

Volume X Seepage

7/30/04 RF

This volume was started for work related to seepage into drift at Yucca Mountain. In part, this is a continuation of the collaboration on dripping and flow in fractures in scientific notebooks:

- #336 Randy Fedors
- #354 Dani Or
- #618 Dani Or (continuation of #354)

Project:

USFIC, 20.06002.01.131

Computer and Programs:

Primary computer running WindowsNT 4.00.1381 is called bubo (Acer, x86 Family 6 Model 4 Stepping 2; AT compatible with 512 MBytes RAM).

- Adobe Acrobat & Distiller version 5.0
- Adobe Illustrator 8.0
- Adobe Photoshop version 5.0.2
- Excel 97 SR-2
- Lahey/Fujitsu Fortran 95 version 5.0
- NIST Standard Reference Database 10, version 2.2
- Sigma Plot2000 version 6.00
- Word 97 SR-2
- Word Perfect version 8.00

UNIX (use uname -X on SUNs and uname -msR) as of March 2003

SUN:

Spock is a SUN sparc Ultra 4 (4 cpu), 64-bit,
running SunOS version (Kernel ID) Generic_108528-17 release 5.8

- Mathematica version 5.0.0
- fortran 77 version 5.0 (SUN Workshop Compiler FORTRAN 77 version 5.0)

Task: Alternative Seepage Model

We are looking for an alternative conceptual model for flow in fractures and matrix that leads to seepage into drifts. Back in August 2000, I tasked Dani with developing seepage curves using the fracture/matrix model he developed when we had him developing a more physically-based model for flow in fractures. The preliminary estimates made in 2000 used properties of the Tiva Canyon tuff, TCw (see Sci Ntbk #354, Volume 3). Assuming a unit gradient, and the fracture flow model, one could derive seepage estimates. At the time, it was a natural progression for the plane and v-notch representation of both the matrix and fracture pore spaces. The plane and v-notch representation allowed for semi-analytical solutions for developing unsaturated zone constitutive relations for the matrix, fracture, and composite domains. At low potentials, film flow occurred on the planes and most flow occurred in the v-notches. Both matrix pore size and fracture aperture ("pore") distributions are needed for his model. The fracture flow model was published in a series of journal articles:

- Or, D. and M. Tuller, Liquid retention and interfacial area in variably saturated porous media: Upscaling from pore to sample scale model, *Water Resources Research*, 35(12), 3591-3605, 1999.
- Or, D. and M. Tuller, Flow in unsaturated fractured porous media: Hydraulic conductivity of rough surfaces, *Water Resources Research*, 36, 1165-1177, 2000.
- Or, D., and M. Tuller, Hydraulic conductivity of unsaturated fractured porous media: Flow in a cross-section. *Advances in Water Resources*, 26(8):883-898, 2003.

The goal now is to use current parameter values for the repository horizon (instead of the Tiva Canyon parameters used a couple years ago, to look at sensitivity analyses), to discuss aperture distributions, and to compare with Finsterle's (2000) Figure 3 Monte Carlo data. Finsterle (2000) and Finsterle et al. (2003) calibrated a fracture continuum model to injection test, then performed a Monte Carlo analysis to cover the a of conditions postulated to possibly occur across the repository.

- Finsterle, S., Using continuum approach to model unsaturated flow in fractured rock. *Water Resources Research* 36, 2055-2066, 2000.
- Finsterle, S., C.F. Ahlers, R.C. Trautz, and P.J. Cook, Inverse and predictive modeling of seepage into underground openings. *Journal of Contaminant Hydrology* 62/63:89-109, 2003.

Collaborators: Dani Or (consultant) and
Markus Tuller (unpaid collaborator)

Markus, who as a student of Dani's, had helped develop the matrix/fracture flow model; he is now an assistant professor at University of Idaho.

The calculations for the model based on the equations in Or and Tuller (2003) are performed in a Excel spreadsheet. Details are inserted in Dani's scientific notebook #618.

My entries in this scientific notebook (#432, Volume X) are restricted to the analysis of maximum aperture data from Yucca Mountain, and documentation and rationale for choosing the hydraulic parameter values for the matrix and fracture domains.

Working Directory

Files for this work are stored on bubo (WindowNT box) in:

E:\DriftSeepage\June2004* (working files)
E:\HydroProperties\FractureDataESF-ECRB (YM aperture source data stored here)

Finsterle (2000) Figure 3 Data

I obtained an ASCII file from Stefan Finsterle so that we directly compare our results with his Figure 3 results in Finsterle (2000). Getting his data allowed us to visually display the

differences, of which the most important difference in preliminary calculations was the difference in slopes for seepage fraction as a function of percolation.

The emails included below explain a mix-up. At first, Stefan sent a file with strange units and mixed up headings. Although I approximated the conversion by scaling to match the figure, we used the 2nd file he sent with the conversions included in the data so that the data set had meaningful units. I renamed the 2nd file Stefan sent from "Threshold2.dat" to `./FinsterleData/FinsterleRevision-of-Data22July2004.dat`

-----Original Message-----

From: Stefan Finsterle [mailto:SAFinsterle@lbl.gov]
 Sent: Thursday, July 22, 2004 12:07 PM
 To: Randy Fedors
 Subject: Re: request based on your WRR 36(8) journal article

Randy,

It seems you figured it all out:

(1) The curve labeled "FCM" in the TEC file corresponds to the crosses in Figure 3, i.e., it is in fact the seepage threshold curve calculated with the FCM using the calibrated parameters and the permeability field during calibration.

(2) The curve labeled "DFNM" in the TEC file is labeled "DFN" in Figure 3.

(3) The curve labeled "mean" in the TEC file is that labeled "FCM" in Figure 3.

(4) Here are the conversion factors:

X-Axis: the value in the TEC file is the percolation rate in kg/s applied over the 6-m wide model. To convert to mm/yr:

$Flux = 10^{**}(Q) * 86400 * 365 / 6$

Y-Axis: the value in the TEC file is the seepage rate in kg/s into the 4-m wide niche. To convert to seepage percentage:

$Seepage\ percentage = Seepage\ rate / Percolation\ rate * (6/4) * 100$

Attached is a TECPLOT file with the converted units and clarified labels. I hope this helps.

Stefan

--Randy Fedors wrote:
 Stefan,

Just to make sure I understood the data you sent, I manipulated the data so that I could reproduce Figure 3 of your Water Resources Research (WRR 36(8)) paper. I suspect the percolation values in your data file were volumetric fluxes over some area. Since I didn't know the units or the area, I just scaled the percolation data to qualitatively match the values in the WRR Figure 3 plot.

The only real question I have is that the data file used different labels than those in the published figure. In creating the attached figure, I presumed that the data file was mislabeled and that the WRR Figure 3 was correct. The "FCM" labeled data in the datafile matched the Calibrated data from your WRR Figure 3. And the "mean" data in the datafile matched the FCM data in the WRR Figure 3 plot.

Can I assume that the WRR Figure 3 is correctly labeled?

Thanks,
 Randy

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The tecplot formatted file from Stefan was imported into Excel and a plot was generated and compared with Figure 3 in Finsterle (2000); a visual check was used as confirmation that the plotted data was the same as those in Figure 3 of Finsterle (2000). The tecplot formatted ascii file and the spreadsheet used to plot the data are in:

`.\FinsterleData\FinsterleFig3.xls`

Maximum Aperture Data from Yucca Mountain

Maximum aperture data was imported into the spreadsheet: .\ParameterValues\fractures.xls
The ascii files from DOE are stored in

bubo: E:\HydroProperties\FractureDataESF-ECRB\ECRB_qualified*

bubo: E:\HydroProperties\FractureDataESF-ECRB\Original* (ESF data)

ECRB TDMS numbers: GS990408314224.001
GS990408314224.002

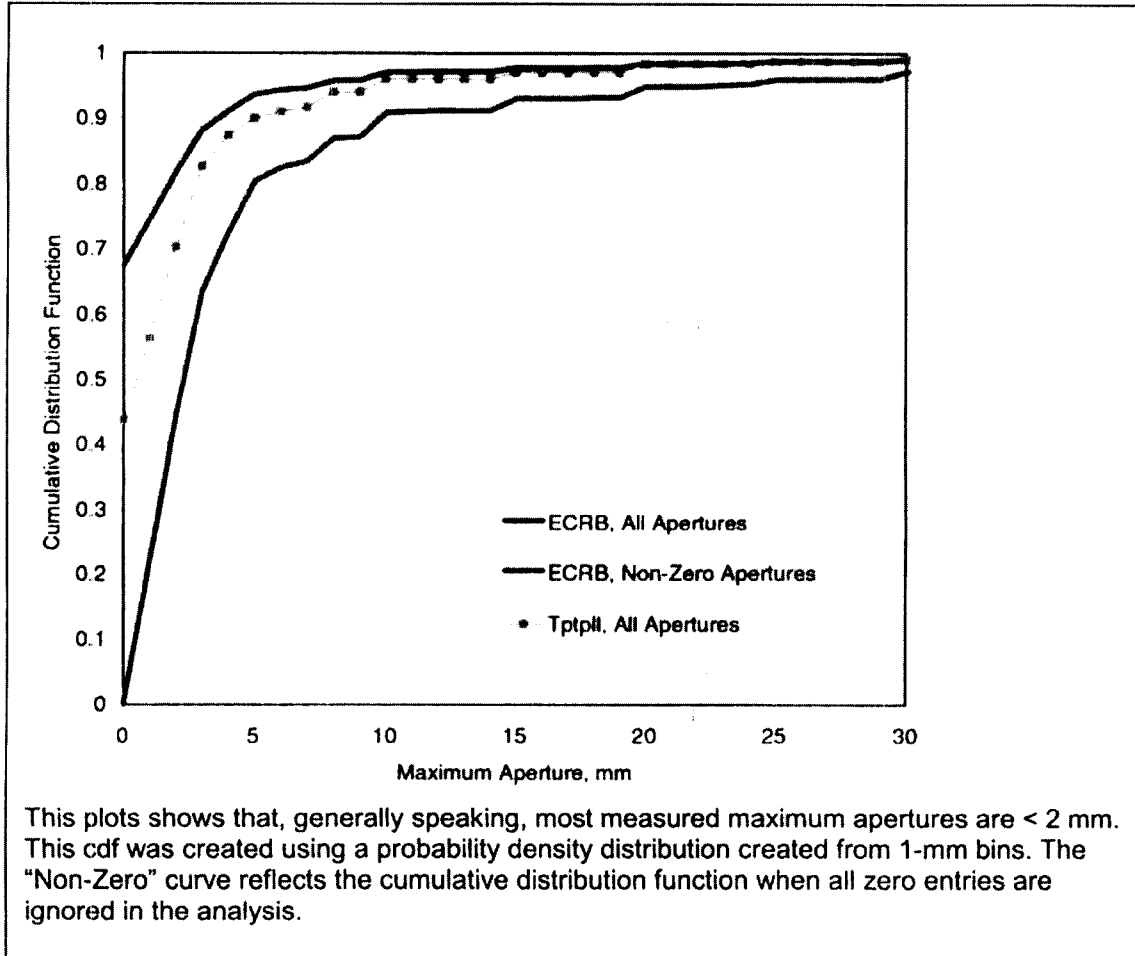
ESF TDMS numbers: GS960708314224.008
GS960708314224.011
GS960708314224.014
GS960708314224.018
GS970208314224.003
GS970608314224.006
GS970808314224.008
GS970808314224.010
GS970808314224.012
GS970808314224.014
GS970908314224.017
GS971108314224.020
GS971108314224.021
GS971108314224.022
GS971108314224.023
GS971108314224.024
GS971108314224.025
GS971108314224.026
GS971108314224.027
GS971108314224.028

The ECRB data included the Topopah Springs upper lithophysal, middle nonlithophysal, lower lithophysal, and lower nonlithophysal units, in other words, only the repository horizons. The records included the stratigraphic information.

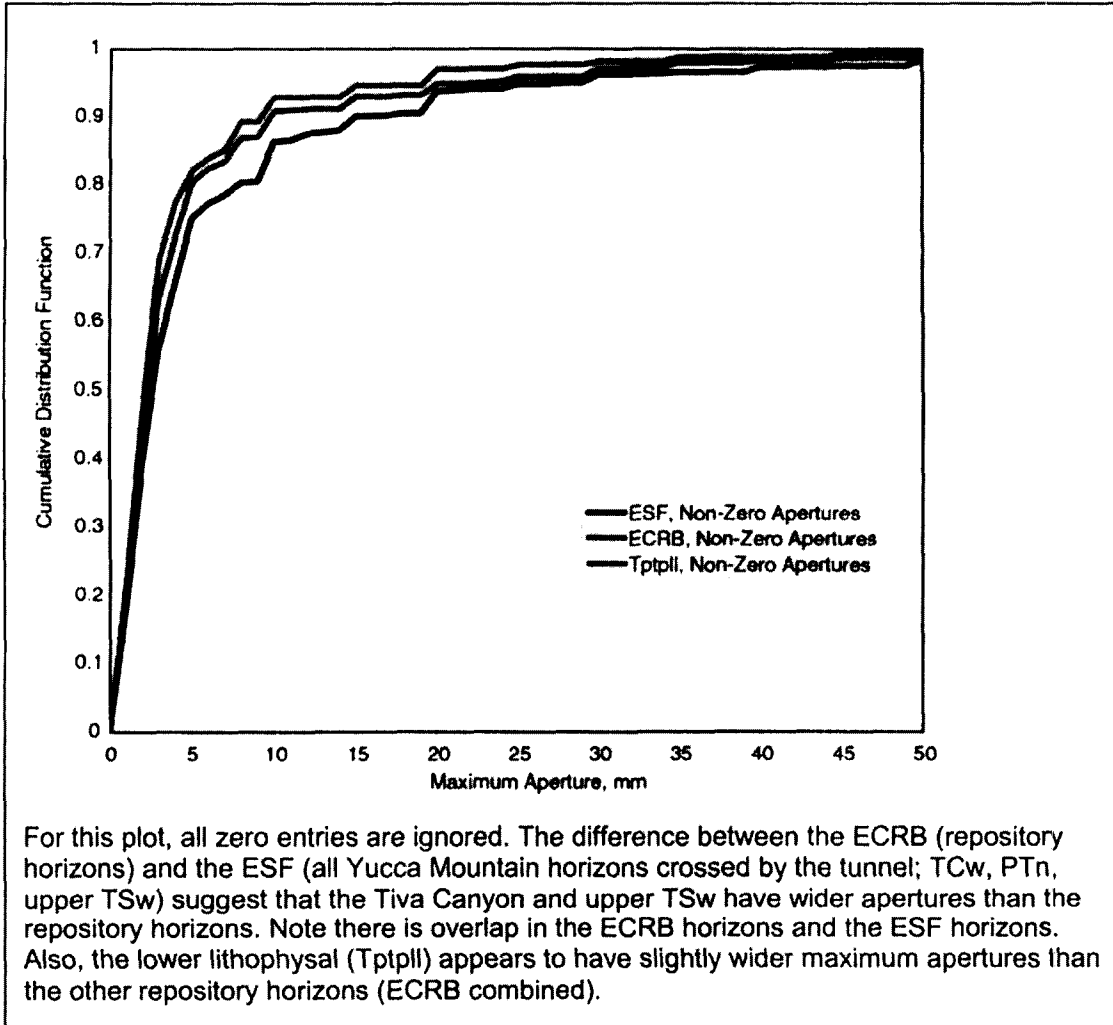
The ESF data did not include the stratigraphic information, and I did not integrate the geologic map data of the ESF into the data set. The ESF includes some Tiva Canyon and nonwelded Paintbrush units, but a majority of the data is the upper part of the Topopah Springs Tuff (down to the middle nonlithophysal; although there are a couple fault slices with lower lithophysal covering small zones of the tunnel). Scanning the data, I noted that the minimum threshold was generally 1 mm. They probably used a feeler gauge. In a couple instances, 0.3 and 0.5 mm maximum apertures were recorded.

This data was plotted for two reasons. One, decide on a reasonable maximum aperture to use in our seepage model. The maximum aperture affects the matching to permeability, but there is not much sensitivity unless large values are used. Two, decide if the distribution of maximum apertures can provide a supporting basis for using the truncated beta distribution for all apertures. The hypothesis is that the shape of the distribution of all fractures may be similar to the shape of the distribution of maximum apertures.

Analysis of the data quickly put to end the second reason. Over half the data records had zero entries for maximum aperture. Cumulative distribution plots were created solely to help justify a choice of maximum aperture to use in our seepage model.



Note that a distinction is made between mechanic aperture and hydraulic aperture in the literature. In fact, mechanical aperture (direct measurement of the opening).can be measured two ways: (1) it makes sense to measure the distance as perpendicular to the plane of the two fracture faces (a direction that varies constantly as you move down the fracture), or (2) more researchers just set an absolute coordinate system and always measure the vertical direction regardless of the local fracture orientation. Hydraulic aperture is a calculated number that is generally derived using permeability measurement (air K), and fracture density information. It is easy to see why mechanical aperture should differ from hydraulic aperture estimates.



Some summary statistics taken directly from the data sets are shown in the table below.

Aperture	All Fractures			Fractures with Non-Zero Apertures		
	ESF	ECRB	Tptpll	ESF	ECRB	Tptpll
>30 mm	0.8%	0.9%	1.0%	3.8%	2.9%	1.8%
>25 mm	1.1%	1.3%	1.3%	5.2%	4.1%	2.4%
>20 mm	1.3%	1.7%	1.7%	6.2%	5.1%	3.0%
>15 mm	2.0%	2.3%	3.3%	9.9%	7.0%	5.9%
>2 mm	12.4%	18.2%	29.7%			
>1 mm	16.8%	25.5%	43.7%			
>0 mm	79.3%	67.4%	56.3%			
# of Fractures	19342	1803	300	3996	588	169

Statically Truncated Gamma Distribution for Apertures

There was some confusion on the distribution used by Markus in his old paper. Dani referred to it as a beta distribution and Markus labeled it as a gamma distribution in his Excel spreadsheet. A beta distribution is bounded by finite numbers (standard is bounded from 0 to 1). The gamma distribution is from 0 to infinity. However, statistically speaking, one can just eliminate the lower and upper tails of the gamma distribution as being insignificant; thus, Dani referred to it as a statistically truncated gamma distribution. Both the beta and gamma distributions use the gamma function, which if the coefficient is an integer, can easily be calculated as $\Gamma(\gamma)=(\gamma-1)!$ (note the factorial). Thus using $\gamma=2$ in the gamma function makes the calculation easy in the gamma distribution. Dani used a substitution to simplify the gamma distribution to the expression used by Markus in the spreadsheet. As described by Dani to Markus and myself (equations thanks to Markus):

Gamma Density Distribution

$$f(B) = \frac{1}{\omega^\gamma \cdot \Gamma(\gamma)} \cdot B^{(\gamma-1)} \cdot c^{\frac{-B}{\omega}} \quad (1)$$

where $\Gamma(\gamma)$ is the complete gamma function that can be expressed as:

$$\Gamma(\gamma) = (\gamma - 1)! \quad (2)$$

Substituting (2) into (1) yields:

$$f(B) = \frac{1}{\omega^\gamma \cdot (\gamma - 1)!} \cdot B^{(\gamma-1)} \cdot c^{\frac{-B}{\omega}} \quad (3)$$

Substituting $\xi=\gamma-1$ into (3) yields the form of the gamma density function we use:

$$f(B) = \frac{B^\xi}{\xi! \cdot \omega^{\xi+1}} \cdot c^{\frac{-B}{\omega}} \quad (4)$$

With $\xi=2$ (4) reduces to:

$$f(B) = \frac{B^2}{2 \cdot \omega^3} \cdot c^{\frac{-B}{\omega}} \quad (5)$$

The cumulative distribution is simply the integral of (5)

$$F(B) = \int_0^B \frac{t^2}{2 \cdot \omega^3} \cdot c^{\frac{-t}{\omega}} dt \quad (6)$$

Hydraulic Parameters

Besides aperture distribution, unsaturated zone hydraulic properties are needed in the model. For the matrix, the pore size distribution is estimated using the unsaturated parameters of the van Genuchten relation. Because there are different flow regimes in the fractures (e.g., water in films and crevices on one side of the fracture at one water potential, and water bridging the aperture at much lower potentials), a fracture aperture distribution needs to be part of the input to constrain the seepage model.

The hydraulic properties of the matrix and fracture should come from a dual-permeability model because overlapping matrix and fracture domains are also inherent in our seepage model. Hence, the parameter values from the DOE seepage model (single continuum) would not be relevant. Note that the DOE seepage models, FCM for heterogeneous fracture continuum model and DFM for discrete fracture model, have both "matrix" and fracture cells. However, the matrix and fracture cells do not overlap. Cells that are not parameterized in the range applicable for fracture flow, are given uniform properties consistent with the matrix (i.e., intrinsic permeability = $1e-18 \text{ m}^2$). Note that the DFM is really a special case of the FCM in that cells with fracture properties are lined up to visually look like a fracture network. The DFM is really a discrete feature model because the cell sizes for fractures are not constrained to the aperture dimension (cell width is 10 cm regardless of whether the cell is a fracture or a matrix). The DFM uses a uniform cell size of 10 cm in both dimensions throughout the grid.

For the Table on page 8, the following two references are used for data:

Flint (1998). Characterization of Hydrogeologic Units Using Matrix Properties, Yucca Mountain, Nevada. USGS Water-Resources Investigations Report 97-4243.

BSC (2003). Calibrated Properties Model. MDL-NBS-HS-000003 Rev01. Bechtel SAIC Company, LLC.

The table on page 8 was used to select parameter values for the alternative seepage model. The fracture properties used in the model come entirely from the 1D calibrated data set provided by DOE in BSC (2003). The matrix values come from Flint (1998) who reported on measurements made on cores. The matrix permeability from Flint (1998), however, is not upscaled much in the 1D calibrations; for example, the $\log(K, \text{m}^2)$ values of the matrix from cores is -17.15 and the calibrated value is -17.35 . Compared to the original analyses from a couple years ago, which used data on the TCw from Wang and Narasimhan (1993), (i) the fracture porosity is now a factor of 20 larger, (ii) there is a large increase in the $1/\alpha_f$ value for the fractures (or decrease in the α_f value), and (iii) the matrix α_m value increased by half an order of magnitude.

The table on page 9 shows fracture continuum parameter values, mostly from the single continuum DOE seepage model. Standard deviations could qualitatively be used to infer standard deviations of fracture continuum in dual-continuum representation.

Note that in the seepage model (fracture-only), $1/a$ is considered an effective property representing average fracture hydraulic properties, connectivity, density, geometry, and orientation. This parameter is also said to incorporate film flow and small scale ceiling roughness. We think it also may include along-wall seepage, change in matrix storage and rewetting fractures (though "late" data is used), and uncertainties in evaporation model. Hence, parameters from the single continuum seepage model should not be used in the alternative seepage model where matrix and fracture inherently overlap.

	Sci.Ntbk #354, Volume 3 Page 4, Table 1	Data to Use				1-D site wide calibration BSC (2003)	1-D site wide calibration, BSC (2003)	uncalibrated (prior) values, BSC (2003)	uncalibrated (prior) values, BSC (2003)	core measurements for matrix, Flint (1998) and Tptpmn (1998) for Tptpmn and Tptpil	Flint (1998); means are in Flint (1998), other statistics developed from L. Flint spreadsheet
	Dani Or Sci Ntbk, TCw	Or and Tuller, TCw	tsw34, middle nonlith	tsw35, lower lithophysal	tsw34, middle nonlith	tsw35, lower lithophysal	tsw34, middle nonlith	tsw35, lower lithophysal	Tptpmn, middle nonlithophysal	Tptpil, lower lithophysal	
Fracture permeability, K(m ²)	4.51E-11	1.18E-12			3.30E-13	9.10E-13					
Fracture permeability, log K(m ²)	-10.35	-11.93	-12.48	-12.04	-12.48	-12.04	same	same			
Standard deviation, log(K)			0.55	0.54			0.55	0.54			
Range, minimum log K (m ²)											
Range, maximum log K (m ²)											
Fracture VG alpha (1/Pa)	7.39E-04				1.04E-04	1.02E-04	6.70E-04	1.00E-03			
Fracture VG 1/alpha (Pa)	1353		9615	9804	9615	9804	1493	1000			
Fracture-Only Continuum VG 1/a (Pa)											
Fracture VG, Range Minimum 1/a (Pa)											
Fracture VG, Range Maximum 1/a (Pa)											
Fracture VG exponent m	0.611		0.633	0.633	0.633	0.633	same	same			
Fracture porosity (fraction)	0.00048	0.00061	0.0085	0.0096	0.0085	0.0096	same	same			
Effective fracture aperture, mean (m)	1.50E-04	1.09E-03									
Fracture aperture frequency (#/m)	3.2	5.5									
Fracture frequency (#/m), ESF, 1-m threshold			3.4	0.7							
Fracture frequency (#/m), ESF, 0.3-m threshold			10	20							
Aperture distrib, xi	2	2									
Aperture distribution, omega (m)	5.0E-05	3.3E-05									
Aperture minimum (m)	1.0E-09	1.0E-09									
Aperture maximum (m)	1.5E-02	5.0E-04									
Matrix permeability, K(m ²)	3.04E-17	2.55E-18			1.77E-19	4.48E-18	4.50E-17	3.17E-17	1.50E-11 m/s	6.96E-11 m/s	
Matrix permeability, log K(m ²)	-16.52	-17.59	-17.81	-17.15	-18.75	-17.35	-16.35	-16.50	-17.81	-17.15	
Standard deviation matrix, log(K)			0.57	0.79			0.97	1.65	0.57	0.79	
Matrix VG alpha (1/bars)									0.064	0.273	
Matrix VG alpha (1/Pa)	6.44E-06	8.39E-07	6.40E-07	2.73E-06	8.45E-06	1.08E-05	1.40E-06	6.00E-04	6.40E-07	2.73E-06	
Standard deviation, matrix VG, from SE=s/sqrt(n)									0.023	0.182	
Matrix VG exponent m (-)	0.236	0.358	0.32	0.227	0.317	0.216	same	same	0.32	0.227	
Matrix porosity (fraction)	0.114	0.114	0.11	0.13	0.111	0.131	same	same	0.110	0.130	
Standard deviation matrix porosity (fraction)			0.02	0.031					0.020	0.031	
Range, minimum matrix porosity (fraction)									0.0547	0.0885	
Range, maximum matrix porosity (fraction)									0.192	0.2576	

Additional Information, not directly used

		Fracture permeability log K(m ²)	Standard deviation, log(K)	Range, minimum log K (m ²)	Range, maximum log K (m ²)	Fracture VG alpha (1/Pa)	Fracture VG 1/alpha (Pa)	Fracture-Only Continuum VG 1/alpha (Pa)	Fracture VG Range Minimum 1/alpha (Pa)	Fracture VG Range Maximum 1/alpha (Pa)	Fracture VG exponent m	Fracture porosity (fraction)
calibrated from seepage model, 20 heterogeneous realizations, fracture-only model; Abstraction of Drift Seepage AMR (2003) Table 6.6-1	tsw34, middle nonlith							0.0	231.1	1840.8		
calibrated from seepage model, 20 heterogeneous realizations, fracture-only model; Abstraction of Drift Seepage AMR (2003) Table 6.6-1	tsw35, lower lithophysal							0.0	427	741		
max range suggested for performance assessment, Abstraction of Drift Seepage AMR (2003) page 128	tsw34-35								297	885		
small scale (0.3 to 1 m) air K tests, Abstraction of Drift Seepage AMR (2003) from In Situ Field Testing of Processes AMR (2003) Table 6.6-3	tsw34, middle nonlith, Niche 3107	-12.14	0.8									
small scale (0.3 to 1 m) air K tests, Abstraction of Drift Seepage AMR (2003) from In Situ Field Testing of Processes AMR (2003) Table 6.6-3	tsw34, middle nonlith, Niche 3107	-11.66	0.72									
small scale (0.3 to 1 m) air K tests, Abstraction of Drift Seepage AMR (2003) from In Situ Field Testing of Processes AMR (2003) Table 6.6-3	tsw34, middle nonlith, Niche 3566	-11.79	0.84									
small scale (0.3 to 1 m) air K tests, Abstraction of Drift Seepage AMR (2003) from In Situ Field Testing of Processes AMR (2003) Table 6.6-3	tsw35, lower lithophysal	-10.95	1.31									
small scale (0.3 to 1 m) air K tests, Abstraction of Drift Seepage AMR (2003) from In Situ Field Testing of Processes AMR (2003) Table 6.6-3	tsw35, lower lithophysal	-10.73	0.21									
fracture only seepage model, Seepage Model for PA Including Drift Collapse AMR (2003) Table 6-3	repository horizon, tsw34-36			-14	-10				100	1000		
Finsterle, et al. (2003), Niche 3107, Tpcpmn tsw34	tsw34	-12.13	0.8					740			0.608	0.001
Finsterle, et al. (2003), Niche 4788, Tpcpmn tsw34	tsw34	-11.79	0.89					550			0.608	0.013
Finsterle (2000) conceptual models, data selection close but not quantifiably supported;single continuum, some cells considered matrix.		-12	1					39.8			0.33	0.006

9/8/04

RF

Recalculation of Critical Percolation Threshold of Philip et al (1989)

Excel worksheet E:\DriftSeepage\June2004\criticalThreshold.xls

The equations for maximum dimensionless matric flux potential ϑ_{\max} and the critical percolation threshold are from Philip, et al. (1989, Unsaturated seepage and subterranean holes: Conspectus, and exclusion problem for circular cylindrical cavities, Water Resources Research 25:16-28).

Inputs that vary are in bold. I used a drift diameter of 2 m just to compare with Dani's first calculations that were put into the paper; then I also used the correct value of 2.75 m.

As part of the technical review, Jim Winterle questioned the dimensionless nature of the equation for ϑ_{\max} . Note that the sorptive length is the inverse of α ; i.e., the units of α are 1/length. Then, I recalculated the numbers using latest values for the matrix and fractures (see previous 2 pages of this scientific notebook). These recalculated values were incorporated into the report.

Thus, for $s=0.5 \cdot \alpha \cdot l$, which is dimensionless, in the first case below,

$$s = 0.5 \cdot 2.68\text{E-}02 \text{ m} \cdot 2.75 \text{ m} = 0.0368$$

To convert units of J/kg to meters, just multiply by the acceleration of gravity (relevant to chemical potential and the α term).

	matrix	matrix	fracture	fracture
$g \text{ (m/s}^2\text{)}$	9.81	9.81	9.81	9.81
$l \text{ (m)}$	2.75	2	2.75	2
$\alpha \text{ (J/kg)}^{-1}$	2.73E-03	2.73E-03	1.02E-01	1.02E-01
$\alpha \text{ (m)}^{-1}$	2.68E-02	2.68E-02	1.00E+00	1.00E+00
$s \text{ (-)}$	3.68E-02	2.68E-02	1.38E+00	1.00E+00
$1/\alpha \text{ (m)} =$	37.3		1.0	
$k \text{ (m}^2\text{)}$	7.08E-18	7.08E-18	9.12E-13	9.12E-13
Philip et al (1989) eqns:				
$\vartheta = 2 \cdot s + 2 - 1/s + 2/s^2 =$	1450	2753	5.1	5.0
critical percolation threshold, $q^* = k / \vartheta$	4.9E-21	2.6E-21	1.8E-13	1.8E-13
ratio, $q^*_m/q^*_f =$	2.7E-08	1.4E-08		

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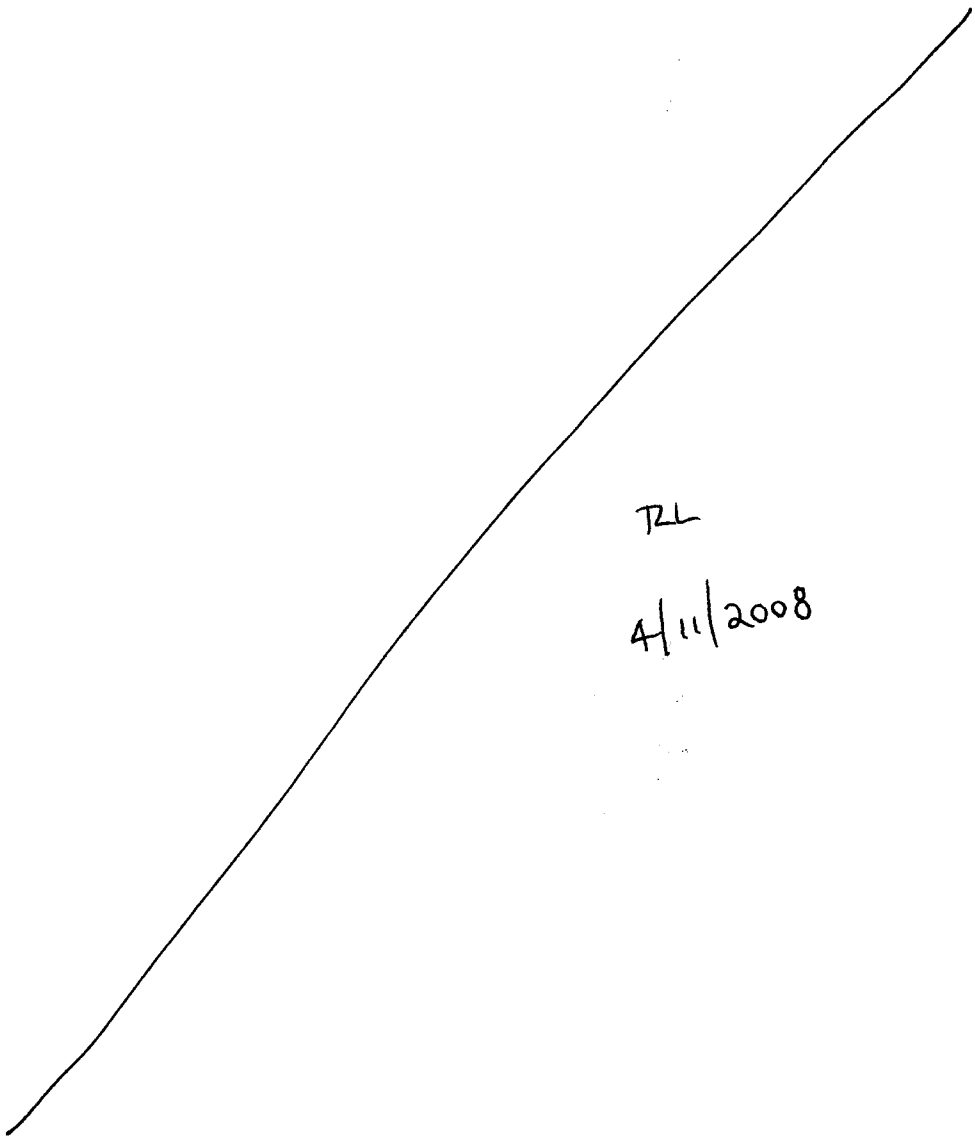
09/20/2004 RF

Entries made into Scientific Notebook #432E Volume X for the period July 2004 to September 30, 2004 have been made by Randall Fedors (September 20, 2004).

No original text or figures entered into this Scientific Notebook has been removed

RF 09/20/2004

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TL
4/11/2008

