 S    15 January   1993   special version for EOS9: sat/unsat. flow
    QU       1.01      2 JULY      1991   ASSEMBLE ALL SOURCE AND SINK TERMS
    LINEQ    0.9 CG   23 April     1993   Interface for linear equation solvers
                                          can call MA28 or a package of conjugate gradient solvers
    CONVER   1.01     27 JUNE      1991   UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED

    OUT      1.0 S     3 May       1994   FOR EOS9: PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
    WRIFI    1.02      5 FEBRUARY  1992   AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*

*****************************************************************************************************

END OF TOUGH2 SIMULATION RUN --- ELAPSED TIME = 9.744E-01 SEC--- CALCULATION TIME = 9.504E-01 SEC--- DATA INPUT TIME = 2.402E-02 SEC
```

```
*************************
File name:  rep.names
*************************

2
M11 1          tcwM1 0.100E+01                        0.5      0.5      -0.5
M12 1          tswM5 0.100E+01                        0.5      1.5      -0.5
```

Appendix B

T2FEHM2 Output Files with Screen Input

```
****************************
Screen Input for T2FEHM2
****************************

picard% ../src/t2fehm2

 This program will re-format TOUGH2 output files
 for FEHM restart files. The following files
 must be present: input, output, and MESH.
 The MESH file should contain 5-character material
 names.

 What is the name of the input file?
TOUGH2.INP

 What is the name of the output file?
TOUGH2.OUT

 What is the name of the MESH file?
mesh.dat

What type of run is this?
1) SNL EOS3
2) SNL EOS9?
3) LBNL EOS9
3

 What reference name would you like to use for the
 FEHM restart files? (no spaces in the name)
QAtest

 In ELEME, how are the elements listed?
 (1) Alternatively with matrix first
 (2) Alternatively with fracture first
 (3) All matrix, then all fractures
 (4) All fractures, then all matrix
2

 For fracture-matrix connections, which element is
 listed first:  (1) Fracture or (2) Matrix?
1

 What is the print-out time (sec) of interest?
3.1536e13

 The fracture volumes will be used as the primary
 control volume for each element.  Have they been
 modified in TOUGH2.INP? (1=yes,  0=no)
0

What is the geometry?
0) 3-D
1) X-Y Plane
2) X-Z Plane
3) Y-Z Plane
0
```

```
 Is there a file with repository element names?
 1 = yes,  0 = no
1

What is the name of the file with repository elements?
rep.names
 Would you like to modify the 2nd character of the
 element name?  1=yes,  0=no
0

 Thank You!  Please wait while I work...
Have read in       24 elements from MESH...
Have read in       40 connections from MESH...
 Have read in state variables from output file...
 Have read in flux variables from output file...
Finished processing printout at   0.3154E+14 sec
 Done!!!
```

Output:

```
QAtest.check
QAtest.dat
QAtest.dpdp
QAtest.files
QAtest.grid
QAtest.ini
QAtest.rock
QAtest.stor
QAtest.zone
QAtest.zone2
```

```
**************************
File name:  QAtest.check
**************************

1 3
2 3
3 3
4 3
5 3
6 3
7 3
8 3
9 3
10 3
11 3
12 3
13 3
14 3
15 3
```

```
**************************
File name:  QAtest.dat
**************************

START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97
# Particle tracking for TOUGH2 flow field
dpdp
file
QAtest.dpdp
perm
1  0  0   0.100E-14 0.100E-14 0.100E-14

rlp
1  0.  0.  1.  1.  0.  1.

1  0  0  1

rock
file
QAtest.rock
flow

time
  0.36525E+09  0.36525E+09      10      10    1997      10

ctrl
     -10  0.10E-03      40
       1        0        0        1
0
      1.00      3.00      1.00
       5  0.20E+01  0.10E-09  0.10E+11
       0        1
iter
  0.10E-04  0.10E-04  0.10E-04 -0.10E-03  0.12E+01
       0        0        0        0  0.14E+05
sol
       1      -1
rflo
air
-1
20.0  0.1
node
1
1
zone
file
QAtest.zone2
ptrk
file
QAtest.ptrk
stop
```

```
*************************
File name:  QAtest.dpdp
*************************

dpdp
1
       -9       0       0     0.2330E-03
      -10       0       0     0.4840E-04
      -11       0       0     0.1300E-03
      -12       0       0     0.3290E-03
      -13       0       0     0.4920E-03
      -14       0       0     0.7140E-04
      -15       0       0     0.1100E-04
      -16       0       0     0.1100E-04

        1       0       0     99.

stop
```

```
***************************
File name:  QAtest.files
***************************

QAtest.dat
QAtest.grid
QAtest.zone
QAtest.out
QAtest.ini
QAtest.fin
QAtest.his
QAtest.trc
QAtest.con

QAtest.stor
QAtest.chk
all
0
```

```
*************************
File name:  QAtest.grid
*************************

coor
        8
        1          0.50          0.50          -0.50
        2          0.50          0.50          -1.50
        3          0.50          1.50          -0.50
        4          0.50          1.50          -1.50
        5          1.50          0.50          -0.50
        6          1.50          0.50          -1.50
        7          1.50          1.50          -0.50
        8          1.50          1.50          -1.50

elem
2  1
1  2  1

stop
```

```
*************************
File name:  QAtest.ini
*************************

START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97
This is a .ini file with saturations, pressures and mass flux values.
0.
air
ptrk
nstr
dpdp
ndua
  0.42804000E-01  0.18497000E-01  0.55351000E-01  0.39015000E-01
  0.28907000E-01  0.22066000E-01  0.40142000E-01  0.92738000
  0.95895000      0.53349000      0.87371000      0.95512000
  0.45117000      0.93434000      0.46551000      0.97286000
  0.92000000E-01  0.92000000E-01  0.92000000E-01  0.92000000E-01
  0.92000000E-01  0.92000000E-01  0.92000000E-01  0.92000000E-01
  0.92000000E-01  0.92000000E-01  0.92000000E-01  0.92000000E-01
  0.92000000E-01  0.92000000E-01  0.92000000E-01  0.92000000E-01
mass flux values
      72      #ntotmfv=       64, nnodes=      16, number of f-m connections=        8
-0.31600000E-07 0.11833000E-09 0.31552000E-07-0.70577000E-10-0.11833000E-09
 0.10751000E-09 0.10578000E-10-0.27061000E-12-0.31552000E-07-0.41600000E-07
 0.74900000E-07-0.17483000E-08-0.10578000E-10-0.74900000E-07 0.53831000E-07
 0.25453000E-07 0.70577000E-10-0.21600000E-07 0.18668000E-10-0.33158000E-09
 0.27061000E-12-0.18668000E-10 0.12376000E-10 0.59297000E-11 0.17483000E-08
 0.33158000E-09-0.11600000E-07 0.90150000E-08-0.25453000E-07-0.59297000E-11
-0.90150000E-08 0.52449000E-07        0.      0.24584000E-08 0.14320000E-08
-0.38905000E-08-0.24584000E-08        0.      0.42930000E-08-0.18341000E-08
-0.14320000E-08        0.      0.14035000E-08 0.29099000E-10-0.42930000E-08
-0.14035000E-08        0.      0.13234000E-08 0.38905000E-08        0.
 0.47716000E-08 0.13180000E-07 0.18341000E-08-0.47716000E-08        0.
 0.29376000E-08-0.29099000E-10-0.13180000E-07        0.      0.13715000E-07
-0.13234000E-08-0.29376000E-08-0.13715000E-07        0.      0.25554000E-15
 0.51366000E-12 0.57876000E-12-0.43731000E-08 0.21842000E-07 0.92120000E-13
 0.50512000E-09-0.17976000E-07
```

```
*************************
File name:  QAtest.rock
*************************

rock
        -1      0      0    0.2480E+04    0.1000E+04    0.6600E-01
        -2      0      0    0.2300E+04    0.1000E+04    0.3690E+00
        -3      0      0    0.2300E+04    0.1000E+04    0.3530E+00
        -4      0      0    0.2480E+04    0.1000E+04    0.1150E+00
        -5      0      0    0.2480E+04    0.1000E+04    0.2000E-01
        -6      0      0    0.2300E+04    0.1000E+04    0.3210E+00
        -7      0      0    0.2300E+04    0.1000E+04    0.2400E+00
        -8      0      0    0.2480E+04    0.1000E+04    0.3600E-01
        -9      0      0    0.2480E+04    0.1000E+04    0.1000E+01
       -10      0      0    0.2300E+04    0.1000E+04    0.1000E+01
       -11      0      0    0.2300E+04    0.1000E+04    0.1000E+01
       -12      0      0    0.2480E+04    0.1000E+04    0.1000E+01
       -13      0      0    0.2480E+04    0.1000E+04    0.1000E+01
       -14      0      0    0.2300E+04    0.1000E+04    0.1000E+01
       -15      0      0    0.2300E+04    0.1000E+04    0.1000E+01
       -16      0      0    0.2480E+04    0.1000E+04    0.1000E+01
       -17      0      0    0.9950E+00    0.1000E+04    0.1000E+01
       -18      0      0    0.2300E+04    0.1000E+04    0.2800E+00

stop
```

```
*************************
File name:  QAtest.stor
*************************

START  *** Verification Run for Option 1 Post-Processing *** C.K.Ho 11/11/97
This is a .stor file with dummy area coefficients
      32         8        41         1
  1.00000000E+00  1.00000000E+00  1.00000000E+00  1.00000000E+00  1.00000000E+00
  1.00000000E+00  1.00000000E+00  1.00000000E+00
       9        13        17        21        25
      29        33        37        41         1
       2         3         5         1         2
       4         6         1         3         4
       7         2         3         4         8
       1         5         6         7         2
       5         6         8         3         5
       7         8         4         6         7
       8
       1         2         3         4         5
       6         7         8         9        10
      11        12        13        14        15
      16        17        18        19        20
      21        22        23        24        25
      26        27        28        29        30
     .31        32         0         0         0
       0         0         0         0         0
       0
      10        15        19        24        27
      32        36        41
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00 -1.00000000E+00
 -1.00000000E+00 -1.00000000E+00
```

```
*************************
File name:  QAtest.zone
*************************

zone
   1       #tcwM1
nnum
           1
           9
   2       #ptnM1
nnum
           1
          10
   3       #ptnM3
nnum
           1
          15
   4       #tswM5
nnum
           1
          11
   5       #tswM7
nnum
           1
          12
   6       #ch3Mv
nnum
           1
          13
   7       #ch3Mz
nnum
           1
          14
   8       #pcM37
nnum
           1
          16
   9       #tcwF1
nnum
           1
           1
  10       #ptnF1
nnum
           1
           2
  11       #ptnF3
nnum
           1
           7
  12       #tswF5
nnum
           1
           3
  13       #tswF7
nnum
           1
           4
  14       #ch3Fv
```

```
nnum
            1
            5
   15       #ch3Fz
nnum
            1
            6
   16       #pwF37
nnum
            1
            8
   17       #topbd
nnum
            0
   18       #botbd
nnum
            0

stop

#Total number of nodes =        16
#Total number of active boundary materials =        2
#Total number of active boundary nodes =        8
```

```
*************************
File name:  QAtest.zone2
*************************

zone
   1      #tcwM1
nnum
          1
          9
   2      #ptnM1
nnum
          1
         10
   3      #ptnM3
nnum
          1
         15
   4      #tswM5
nnum
          1
         11
   5      #tswM7
nnum
          1
         12
   6      #ch3Mv
nnum
          1
         13
   7      #ch3Mz
nnum
          1
         14
   8      #pcM37
nnum
          1
         16
   9      #tcwF1
nnum
          1
          1
  10      #ptnF1
nnum
          1
          2
  11      #ptnF3
nnum
          1
          7
  12      #tswF5
nnum
          1
          3
  13      #tswF7
nnum
          1
          4
  14      #ch3Fv
```

```
nnum
         1
         5
  15     #ch3Fz
nnum
         1
         6
  16     #pwF37
nnum
         1
         8
  17     #topbd
nnum
         0
  18     #botbd
nnum
         0
 500    #fracture repository nodes
nnum
         2
         1          3
 501    #matrix repository nodes
nnum
         2
         9          11

stop

#Total number of nodes =        16
#Total number of active boundary materials =        2
#Total number of active boundary nodes =        8
```

Appendix C
Program Listing for T2FEHM2

```
*************************
File name:  t2fehm2.f
*************************

C*****************************************************************
c     This program creates column formatted files from TOUGH2.OUT
c     files of EOS3 simulations.
c     Files  MESH, TOUGH2.INP, and TOUGH2.OUT must be present.
c     The format of the output files are amenable for an FEHM
c     restart.
c                          C.K.Ho 5/27/97
c  This version now re-formats TOUGH2.OUT files in either EOS3 or
c  EOS9 format. Multidimensional files can be post-processed. This
c  version assumes that the elements listed in ELEME alternate
c  between fractures and matrix, starting with a fracture element.
c  This can be generalized in the loop (do 3000...) by knowing how
c  how the fracture and matrix elements were listed and by arranging
c  the arrays accordingly.  I started this by asking the user to
c  specify the ordering, but I didn't do much with it in this version.
c  So for now, the elements should be listed alternately starting with
c  a fracture element. Also, the matrix materials are assumed to be listed
c  first in the ROCKS card.
c
c     C.K.Ho
c     9/2/97-9/12/97,9/19/97
c  This version (op1postv3.f) is tailored specifically for LBL site-scale
c  runs. The previous version (option1postv2.f) is still good for SNL
c  TOUGH2 simulations of flow fields.  The major revisions include reading
c  information from external files (MESH, GENER). In MESH, the material
c  identifier is a 5-character name--not an integer, which was assumed in
c  the previous version.  The coordinates will have to be
c  read from MESH. Changes will have to be made for recognizing
c  fracture or matrix materials to accomodate all the materials (there
c  are greater than 100 materials) in the site-scale model. The dimensions
c  will have to be greatly increased to accommodate the 80,000 element
c  site-scale model.
c     C.K.Ho
c     10/23/97
c
c  This version (op1postv4.f) does not assume any ordering in the ROCKS
c  card.  There can be different numbers of matrix and fracture
c  materials written to the FEHM zone macro.  Also, this version can read
c  in a file containing repository element names to create a separate zone.
c  Another assumption is that the active elements are listed before any
c  boundary elements ('TP' or 'BT') in ELEME.
c     C.K.Ho
c     11/5/97
c
c  A few things have been cleaned up and it appears to work for the LBNL
c  3-D site scale model.  The current version is 't2fehm2.f'.
c     C.K.Ho
c     11/6/97
C*****************************************************************
c2345678901234567890123456789012345678901234567890123456789012
C
      implicit double precision (a-h,o-z)
      DIMENSION X(99000),Y(99000),z(99000),SL(99000),vol(99000)
      dimension PG(99000)
```

```
      dimension gelem(99000),ifm(99000)
      dimension flux1(990000),fmlfm(99000),ncord(99000)
      dimension icon2(990000),flo12(990000),istrw(990000)
      dimension drok(500),por(500),nelmdg(99000),ncon2(99000)
      double precision lblpor
      CHARACTER*22 BLOCK
      CHARACTER*5  ELEMN(99000),ELEM1(490000),ELEM2(490000),ELEMX
      character*5  genname,matname(500),matb,mat(99000)
      character*80 header
      character*40 filen,control,dat,grid,ini,stor,dpdp,rock,zone
      character*40 filein,fileout,meshfile,repfile,zone2,check
      character*1 char2
      character*5 repname(1003)
      common/int/ ncon(99000),icon(99000,35)
      common/flux/ flol(99000,35)
c
      write(*,*) 'This program will re-format TOUGH2 output files'
      write(*,*)'for FEHM restart files. The following files'
      write(*,*)'must be present: input, output, and MESH.'
      write(*,*)'The MESH file should contain 5-character material'
      write(*,*)'names.'
      write(*,*)
      write(*,*)'What is the name of the input file?'
      read(*,*) filein
      write(*,*)'What is the name of the output file?'
      read(*,*) fileout
      write(*,*)'What is the name of the MESH file?'
      read(*,*) meshfile
      write(*,4)
4     format('What type of run is this?'/,'1) SNL EOS3'/,'2) SNL EOS9?'/
     & ,'3) LBNL EOS9')
      read(*,*) neos
      write(*,*)'What reference name would you like to use for the'
      write(*,*)'FEHM restart files? (no spaces in the name)'
      read(*,*) filen
      write(*,*)'In ELEME, how are the elements listed?'
      write(*,*)'(1) Alternatively with matrix first'
      write(*,*)'(2) Alternatively with fracture first'
      write(*,*)'(3) All matrix, then all fractures'
      write(*,*)'(4) All fractures, then all matrix'
      read(*,*) norder
      write(*,*)'For fracture-matrix connections, which element is'
      write(*,*)'listed first:  (1) Fracture or (2) Matrix?'
      read(*,*) nfmc
      write(*,*)'What is the print-out time (sec) of interest?'
      read(*,*) tsec
      write(*,*)'The fracture volumes will be used as the primary'
      write(*,*)'control volume for each element.  Have they been'
      write(*,*)'modified in TOUGH2.INP? (1=yes,  0=no)'
      read(*,*) nvol
      volscale=1.
      if(nvol.eq.1) then
        write(*,*)'What is the scaling factor to retrieve correct',
     &  ' primary volumes from fracture volumes?'
        read(*,*) volscale
      end if
      write(*,7)
7     format('What is the geometry?'/'0) 3-D'/'1) X-Y Plane'/
```

```
     &        '2) X-Z Plane','3) Y-Z Plane')
      read(*,*) icnl
      write(*,*)'Is there a file with repository element names?'
      write(*,*)'1 = yes,  0 = no'
      read(*,*) nrepans
      if(nrepans.eq.1) then
        write(*,9)
9     format('What is the name of the file with repository elements?')
        read(*,*) repfile
        write(*,*)'Would you like to modify the 2nd character of the'
        write(*,*)'element name?  1=yes,  0=no'
        read(*,*) n2nd
        if(n2nd.eq.1) then
          write(*,*)'What character would you like to use?'
          read(*,'(a1)') char2
        end if
        open(19,file=repfile,status='old')
      end if

      if(norder.eq.1.or.norder.eq.2) then
        nalt=2
      else
        nalt=1
      end if

c...Define FEHM restart files based on reference name
      kend=index(filen,' ')
      control=filen(1:kend-1)//'.files'
      dat=filen(1:kend-1)//'.dat'
      grid=filen(1:kend-1)//'.grid'
      ini=filen(1:kend-1)//'.ini'
      stor=filen(1:kend-1)//'.stor'
      dpdp=filen(1:kend-1)//'.dpdp'
      rock=filen(1:kend-1)//'.rock'
      zone=filen(1:kend-1)//'.zone'
      zone2=filen(1:kend-1)//'.zone2'
      check=filen(1:kend-1)//'.check'

      if(neos.eq.1) then
        nlin1=5
        nlin2=3
        nlin3=3
      elseif(neos.eq.2) then
        nlin1=6
        nlin2=4
        nlin3=4
      elseif(neos.eq.3) then
        nlin1=6
        nlin2=3
        nlin3=4
      end if

      write(*,*) 'Thank You!  Please wait while I work...'
      open(1,file=meshfile,status='old')
      open(2,file=fileout,status='old')
      open(3,file=filein,status='old')
      open(11,file=control,status='unknown')
      open(12,file=dat,status='unknown')
```

```
      open(13,file=grid,status='unknown')
      open(14,file=ini,status='unknown')
      open(15,file=stor,status='unknown')
      open(16,file=dpdp,status='unknown')
      open(17,file=rock,status='unknown')
      open(18,file=zone,status='unknown')
      open(22,file=check,status='unknown')
      open(23,file=zone2,status='unknown')

c....Data
      spht=1.e3
      per1=1.e-15
      per2=1.e-15
      per3=1.e-15
      day=365.25e6
      tims=365.25e6
      nstep=10
      iprtout=10
      iyear=1997
      month=10
      maxit=-10
      epm=1.e-4
      north=40
      ja=1
      jb=0
      jc=0
      igaus=1
      as=1.
      grav=3.
      upwgt=1.
      iamm=5
      aiaa=2.
      daymin=1.e-10
      daymax=1.e10
      lda=1
      g1=1.e-5
      g2=1.e-5
      g3=1.e-5
      tmch=-1.e-4
      overf=1.2
      irdof=0
      islord=0
      iback=0
      icoupl=0
      rnmax=14400.
      ntt=1
      intg=-1
      zero=1.d-10
      ra=287.
      rv=461.52
c
c...Read header from TOUGH2.INP
      read(3,'(a80)') header

c_____________________________________________________________________
c...Write information to .dat file
      write(12,510) header
510   format(a80/'# Particle tracking for TOUGH2 flow field')
```

```
c...Write dpdp macro
      write(12,516) dpdp
516   format('dpdp'/'file'/a)

c...Write perm macro
      write(12,518) per1,per2,per3
518   format('perm'/'1  0  0  ',3e10.3/)

c...Write rlp macro
      write(12,520)
520   format('rlp'/'1  0.  0.  1.  1.  0.  1.'//'1  0  0  1'/)

c...Write rock macro
      write(12,522) rock
522   format('rock'/'file'/a)

c...Write flow macro
      write(12,524)
524   format('flow'/)

c...Write time macro
      write(12,526) day,tims,nstep,iprtout,iyear,month
526   format('time'/2e13.5,4i8/)

c...Write ctrl macro
      write(12,528) maxit,epm,north,ja,jb,jc,igaus,as,grav,upwgt,
     & iamm,aiaa,daymin,daymax,icnl,lda
528   format('ctrl'/i8,e10.2,i8/4i8/'0'/3f10.2/i8,3e10.2/2i8)

c...Write iter macro
      write(12,530) g1,g2,g3,tmch,overf,irdof,islord,iback,icoupl,
     & rnmax
530   format('iter'/5e10.2/4i8,e10.2)

c...Write sol macro
      write(12,532) ntt,intg
532   format('sol'/2i8)

c...Write rflo macro
      write(12,534)
534   format('rflo'/'air'/'-1'/'20.0  0.1')

c...Write node macro
      write(12,536)
536   format('node'/'1'/'1')

c...Write zone macro that corresponds to the repository nodes
      write(12,515) zone2
515   format('zone'/'file'/a)

c...Write ptrk macro
      write(12,538) filen(1:kend-1)
538   format('ptrk'/'file'/a,'.ptrk')

c...Write stop
      write(12,540)
540   format('stop')
```

```
c_______________________________________________________________________

c...Write information to control file
       write(11,501) dat,grid,zone,filen(1:kend-1),ini,filen(1:kend-1)
      &,filen(1:kend-1),filen(1:kend-1),filen(1:kend-1),stor,
      &filen(1:kend-1)
501    format(a/a/a/a,'.out'/a/a,'.fin'/a,'.his'/a,'.trc'/a,'.con'//
      & a/a,'.chk'/'all'/'0')

c...Read in repository element names
       if(nrepans.eq.1) then
         read(19,*) nrepelem
         numrep=nrepelem
         do i=1,nrepelem
           read(19,'(a5)') repname(i)
           repname(i)(1:1)='F'
           if(n2nd.eq.1) repname(i)(2:2)=char2
         end do
       end if

c...Read in grid information from MESH
      nbelm=0
      nbmat=0
      matb='     '
      N=1
      read(1,1000) block
1000  format(a22)
99    read(1,65) elemn(n),mat(n),vol(n),x(n),y(n),z(n)
65    format(a5,10x,a5,e10.4,20x,3e10.4)
      if(elemn(n).eq.'     ') go to 98
      if(elemn(n)(4:4).eq.'0') elemn(n)(4:4)=' '
c...Count number of boundary elements, nbelm, and number of boundary
c...materials, nbmat.
      if(elemn(n)(1:2).eq.'TP'.or.elemn(n)(1:2).eq.'BT') then
        nbelm=nbelm+1
        if(mat(n).ne.matb) then
          nbmat=nbmat+1
          matb=mat(n)
        end if
      end if
      N=N+1
      GO TO 99
98    CONTINUE
      NMAX = N - 1
c...NMAX is the total number of elements read from MESH
      write(*,107) nmax
107   format('Have read in ',i8,' elements from MESH...')
c...nnodes is the total number of active nodes
      nnodes=nmax-nbelm

c...Find maximum number of materials used in ROCKS (nmat)
c      nmat=0
c      do i=1,nmax
c        nmat=max(mat(i),nmat)
c      end do
c      write(*,222) nmat
c222   format('Maximum number of active materials = ',i8,'...')
```

```
c...nfmat is the number of fracture materials
c     nfmat=(nmat-nbmat)/2

c...Read in connection information from MESH
      N=1
      READ(1,1500) BLOCK
1500  FORMAT(A22,3X,25X,E10.4)
199   read(1,1502) elem1(n),elem2(n),ifm(n)
c...ifm(n) is a flag in the 75th column of the CONNE card that Yu-Shu has
c...specified as equal to '2' for fracture-matrix connections
1502  format(2a5,64x,i1)
      IF(elem1(n)(1:5).EQ.'     '.OR.elem1(n)(1:3).EQ.'+++') GO TO 198
      if(elem1(n)(4:4).eq.'0') elem1(n)(4:4)=' '
      if(elem2(n)(4:4).eq.'0') elem2(n)(4:4)=' '
      N=N+1
      GO TO 199
198   CONTINUE
      NCMAX = N - 1
c...NCMAX is the total number of connections read from MESH
      write(*,203) ncmax
203   format('Have read in ',i8,' connections from MESH...')

c...Read in ROCKS information from TOUGH2 input file
18    read(3,1000) block
      if(block(1:5).ne.'ROCKS') go to 18

      i=1
      nfmat=0
      nmmat=0
408   read(3,410) matname(i),drok(i),por(i)
410   format(a5,5x,2e10.4)
      if(matname(i).eq.'REFCO') go to 408
      if(matname(i).eq.'     ') then
c...ntotmat is the total number of materials in the ROCKS card
c...nmat is the number of materials associated with non-boundary
c...elements
        ntotmat=i-1
        nmat=ntotmat-nbmat
        go to 27
      end if
c...LBNL uses columns 71-80 in the second line of each material card to
c...identify the fracture porosity
      read(3,415) lblpor
415   format(70x,e10.4)
c...nfmat is the total number of fracture materials
      if(matname(i)(3:3).eq.'F'.or.matname(i)(4:4).eq.'F') then
        nfmat=nfmat+1
        if(neos.eq.3) por(i)=lblpor
c...The perched water fractures do not have porosities listed in ROCKS.
c...Yu-Shu said that they have the same porosity as the zeolitic fractures,
c...which is 1.1e-5 (phone message 10/31/97).
        if(por(i).eq.0.) por(i)=1.1d-5
      end if
c...nmmat is the total number of matrix materials
      if(matname(i)(3:3).eq.'M'.or.matname(i)(4:4).eq.'M') nmmat=nmmat+1
      read(3,*)
      read(3,*)
      i=i+1
```

```
      go to 408

 27   continue

 c...10/27/97 Ho

 c...Write grid macro file
      write(13,202) nnodes/2
 202  format('coor'/i8)
 c...This assumes that all boundary elements ('TP' and 'BT') are listed
 c...after the active elements in ELEME
      do i=1,nnodes/2
        write(13,204) i,x(i*nalt),y(i*nalt),z(i*nalt)
 204    format(i8,3(3x,f10.2))
      end do
      write(13,206)
 206  format(/'elem'/'2  1'/'1  2  1'//'stop')

 c...Initialize generation array
      do i=1,nmax
        gelem(i)=0.
      end do

 c...Read in generation information from TOUGH2.INP
      i=1
 33   read(3,1000,end=299) block
      if(block(1:5).ne.'GENER') go to 33
 74   read(3,75) genname,g
 75   format(a5,35x,e10.4)
      if(genname.eq.'     ') go to 77
      if(genname(4:4).eq.'0') genname(4:4)=' '
      do ik=1,nmax
       if(genname.eq.elemn(ik)) then
 c...Assign a generation term for each element (flow into an element
 c...is defined as negative)
 c...The method used here is different than in v3.  It eliminates a
 c...separate do-loop and the need for arrays igen and g.
         gelem(ik)=-g
         i=i+1
         go to 74
       end if
      end do
      write(*,*)'Could not find element name for generation'
      write(*,79) i,genname
 79   format('element ',i8,': ',a5)
      stop

 299  write(*,*)'***Warning*** No generation card in TOUGH2.INP'

 77   ngentot=i-1

 c...Write zone macro
      ntotin=0
      write(18,'(a4)') 'zone'
      write(23,'(a4)') 'zone'
      do i=1,ntotmat
        write(18,512) i,matname(i)
        write(23,512) i,matname(i)
```

```
512     format(i4,5x,'#',a5)
        write(18,'(a4)') 'nnum'
        write(23,'(a4)') 'nnum'
        nin=1
        do j=1,nmax
c...Match nodes to respective materials. This assumes that the
c...fractures and matrix elements are listed alternately in ELEME
c...starting with the fractures first
c...If element is a boundary element, go to next element
          if(elemn(j)(1:2).eq.'TP'.or.elemn(j)(1:2).eq.'BT') goto 517
          if(mat(j).eq.matname(i)) then
            if(mat(j)(3:3).eq.'F'.or.mat(j)(4:4).eq.'F') then
              ncord(nin)=(j+1)/nalt
              nin=nin+1
              go to 517
            end if
            if(mat(j)(3:3).eq.'M'.or.mat(j)(4:4).eq.'M') then
              ncord(nin)=j/nalt+nnodes/2.
              nin=nin+1
            end if
          end if
517     end do
        nin=nin-1
        ntotin=ntotin+nin
        write(18,'(i10)') nin
        write(23,'(i10)') nin
        if(nin.gt.0) write(18,'(8i10)') (ncord(k),k=1,nin)
        if(nin.gt.0) write(23,'(8i10)') (ncord(k),k=1,nin)
      end do
      write(18,*)
      write(18,'(a4)') 'stop'

c...Now write zones for nodes corresponding to repository elements
      nrp=1
      do i=1,nmax
        do j=1,numrep
          if(elemn(i).eq.repname(j)) then
            ncord(nrp)=(i+1)/nalt
            nrp=nrp+1
            go to 527
          end if
        end do
527   end do

      nrp=nrp-1
      write(23,*) '500    #fracture repository nodes'
      write(23,'(a4)') 'nnum'
      write(23,'(i10)') nrp
      if(nrp.gt.0) write(23,'(8i10)') (ncord(k),k=1,nrp)
      write(23,*) '501    #matrix repository nodes'
      write(23,'(a4)') 'nnum'
      write(23,'(i10)') nrp
      do i=1,nrp
        ncord(i)=ncord(i)+nnodes/2.
      end do
      if(nrp.gt.0) write(23,'(8i10)') (ncord(k),k=1,nrp)
      write(23,*)
      write(23,'(a4)') 'stop'
```

```
c...Now write some additional information to the zone file
      write(18,*)
      write(23,*)
      write(18,514) ntotin,nbmat,nbelm
      write(23,514) ntotin,nbmat,nbelm
514   format(/'#Total number of nodes = ',i8/'#Total number of',
     & ' active boundary materials = ',i8/'#Total number of active',
     & ' boundary nodes = ',i8/)

c...Write dpdp macro file
      write(16,550)
550   format('dpdp'/'1')
c...Loop over the materials and print out fracture porosities
      do i=1,ntotmat
        if(matname(i)(3:3).eq.'F'.or.matname(i)(4:4).eq.'F') then
          write(16,552) -i,jb,jc,por(i)
552       format(3i8,5x,e10.4)
        end if
      end do
      write(16,554) ja,jb,jc
554   format(/,3i8,5x,'99.'//'stop')

c...Write rock macro file
      write(17,556)
556   format('rock')
      do i=1,ntotmat
        porock=por(i)
        if(matname(i)(3:3).eq.'F'.or.matname(i)(4:4).eq.'F')porock=1.
        write(17,558) -i,jb,jc,drok(i),spht,porock
558     format(3i8,5x,e10.4,5x,e10.4,5x,e10.4)
      end do
      write(17,559)
559   format(/'stop')

c...Search for "TOTAL TIME" in TOUGH2.OUT and then read in variables
89    READ(2,1000,END=90) BLOCK
      IF(BLOCK(1:12).NE.'  TOTAL TIME') GO TO 89
      READ(2,1001) TIME
      if(time.ne.tsec) go to 89
1001  FORMAT(E13.5)
      do nl=1,nlin1
        READ(2,1000) BLOCK
      end do
c
c23456789012345678901234567890123456789012345678901234567890123456789012

c...Read in state variables from TOUGH2.OUT
115   N1=1
      N2=MIN(NMAX,45)
      DO 2000 I=N1,N2
      if(neos.eq.1) then
c...    This is EOS3 format
        READ(2,1002) PG(I),SL(I)
1002    FORMAT(12x,e12.5,24x,7e12.5)
      else
c...    This is EOS9 format
        read(2,118) pg(i),sl(i)
```

```
118     format(12x,2e12.5)
      end if
2000  CONTINUE
C
2100  CONTINUE
c...Check to see if we've read in all the element variables
      IF(N2.EQ.NMAX) GO TO 91
      N1=N2+1
      N2=MIN(NMAX,N1+56)
      do n1=1,nlin2
        READ(2,1000) BLOCK
      end do
      DO 2010 I=N1,N2
      if(neos.eq.1) then
c...    This is EOS3 format
        READ(2,1002) PG(I),SL(I)
      else
c...    This is EOS9 format
        read(2,118) pg(i),sl(i)
      end if
2010  CONTINUE
      GO TO 2100
C
91    CONTINUE
C
c...Write saturations to .ini file (fractures saturations first followed
c...by matrix saturations)
      write(14,302) header
302   format(a80/'This is a .ini file with saturations, pressures',
     & ' and mass flux values.'/'0.'/'air'/'ptrk'/'nstr'/
     & 'dpdp'/'ndua')
      write(14,304) (sl(i),i=1,nnodes,2),(sl(i),i=2,nnodes,2)
304   format(4g16.8)

c...Write pressures to .ini file in MPa (fractures first, then matrix)
      write(14,304) (pg(i)*1.d-6,i=1,nnodes,2),
     & (pg(i)*1.d-6,i=2,nnodes,2)

      write(*,*)'Have read in state variables from output file...'
C
c...Read in flux variables from TOUGH2.OUT
289   READ(2,1500,END=190) BLOCK
      IF(BLOCK(11:22).NE.'ELEM1  ELEM2') GO TO 289
      READ(2,1500) BLOCK
      READ(2,1500) BLOCK
C
c...Read in mass flow liquid for each connection pair
      N1=1
      N2=MIN(NCMAX,53)
      DO 1600 I=N1,N2
      if(neos.eq.1) then
        READ(2,1003) fluxl(I)
1003    FORMAT(80x,4e13.5)
      else
        read(2,121) fluxl(i)
121     format(29x,e13.5)
      end if
1600  CONTINUE
```

```
C
2150  CONTINUE
      IF(N2.EQ.NCMAX) GO TO 191
      N1=N2+1
      N2=MIN(NCMAX,N1+56)
      do n1=1,nlin3
        READ(2,1500) BLOCK
      end do
      DO 2020 I=N1,N2
      if(neos.eq.1) then
        READ(2,1003) fluxl(I)
      else
        read(2,121) fluxl(i)
      end if
2020  CONTINUE
      GO TO 2150
C
191   CONTINUE

C
190   CONTINUE

c...Check
      write(*,*)'Have read in flux variables from output file...'

c...Check
c       do i=1,ncmax
c         write(15,444) i,elem1(i),elem2(i),fluxl(i)
c444     format(i8,2x,2(a5,2x),e10.4)
c       end do
c       stop
c...End check
C
c...Loop over all elements to determine connections and fluxes for each
c...element
      nmlfm=1
c...nmlfm is the total number of fracture-matrix connections
      DO 3000 I=1,NMAX

        if(mod(i,1000).eq.0) write(*,472) i
472     format('Still working...  Element ',i8)

c...fmlfm(i) is the flow (kg/s) between fracture and matrix
        fmlfm(i)=0.d0

c...jj is the number of connections for each element
        do jj=1,35
          flol(i,jj)=0.d0
c...icon(i,jj) is the node number of the element for connection jj to element
i
          icon(i,jj)=0
        end do

       ELEMX=ELEMN(I)

c...If element is a boundary element, go to next element
       if(elemx(1:2).eq.'TP'.or.elemx(1:2).eq.'BT') go to 3000
```

```
c...Write the element number and the number of connections for that element
      if(i.gt.1) write(22,*) i-1,ncon(i-1)
c_____________________________________________________________________________
c...For each element, loop over all connections to determine if
c...the element is either the first or second element in each connection
c...nc is the number of connections per element

      nc=1
      DO 3001 J=1,NCMAX

c...Say element is the first element in the connection
       if(elem1(j).eq.elemx) then
        nsign=-1
c...If connecting element is the top boundary, go to next connection
        if(elem2(j)(1:2).eq.'TP') go to 3001
c...If connecting element is the bottom boundary, treat the flow to the
c...bottom boundary as a sink/source term and move on to the next connection
        if(elem2(j)(1:2).eq.'BT') then
          gelem(i)=flux1(j)*nsign
          go to 3001
        end if
c...What is the second element in the connection?
        do ii=1,nmax
         if(elem2(j).eq.elemn(ii)) then
          k2nd=ii
c...Determine if the connection is between a fracture and matrix element
c...If it is a fracture-matrix connection (both elements have the same
c...coordinates, or ifm=2), store this flux separately from fracture-fracture
c...or matrix-matrix fluxes.
          dx=dabs(x(k2nd)-x(i))
          dy=dabs(y(k2nd)-y(i))
          dz=dabs(z(k2nd)-z(i))
          if(dx.le.zero.and.dy.le.zero.and.dz.le.zero.or.
     &       ifm(j).eq.2) then
c...If the first element of f-m connection is a fracture, then process this
            if(nfmc.eq.1) then
              go to 3017
            else
              go to 3001
            end if
          end if
          icon(i,nc)=ii
          flo1(i,nc)=flux1(j)*nsign
          nc=nc+1
          go to 3002
         endif
        end do
        write(*,7001) elemx,j,elem2(j),elem2(j-1),elem2(j+1)
7001    format('***Could not find 2nd element in connection for',
     &  ' first element ',a5,'***'/'Connection index = ',i8/
     &  'Second element = ',a5/'j-1= ',a5/'j+1= ',a5)
        stop
       end if

c...If no match in first element of connection, try second element
       if(elem2(j).eq.elemx) then
        nsign=1
c...If connecting element is the top boundary, go to next connection
```

```
        if(elem1(j)(1:2).eq.'TP') go to 3001
c...If connecting element is the bottom boundary, treat the flow to the
c...bottom boundary as a sink/source term and move on to the next connection
        if(elem1(j)(1:2).eq.'BT') then
          gelem(i)=flux1(j)*nsign
          go to 3001
        end if
c...What is the first element in the connection?
        do ii=1,nmax
         if(elem1(j).eq.elemn(ii)) then
          k2nd=ii
c...Determine if the connection is between a fracture and matrix element
c...If it is a fracture-matrix connection (both elements have the same
c...coordinates), store this flux separately from fracture-fracture or
c...matrix-matrix fluxes.
           dx=dabs(x(k2nd)-x(i))
           dy=dabs(y(k2nd)-y(i))
           dz=dabs(z(k2nd)-z(i))
           if(dx.le.zero.and.dy.le.zero.and.dz.le.zero.or.
     &        ifm(j).eq.2) then
c...If the second element of f-m connection is a fracture, then process this
             if(nfmc.eq.2) then
               go to 3017
             else
               go to 3001
             end if
           end if
           icon(i,nc)=ii
           flol(i,nc)=flux1(j)*nsign
           nc=nc+1
           go to 3002
         end if
        end do
        write(*,7000) elemx,j,elem1(j)
7000    format('***Could not find 1st element in connection for',
     &  ' second element ',a5,'***'/'Connection index = ',i8/
     &  '1st element = ',a5)
        stop
       end if

c...If neither element 1 or 2 for connection j is equal to elemx, then
c...go on to the next connection
       goto 3001

3002   continue

c_________________________________________________________________________
c...go to next connection
       go to 3001
c_________________________________________________________________________
c...Come here if this is a fracture-matrix connection AND the element
c...being considered (elemx=elemn(i)) is a fracture
c...Consider outflow to be positive and
c...that the first element in the connection is a fracture
3017  continue
      fmlfm(nmlfm)=nsign*flux1(j)
      nmlfm=nmlfm+1
```

```
c...Go to next connection
c________________________________________________________________
3001  continue

c...ncon(i) is the total number of connections for node i
      ncon(i)=nc-1
c
c...Check
c        write(15,446) i,ncon(i),(icon(i,j),j=1,ncon(i))
c446     format(10(i8,2x))
c        write(15,448) i,ncon(i),(flol(i,j),j=1,ncon(i))
c448     format(2(i8,2x),8(e10.4,2x))
c...End check

c...Go to next element
3000  CONTINUE

c...nmlfm is the total number of fracture-matrix connections
      nmlfm=nmlfm-1

c...Add connection for each element to itself using generation array
c...nmfluxval is the total number of mass flux values
c...Note: nodes 1-nnodes are still assumed to alternative between
c...fractures and matrix. This will be adjusted later in the print-out
c...to the FEHM files.
      nmfluxval=0
      do i=1,nnodes
        ncon(i)=ncon(i)+1
        icon(i,ncon(i))=i
        flol(i,ncon(i))=gelem(i)
        nmfluxval=nmfluxval+ncon(i)
c...Check
c        write(15,448) i,ncon(i),flol(i,ncon(i)),nmfluxval
c448     format(2(i8,2x),e10.4,2x,i8)
c...End check
c...nmfluxval is the total number of flux values for fracture and matrix
c...elements excluding f-m fluxes
      end do

c...Call sort subroutine to sort the necessary arrays in ascending order
c...of elements for each connection pair of a given element

      call sort(nnodes)
c
c...Create 1-D arrays containing icon and flol information.  The arrays
c...will be icon2 and flol2. This assumes that the fractures and matrix
c...elements alternate in ELEME and fractures are listed first.
      k=1
      jj=1
      ncont1=0
c...ncont1 is the total number of connections for each continuum
c...do the fracture continuum first
      do i=1,nnodes,2
        do j=1,ncon(i)
c...The index k+nnodes/2+1 accounts for the leading pointer information
          icon2(k+nnodes/2+1)=(icon(i,j)+1)/2
          flol2(k)=flol(i,j)
          k=k+1
```

```
          end do
          ncont1=ncont1+ncon(i)
c...ncon2(jj) is the number of connections for fracture node jj, where jj is
c...now icremented 1,2,3...nnodes/2
          ncon2(jj)=ncon(i)
          jj=jj+1
        end do

c...Now do the matrix continuum
        do i=2,nnodes,2
          do j=1,ncon(i)
            flol2(k)=flol(i,j)
            k=k+1
          end do
        end do
c...ntotmfv is the total number of connections.  This can be compared to
c...nmfluxval as a cross-check to see if they're equal.
        ntotmfv=k-1

c...Write mass flux values to .ini file
        write(14,602) nmlfm+nmfluxval,ntotmfv,nnodes,nmlfm
602     format('mass flux values'/i8,5x,'#ntotmfv=',i8,', nnodes=',i8,
     & ', number of f-m connections= ',i8)
        write(14,604) (flol2(i),i=1,ntotmfv),(fmlfm(i),i=1,nmlfm)
604     format(5g15.8)

c...Write .stor file
        write(15,702) header
702     format(a80/'This is a .stor file with dummy area coefficients')

c...Add the pointer information (number of fracture nodes+1) to ncont1
        neq=nnodes/2
        ncont=ncont1+(neq+1)
        iwtotl=ncont-(neq+1)

        write(15,704) iwtotl,neq,ncont,1
704     format(4(i8,2x))

c...Write primary volume for each node to .stor
c...If this is an LBNL run, then divide the fracture volumes by the
c...fracture porosity, since the volumes in ELEME were multiplied by .
c...the fracture porosity.
        if(neos.eq.3) then
          do i=1,nnodes,2
            do j=1,ntotmat
              if(mat(i).eq.matname(j)) then
                vol(i)=vol(i)/por(j)
                go to 833
              end if
            end do
833       end do
        end if
c...If the fracture volumes were globally modified, multiply the volume
c...by a scaling factor, volscale, specified by the user to get the original
c...volume back.
        write(15,706) (vol(i)*volscale,i=1,nnodes,2)
706     format(1p5e16.8)
```

```
c...Compile and write ncon and pointer information
c...Fill the icon2(i) array from i=1,neq+1 (recall that icon2(i) has
c...already been filled from neq+2 to ncont1 (the total number of connections
c...for the fracture continuum
      icon2(1)=neq+1
      do i=2,neq+1
        icon2(i)=icon2(i-1)+ncon2(i-1)
      end do
      write(15,708) (icon2(i),i=1,ncont)
708   format(5(i8,2x))

c...Compile and write istrw information to .stor file
      do i=1,ncont
        if(i.le.iwtotl) then
          istrw(i)=i
        else
          istrw(i)=0
        end if
      end do
      write(15,708) (istrw(i),i=1,ncont)

c...Compile and write nelmdg information to .stor file
      do i=1,neq
        do j=icon2(i)+1,icon2(i+1)
          if(icon2(j).eq.i) nelmdg(i)=j
        end do
      end do
      write(15,708) (nelmdg(i),i=1,neq)

c...Write dummy area coefficients to .stor file
      do i=1,3
        write(15,706) (-1.0,j=1,iwtotl)
      end do
c______________________________________________________________________

      write(*,1153) time
1153  format('Finished processing printout at ',e12.4,' sec')
      go to 722
c
90    CONTINUE
      write(*,*)'**Did not find desired print-out time in TOUGH2.OUT**'
c
722   write(*,*) 'Done!!!'

      stop
      END


      subroutine sort(nnodes)
c______________________________________________________________________
c  This subroutine sorts variables using a multipass method.
c     C.K.Ho
c     9/8/97
c______________________________________________________________________

      implicit double precision (a-h,o-z)
      common/int/ ncon(99000),icon(99000,35)
      common/flux/ flol(99000,35)
```

```
c...The objective here is to arrange the connections in ascending order
c...of connecting node number. The associated flux should also be sorted.

      nsort=1
      do i=1,nnodes
5       if(nsort.eq.1) then
          nsort=0
          do j=1,ncon(i)-1
            if(icon(i,j).gt.icon(i,j+1)) then
              itempicon=icon(i,j)
              icon(i,j)=icon(i,j+1)
              icon(i,j+1)=itempicon
              tempflol=flol(i,j)
              flol(i,j)=flol(i,j+1)
              flol(i,j+1)=tempflol
              nsort=1
            end if
          end do
          go to 5
        end if
        nsort=1
      end do
      return
      end
```