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Date: 7/30/01 12:31PM
Subject: The Contribution of Geologic Data To Fracture Hydrologic Properties in the UZ

Structural Deformation and Seismicity KTI geologists asked me to describe how geologic data is incorporated by DOE into the hydrologic parameters used to model flow and transport in the unsaturated zone. As part of this task, I have completed the attached report. It briefly documents how geologic data is used in deriving hydrologic properties from site characterization data for the fractures in the unsaturated zone site-scale hydrologic units and faults. It also briefly describes how the fracture hydrologic properties change through calibration and modeling exercises, until they are used to model the site scale groundwater flow field in DOE's total system performance assessment.

In summary, fracture hydrologic properties for each hydrologic unit are related to the degree of welding and for non-welded units beneath the Topopah Springs unit, they are also related to the degree of zeolitization. The site-scale model grid, the fracture porosity, and the fracture van Geunuchten curve fitting parameters were derived from site characterization geologic data. Grid and porosity values are unaffected by the calibration process and are directly incorporated into DOE's total system performance assessment model. However, while the van Geunuchten curve fitting parameters were modified from their initial estimates by subsequent modeling exercises; van Geunuchten curve fitting parameters above the Calico Hills unit are little changed from their values derived from field data.

In future reports, I hope to describe how geologic data is incorporated by DOE into unsaturated zone fracture hydrologic properties for drift scale near-field modules and into near-field and far-field transport parameters. This is an internal report to aid the staff's review of the characterization program. If this report contains any errors, please let me know. I welcome constructive comments and questions.

tracing parameters back –
some failures dtns }?
a lot of failures → can't trace it
through – computer
but can access when
call someone

Leg-c-s /ma... 2.0

question – TSPA → 3-D site scale → 3-D model calibration → 1-D calibrations → site interpretations
use of fracture permeability → air injection test

How Geologic Data Contributes to Fracture-Hydrologic Properties in DOE's Site-Scale Unsaturated Zone Groundwater Flow Modules

porosity → 1 test

telling what did V. Genuchten / fracture / porosity frequency aperture

By
William Ford
NRC
July 30, 2001

DOE's Total System Performance Assessment assigns hydrologic properties to fractures to each hydrologic unit and fault to simulate groundwater flow in the "unsaturated zone flow" and "unsaturated zone flow and transport" modules of DOE's total system performance assessment . Fracture hydrologic properties for each hydrologic unit are related to the degree of welding and for non-welded units beneath the Topopah Springs unit they are also related to the degree of zeolitization.

The "unsaturated zone flow" and "unsaturated zone flow and transport" modules of DOE's total system performance assessment obtains fracture hydrologic properties for the groundwater flow field from the site-scale model (DOE, 1999 and DOE, 2000A). Fracture hydrologic properties for the site-scale model are obtained from site-scale model calibrations (DOE, 2000B). Initial parameter input for the site-scale model calibrations are obtained from one and two dimensional calibrations (DOE, 2000C). Initial parameter inputs for the one and two dimensional calibrations are obtained from analysis and numerical manipulation of site characterization data (DOE, 2000D).

The physical dimensions of the hydrologic units and faults are obtain from the Geologic Frame Work Model. The physical dimensions remain unchanged through any model calibrations and are carried forward unchanged through to the performance assessment module. Fracture porosities are derived for each unit by modifying the porosity values obtained from a single gas tracer test in the Topopah Spring middle nonlithophysal welded tuff. These values were modified using fracture intensity data from the Exploratory Studies Facility (ESF) and fracture frequency data from borehole data (DOE, 2000D pages 42 & 43). Porosity data is not calibrated by subsequent modeling exercises and are the final values used in the performance assessment module (DOE, 2000D, page 61).

# of calibration parameters

Values for fracture permeability, the van Geunuchten curve fitting parameters, and the active fracture parameter are modified from their initial estimates by subsequent modeling exercises. Initial values for fracture permeability are derived from air injection tests in the ESF and boreholes. However, van Geunuchten curve fitting parameters which are used in the modeling to adjust the permeability values as water contents change are derived from fracture frequency, fracture permeability, and fracture aperture data (DOE, 2000D pages 32 to 41). The active fracture parameter is estimated based on the degree of welding (DOE, 2000C pages 24 and 36). Equations to derive fracture frequency, fracture intensity, fracture interface area, and fracture aperture from geologic data from the ESF and boreholes is contained in pages 24 to 39 of DOE, 2000C. Calculated results for these parameters for each hydrologic unit is contained in Table 6 of DOE, 2000C (pages 40 and 41).

Initial values for fault-fracture permeability are derived from air injection tests performed in Alcoves 2, 6, and 7, the Bow Ridge Fault Alcove, the North Ghost Dance Fault Access Drift,

only used packed water → for TSPA values and the South Ghost Dance fault Access Drift. All other fault properties are calculated directly as averages of previously determined values for the hydrologic units crossed by a fault.

As previously stated, the fracture hydrologic parameters obtained from analysis and numerical manipulation of site characterization data are used as initial guesses for model calibration. Data from 11 boreholes were used to calibrate fracture hydraulic conductivity, fracture van Geunuchten curve fitting parameters, and the active fracture parameter. Calibrated values were obtained by fitting one dimensional model results to water content, matrix potential, and air pressure changes. Water and gas flow are simulated simultaneously in all 11 boreholes to produce hydrologic layer averaged effective parameters (DOE, 2000C, page 32). To reflect base case infiltration uncertainty, calibrated hydrologic parameters were obtained for three different infiltration scenarios (low, average, and high). This produced three different tables of hydrologic parameters for the base case (DOE, 2000C, Tables 13, 14, and 15).

Calibration was carried out in a series of steps. First, the parameters were calibrated by inversion of water saturation and water potential data. Second, the calibrated parameters from the first step were used as initial estimates for calibration by inversion of pneumatic data. Third, the calibrated parameter set from the second step was checked against the saturation and water potential data and further calibrated if needed. If further calibration was carried out in the third step, then the new parameter set was checked against the pneumatic data and so on until acceptable matches to the original data set were obtained (DOE, 2000C, page 44).

Fracture properties for faults were derived by calibration modeling to data collected from borehole USW UZ-7a on the Ghost Dance Fault. A two dimensional model that simulated an east-west vertical cross section through borehole "USW UZ7a" was used to derive calibrated parameters for all hydrologic layers from the Topopah Spring welded unit to the surface. Hydrologic parameters for units deeper than the Topopah Springs welded unit were not calibrated, but were derived directly from field data. This calibration exercise was carried out in the same manner and against the same kind of parameters as the one dimensional modeling exercise, with the exception that fracture permeabilities were fixed during the saturation and water potential inversion and are the only parameters calibrated to the pneumatic data. Also, unlike the one dimensional site-scale calibrations, only one set of calibrated parameters are derived for the base case (DOE, 2000c, pages 62 and 63 and Table 20).

Uncertainties in the calibrated properties from the one dimensional and two dimensional modeling were impossible to characterize. However, in most cases the calibration exercises did not change the properties very much from the initial estimates derived from the field data (DOE, 2000C, page 69). Therefore, the uncertainty in the original data set is considered by DOE to be a reasonable estimate of the parameter uncertainty.

Fracture hydrologic parameters obtained from the one dimensional and two dimensional calibration runs were used as initial guesses for calibration of the three dimensional site-scale model. Modeling exercises were conducted against tests in the ESF, unsaturated zone geochemical data, perched zone occurrence, and data from the eleven boreholes simulated in the one dimensional modeling exercises. However, only calibration exercises against perched water occurrence were used to develop calibrated data for the three dimensional site-scale model.

Calibration exercises were conducted for all three infiltration scenarios for the base case for two different conceptual models of perched water formation. These exercises produced six tables of calibrated hydrologic properties (DOE, 2000D). In conceptual model #1, matrix properties of potential perched zones are based on average matrix permeabilities while fracture permeabilities are calibrated to match the observed perched zone data. Conceptual model #2 parameters were not calibrated. In this conceptual model, fracture properties of potential perched zones were set equal to the average matrix properties. Both perched water models generally matched the water perching water occurrence observed in seven boreholes at Yucca Mountain. The perched water exercises produced revised fracture parameters in the zeolitized nonwelded units beneath Yucca Mountain. Fracture parameters for nonzeolitized units and all hydrologic units overlying the Calico Hill non-welded unit, essentially remained unchanged from the one dimensional calibration exercises.

With the exception of hydrologic units with significant zeolitization, the same hydrologic properties are assigned to any given hydrologic unit where ever it occurred in the site-scale model. For hydrologic units that contain areas of significant zeolitization, the hydrologic properties were varied laterally depending on whether it was considered to be zeolitized or not. Hydrologic properties for all faults were derived from the two dimensional calibration exercises are identical to each other and were the same irrespective of the infiltration rate.

As previously mentioned the three dimensional calibration exercise produced six tables of calibrated values for the base case (DOE, 2000B, Attachment II). The values from these tables were used by the three dimensional site-scale model to produce eighteen steady state flow fields; six base case scenarios, six scenarios for the monsoon climate, and six scenarios for the glacial climate (DOE, 2000A, Table 3.5-4). The hydrologic properties, matric potentials, and water contents from these steady state runs were placed in tables. These tables are accessed by the three dimensional dual continuum code FEHM, to reproduce the steady state flow fields of the site-scale model when it is run as part of the "unsaturated zone flow" and "unsaturated zone flow and transport" modules in DOE's Total System Performance Assessment.

Summary

In summary, the site-scale model grid, the fracture porosity and the fracture van Geunuchten curve fitting parameters are derived from site characterization geologic data. Grid and porosity values are unaffected by the calibration process. Fracture van Geunuchten parameters above the Calico Hills unit are little changed from their values derived from field data.

Additional Reading

Additional observations from other reviewers on this subject can be found in Winterle, et al, 2001.

References Cited

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