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Scientific Notebook #171

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Scientific Notebook for KTI on UZ & SZ Isothermal conditions. Task 3 (Applied Technical Investigations) & Task 2 (SUFLAT)

Initial Entries & Signatures.

R. Baptzoglou [signature]
T. Tolley [signature: Timothy S Tolley] TST
M. Muller
E. PEARCY ECP

The first 100 pages of this notebook pertain to the perched-water activity of Task 3. The last 60 pages will include entries on Task 2 (SUFLAT modification) & geological model conditioning of Task 3. The first part will begin w/ some duplication from the SUBREGIONAL Research Project notebook for continuity purposes since this work had started under that project.

[signature] 4/5/1996

Timothy J Tolley May ~~24~~ 23 19~~97~~ '96 TJT

Hypothesis

Draining:

Because of the different properties of the different layers in Yucca Mountain there exist a potential for trapping to occur thus producing perched water bodies. A 1 dimensional model has already been used as a preliminary indication of the trapping potential of the area (pp. 25-37). A one dimensional simulation, though, gives a projection that is likely not very realistic so a 2 dimensional representation now being used to give a more realistic assessment of the movement of water in the area.

Initially some certain amount of water resided in the subsurface and it was assumed to be uniformly distributed throughout. This was allowed to drain on its own with no inflow. The orientation of the beds and the contrasting hydrologic properties of the various layers will cause the flow of the water to be channeled as it drains instead of just draining straight downward. This redistribution of the initial water may cause it to become more concentrated at some areas and less concentrated at others. The saturation levels at the regions of concentration may become high enough that it forms a region that is for all practical purposes a perched water body. Given enough time, all of the initial water will drain leaving the saturation levels at their irreducible minimum water content.

Flux:

The next step is to try to determine if it is possible for a perched water body

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to form and be maintained from the completely drained system, (from the previous step), with a flux added uniformly at the top. If this is possible, then the smallest flux to produce this perching needs to be determined.

At some time in the past, the climate in the Yucca Mountain region was cooler and wetter than at present. This would have produced a greater overall saturation level and a higher water table than exists at present. If a particular flux could have produced a perched water body from a completely drained initial condition then it stands to reason that the same flux could produce and maintain a perched water table from a starting condition of higher overall saturation levels.

If a perching situation could be produced and maintained from a totally drained starting condition and from a relatively more saturated initial condition, (representing cooler and wetter climatic conditions of the past), then three questions are asked: 1) what is the volume of water in the perched water body produced from the drained initial condition, 2) what is the volume of water in the perched water body produced from the relatively saturated initial condition, 3) assuming the same flux and same location for both situations, how do the volumes compare. If the volumes are nearly the same (and remain so indefinitely) then it is reasonable to assert that the volume of water produced in the perched water bodies is independant of the initial saturation of the rock units involved.

Modeled area:

The region of consideration for this work is around the intersection of the

Ghostdance fault and the Sundance fault in the repository area of Yucca Mountain (figure 1). It is approximately 1100 meters X 650 meters, (width X depth). The plane of view for the simulations is the plane of the Sundance fault looking northward. The area of importance is above the water table and primarily updip from the fault. The right border of this model represents an "artificial" no-flow boundary. This causes water to accumulate here in the model whereas in actuality the flow would continue downdip here. The beds that we are dealing with are (from top to bottom : Tiva Canyon (bed 1), Paintbrush Tuff (bed 2), Topopah Spring 1,2,3 (bed 3), Calico Hills (bed 4) and Prow Pass (bed 5).

Directory and file naming convention:

All of the computer simulations were run in sebastian/ttolley/bigflo.

The code used was "BIGFLOW: A Numerical Code for Simulating Flow in Variably saturated, Heterogeneous Geologic Media", version 1.1, May 1993, by R. Ababou and A. C. Bagtzoglou, NUREG/6028, CNWRA 92-026. The individual runs of bigflo2.x. were run under directory /bigflo/run. The results of each run were placed in another directory named for the run number. For example, /bigflo/run/R01 for run #1 and no flux is indicated so this is a draining simulation. For runs where a flux was added, the word flux is added and a number indicating the amount of flux is indicated. For example, "Rflux=05." indicates that for this run 5.0 mm/year of flux was applied to the simulation. These directories contained the head levels taken at time increments in the simulation. File "HEAD_T2" indicates that the these head levels were taken at

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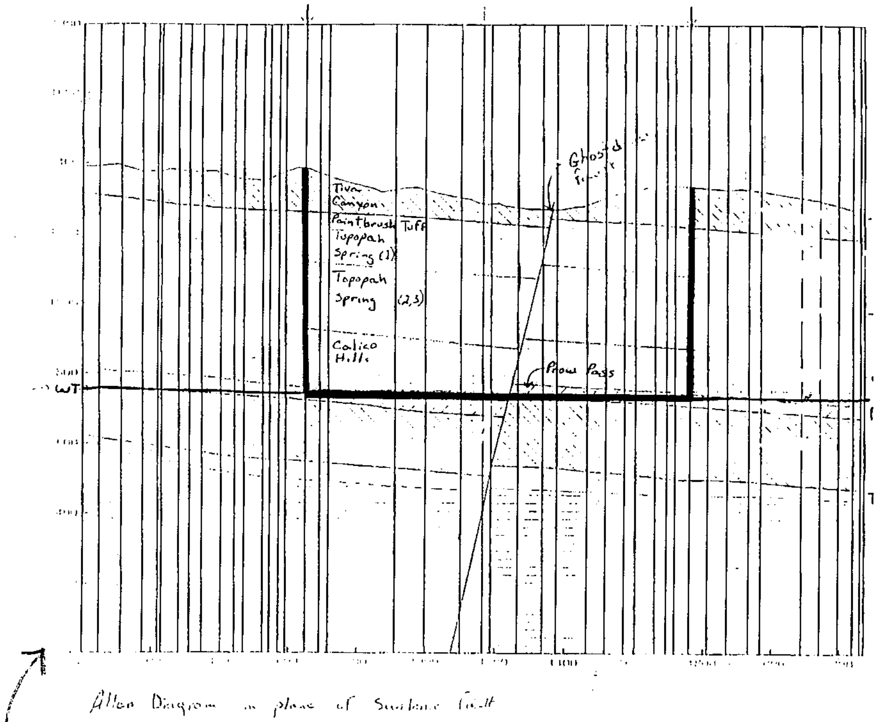

FIGURE 1A

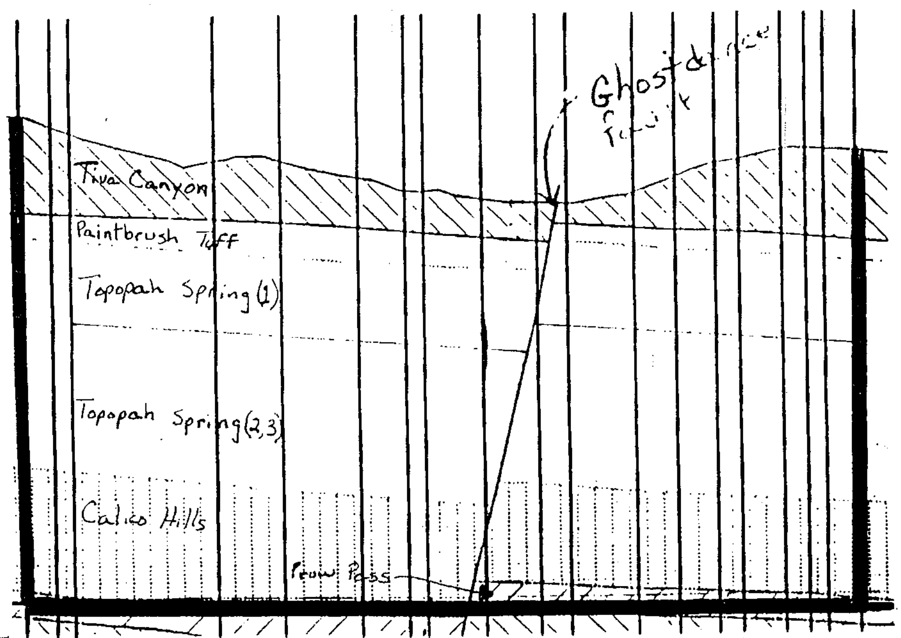

FIGURE 1B

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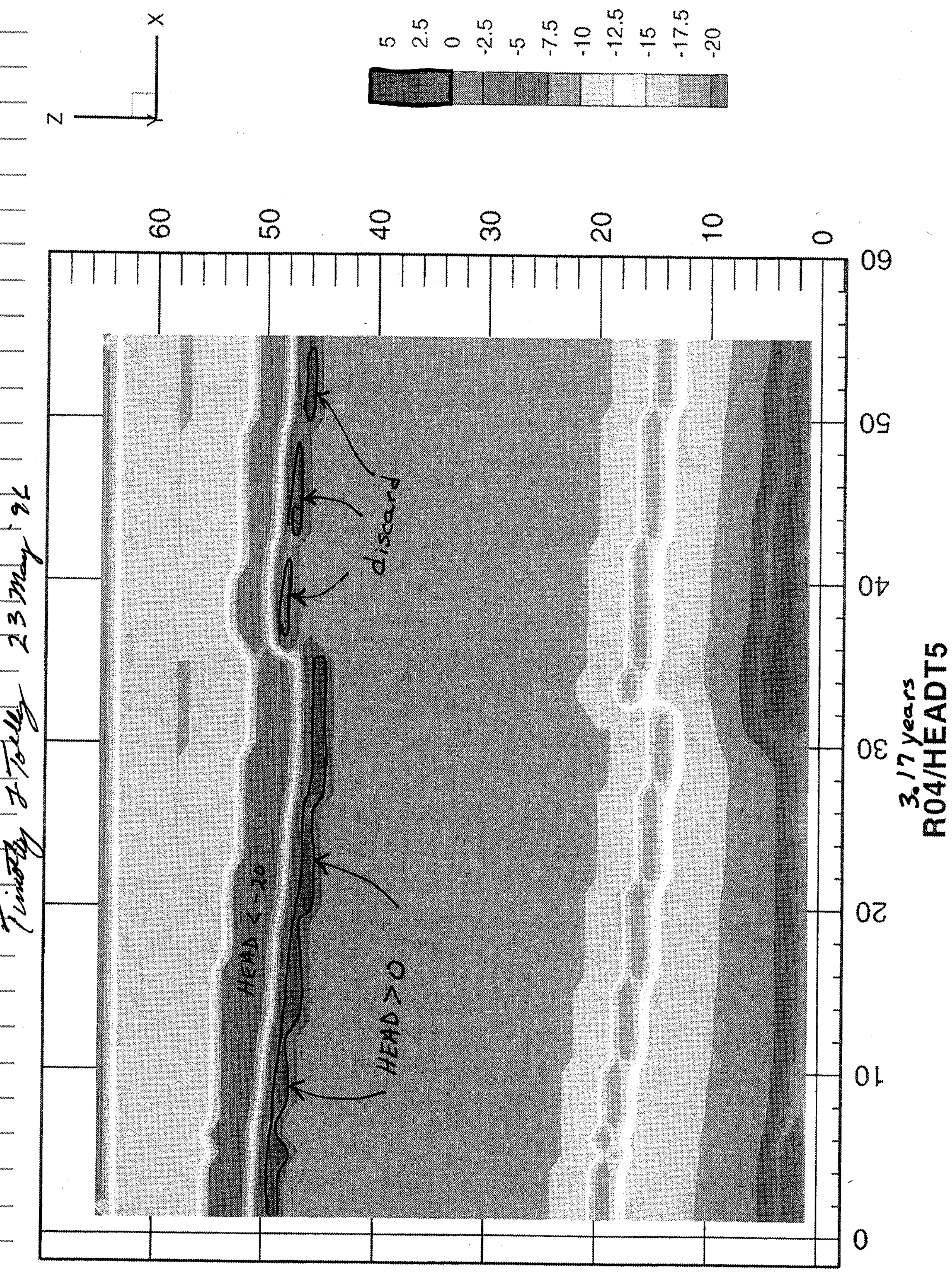
the second time interval in the simulation. These head values were processed for graphing in "Tecplot" in the directory /bigflo/tec. Once again individual directories were made for the individual runs using the same naming method. In these directories, (ie. /tec/R06), the head values were preplotted for "Tecplot" and the resulting Tecplot figures for head levels were stored here. In each of these directories another directory, called "flux", was created to compute the saturations, preplot the results and store the resulting graphs.

Procedures & Results

10-24-95 TT

An initial head level was assumed to be -10 meters throughout the area of simulation and from this level a simulation of was run in in the code "figflo2.x" in increments for a cummulative time of about 158,000 years. (This was done on Sebastian/ttolley/bigflo/run/R01 ... R10, with R01 through R10 being directories for the individual increments or 'runs" of the 158,000 years). These results were further processed in sebastian/ttolley/bigflo/tec/R01.../R10 to produce an output ready to plot with "Tecplot". In Tecplot the head levels were contoured and plotted to give a visual representation of the numerical values. The head levels were initially relatively uniform. With the progression of time in the simulation, the head levels in certain areas decreased. Specifically these areas were: the updip portions of all layers, and all of bed 2 and bed 4 (except near the fault in the updip side of bed 2), (Figure 2). The interface between bed 2 and bed 3 seems to act as a barrier to vertical flow, instead channeling the water in bed 2 downdip until it encounters the fault. This point,



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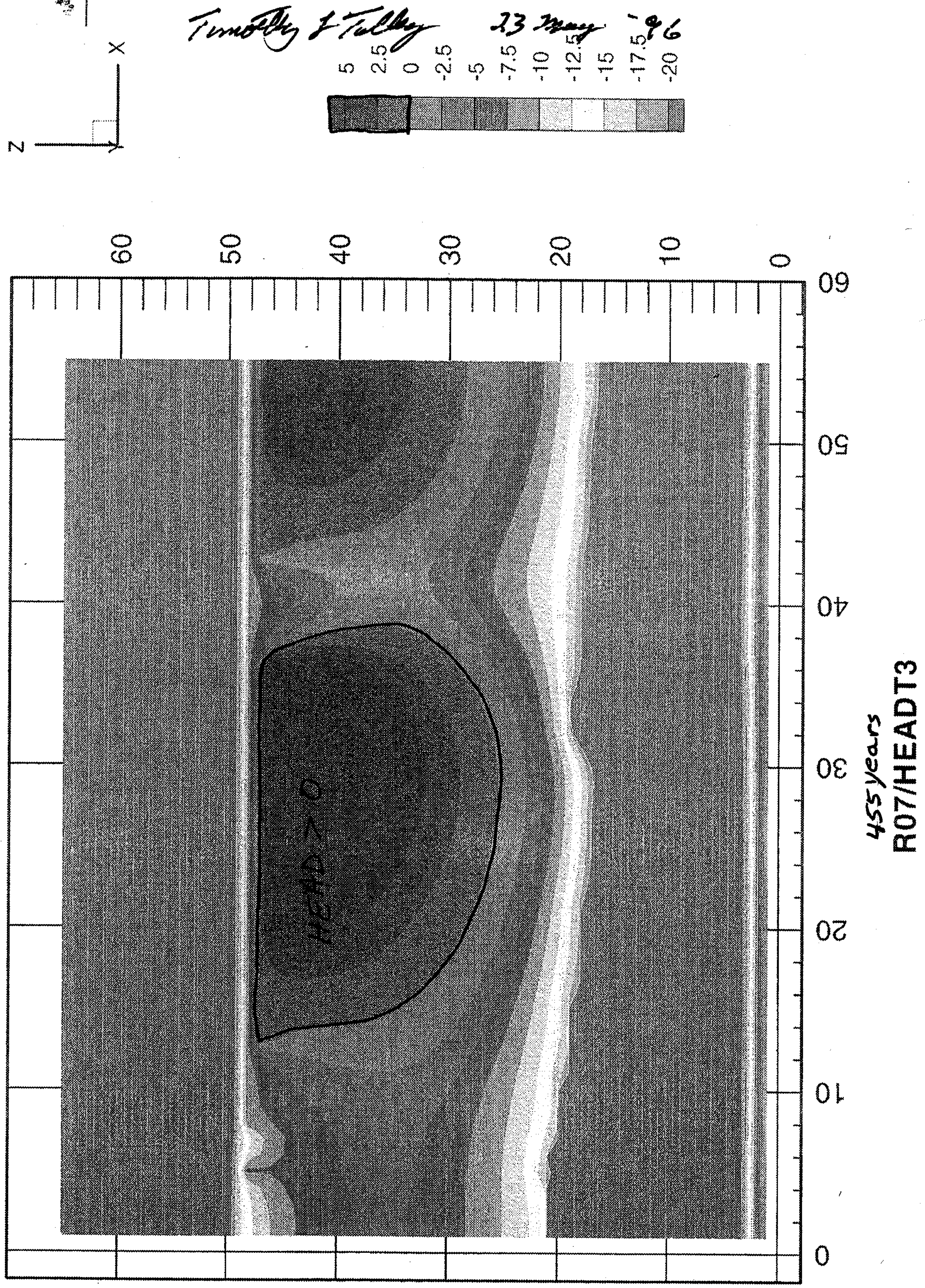
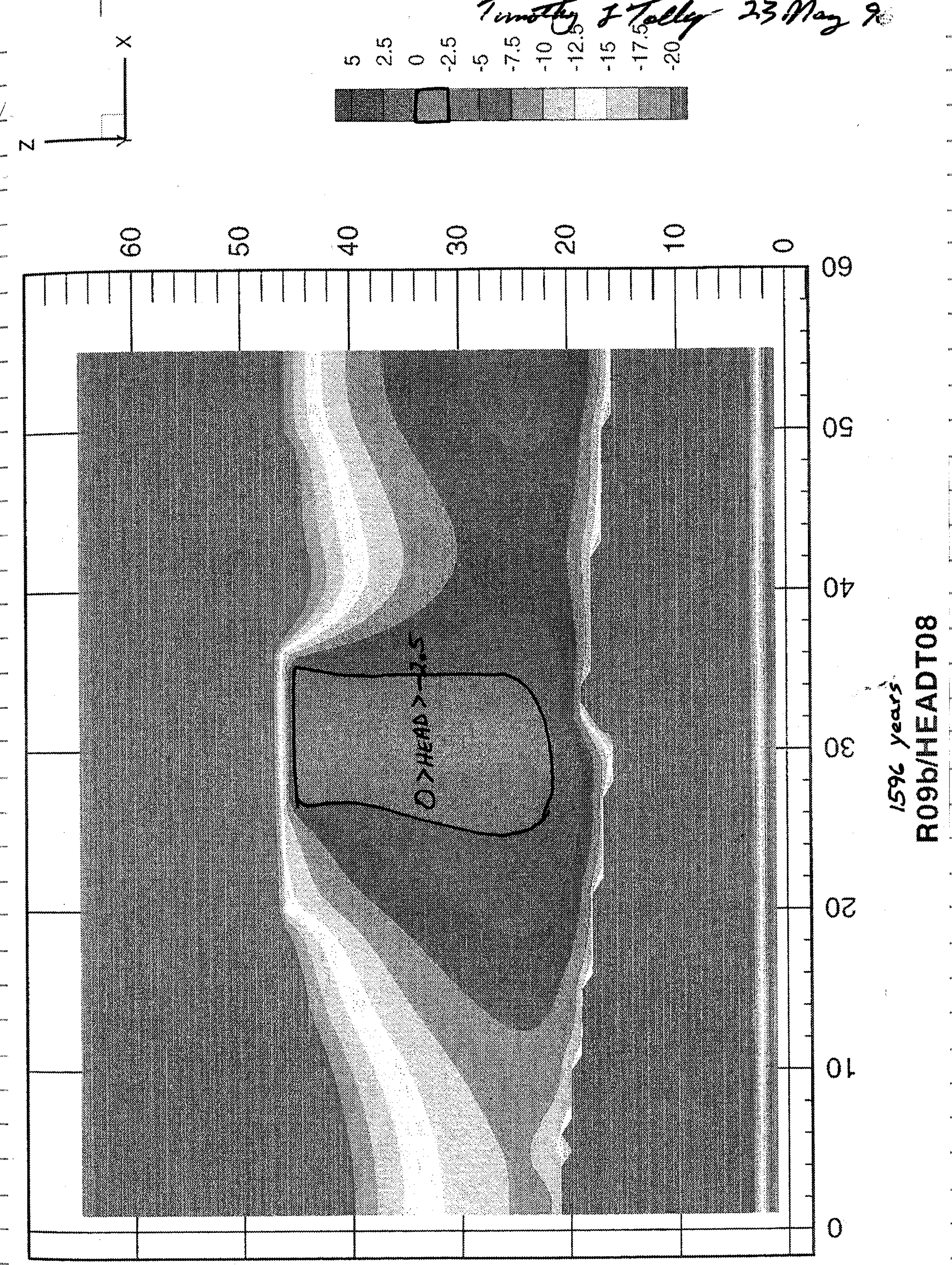
the intersection of bed 2, bed 3 and the fault, is the location where the higher head values begin. This region of high head values indicates higher saturation levels. Thus the water is becoming "backed up" at this point.

Although the water begins to accumulate at this point, it is, of course, not a total barrier. Rather, the water does pass across the interface from bed 2 to bed 3 but the lower hydraulic conductivity, K, of bed 3 slows the flow across the interface and instead channels it downdip until it encounters the fault. From the accumulation of water at this 3-point intersection, the flow is downward and outward. The lower K of bed 2 keeps the water from dispersing more rapidly than it accumulates thus causing a rather large region of high head values in bed 3, originating at the 3-point intersection and extending downward and outward. The fault further inhibits flow thus most of the region of high head values in bed 3 is updip from the fault.

The head values then, are initially the same throughout the simulation area. With time a region of high head values develops at the intersection of bed 2, bed 3 and the fault and extends downward and outward from this point with the main area being updip from the fault. This culminates with the maximum area of head values higher than "0" occurring at about 450 years (R07/HEAD_T03), (Figure 3). From this time onward less water is available, since the system is receiving no recharge, and the dispersion rate becomes greater than the accumulation rate. The area of head > 0 decreases and by 1600 years, (R09b/HEAD_T08), it is completely gone (Figure 4).

From each of the directories of the individual runs, (sebastian/ttolley/bigflo/tec/R01.../R10), another directory, called "flux", was created


5 2.5 0 -2.5 -5 -7.5 -10 -12.5 -15 -17.5 -20
X
Z
60 50 40 30 20 10 0
60 50 40 30 20 10 0
HEAD > 0
455 years
R07/HEADT3


5 2.5 0 -2.5 -5 -7.5 -10 -12.5 -15 -17.5 -20
X
Z
60 50 40 30 20 10 0
60 50 40 30 20 10 0
0 > HEAD > -2.5
1596 years
R09b/HEADT08

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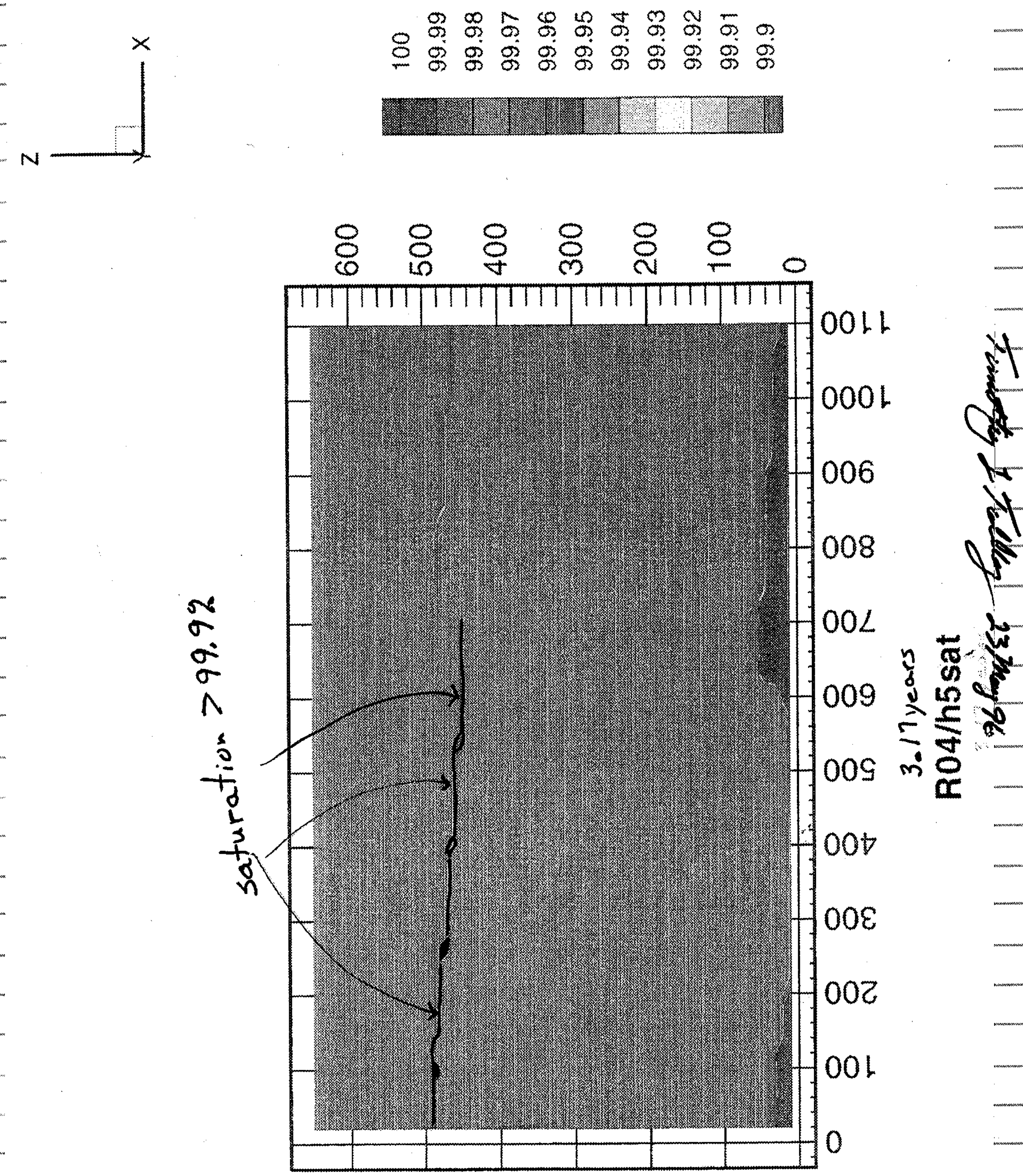
to calculate the saturation levels for the corresponding head values. The head values, (output of bigflo2.x), post-processed to produce either unsaturated moisture content files, "out2_ttuns", stored as "hxx.ttuns", and saturation files stored as "hxx.sat". In all this, "xx" indicates the particular head file. These saturation levels were also plotted in "Tecplot". Only saturation levels of 99.9% or greater were considered to be fully saturated. The overall pattern for saturation levels was the same as for the head levels; regions of saturation begin to occur along the bed2/bed3/fault interface, the maximum area of saturation occurs at about 450 years, (R07h3sat), and by 1628 years, (R09b_h09sat) no saturated regions remain (Figures 5, 6, 7). The region of saturation, of course, is basically the same as the region of maximum head values.

Adding flux from completely drained

11-28-95

After determining the behavior of water in a draining simulation, (with no flux added), the question is "can a saturated zone be produced by adding flux to a completely drained system". A flux was added to the drained system in a simulation to answer this question. The system was allowed to drain for about 158,000 years with no flux, in order to assure a completely drained initial condition for the system. The head levels at the end of the draining period, R10HEAD_Txx, were now the initial head levels. The simulation was now run with the same system except that the initial head levels were the completely drained values from R10HEAD_Txx and a flux was now added. Initially a flux of .1mm/year was added uniformly at the top. When this failed to produce a zone in which the saturation was greater than 99.9%, (essentually fully saturated), 1mm/year was



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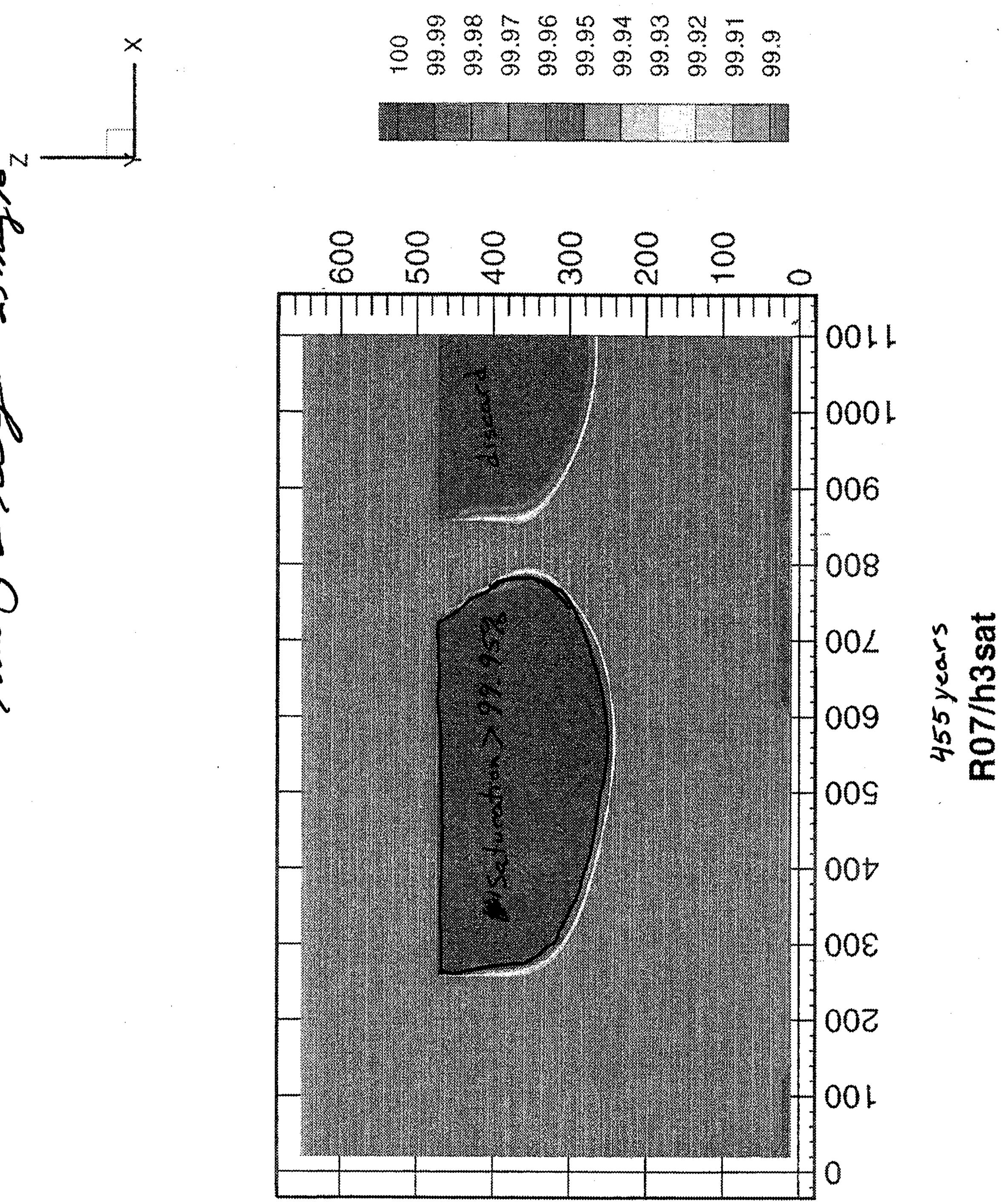

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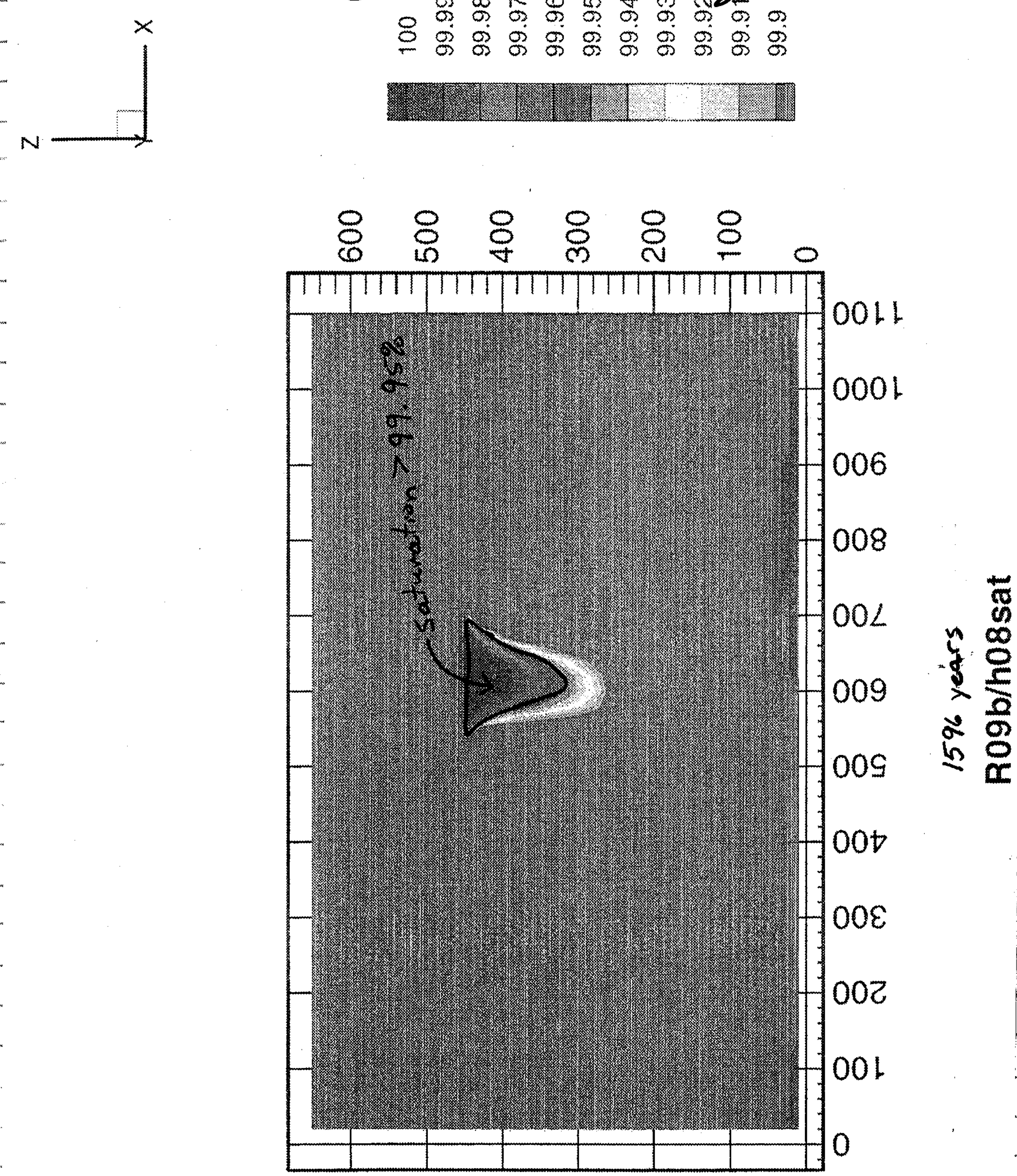

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added then 2mm/year, then 4mm/year was added. Finally, 8mm/year produced an perched zone, (saturation > 99.9%). Upon further evaluation it was determined that a flux of 5mm/year did not produce a perched water body but a flux of 6mm/year did produce a perched water body. The area of perching reached a maximum at about 7000 years after the flux was first added and it remained at this level for the remainder of the 19000 year simulation. While a flux of less than 5mm/year or less produced no saturated zone, one particular region, the same general region that became saturated in the draining simulation, had a progressively increasing saturation level as the flux was increased.

Thus it is possible to produce and maintain a perched water body in the region with a sustained flux.

Flux added to the maximum perched volume in draining simulation 12-6-95

Knowing that perched water bodies can be produced during the course of draining-only and from a completely drained system with a flux added uniformly to the top, it seems reasonable that adding flux to a system that already has a saturated region will sustain saturation at some level. To confirm this, another simulation was run in which the initial head levels were taken from R07HEADT3, (Figure 3), the time in the draining simulation at which the greatest area of perching occurred, (450 years). As in the case of adding flux to a completely drained system, a flux of 5mm/year did not sustain perching while with 6mm/year perching was sustained.

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Compare "flux added to drained system" simulation with "flux added to a saturated system" simulation

The question now is, "how do the volumes of perched water compare from these two senarios". To get a more precise value of the volumes than can be discerned from the colored contour graphs of saturation, the volume of water in each cell was computed based on its porosity and saturation and then totals the volumes of the cells that have greater than a user specified saturation level, (99.9% saturated in this case). Also in this case, 12 columns, (240 meters), on the sides, and 5 rows, (50 meters), on the bottom were ignored to eliminate "edge effects". The volumes for the simulation that added 6mm/year of flux to a drained initial condition had a final sustained volume of 5670 m^3 in the saturated zone. For the simulation that used the head values from the time of greatest perching in the draining simulation, the final sustained volume of the perched zone was 6087 m^3. The values are within about 400 m^3 of each other (or about 7%), (Figure 8). The difference is considered acceptable and is attributed to the nonlinear nature of the unsaturated flow equation.

More simulations were run with a flux between 5mm/year and 6mm/year. The initial head levels for these simulations were those of R07/HEAD_T3, (the maximum saturated condition from the draining simulation). Thus far only the volumes after about 19,000 years has been computed and only for the following fluxes: 5.0mm/year, 5.1mm/year, 5.2mm/year, 5.3mm/year, 5.5mm/year and 6mm/year.

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The volumes for each are:

5.0mm/year	55.54 m^3
5.1mm/year	639 m^3
5.2mm/year	1195 m^3
5.3mm/year	1640 m^3
5.4mm/year	xxxx m^3
5.5mm/year	2668 m^3
6.0mm/year	6087 m^3 (shown in graph below)

Thus it seems that for a given area that will allow perching to develop, the volume of perched water will be dependant upon the flux rate.

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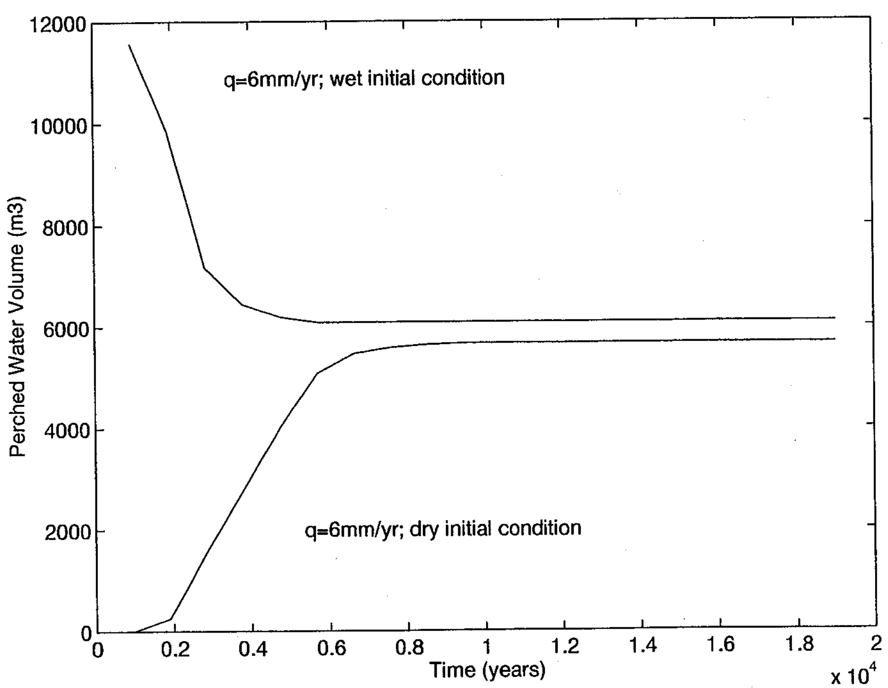

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Directory structure

The files used and produced in this profect are, for the most part stored on "thumper" or "yucca". The basic directory structure is the same on both machines and is shown at the end of this section. The main directory on each machine is: "/home/thumper/ttolley/bigflo" on thumper and "/home/yucca/ttolley/bigflo" on yucca. On thumper all the "source" files are stored under "src". These are things such as data files that are to be used several times and routines that are to be executed. The routines are usually executed under the "run" directory and the resultant "HEAD" files are also stored under the "run" directory; exactly where they will be stored is determined by the amount of flux, if any, is added, which realization, (i.e. which input files are used) and according to the run number. The saturation and volume files are produced and stored under "tec", ("tec" is parallel with "run" and "src"). As in "run", directories are created to indicate the realization, flux and run number. Subdirectories are then created for saturation files and volumes of perched water bodies.

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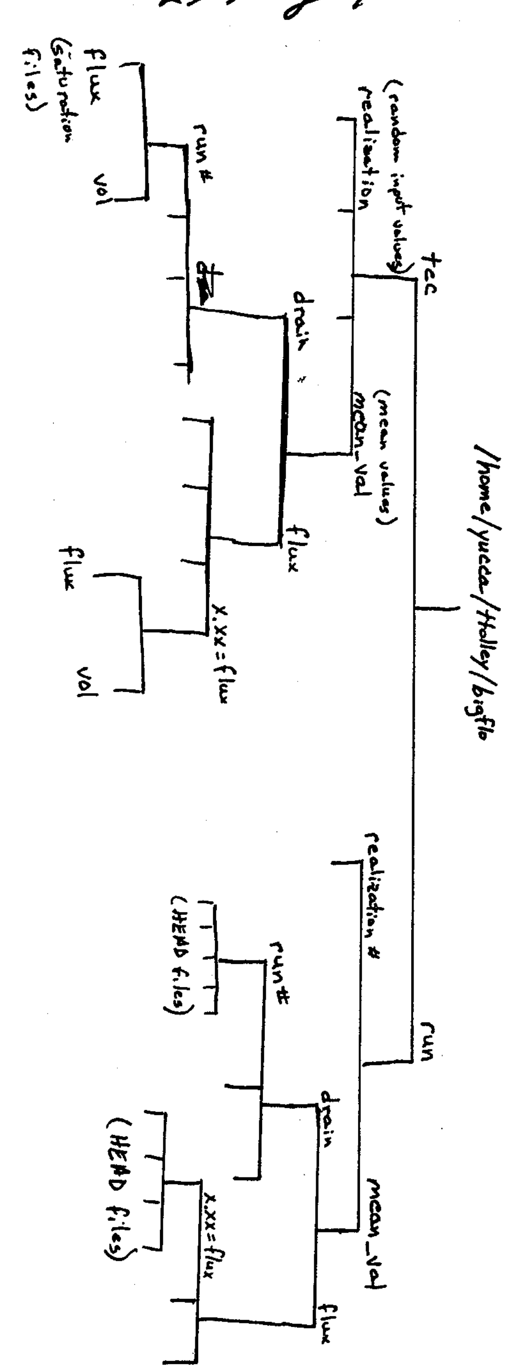

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Mar 10 1996

Approximating the Volume of an Actual Perched Water Body

A perched water table has been found in Yucca Mountain and this saturated region is estimated to contain approximately 500 cubic meters of water. The simulation that produced a sustained perched volume closest to this was the simulation with 5.1mm/year of flux added uniformly to the top of the model. This produced a sustained perched volume of about 639 cubic meters.

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March 06 1996

Change of Alpha (in6_alfa)

Upon re-evaluating the input date used for the simulations, (input files: in10_vgn, in11_ttdry, in5_ksat, in6_alfa, in7_tsat, in8_beta), it was discovered that the values for "in6_alfa", (alpha), were incorrect. The error occurred when the alpha values were copied from the reference sheet. The values for Topopah Spring 1, (TS1), and Topopah Spring 2&3, (TS2,3), should have been averaged based on their thicknesses as determined from the cross section. Instead the first five alpha values of the reference sheet were copied directly to the five units used in our simulation. This caused the Topopah Spring unit (from this simulation) to be assigned the value of the TS1 unit instead of the weighted average of TS1 and TS2,3. Of course the values of the units below Topopah Spring were then also incorrect, (see chart below).

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incorrect (WRONG) alpha values

Layer	ID	Ksat	THsat	THr	Beta (σ)	Van n (β)	Alpha	Bub head	layer (#)
TCw	GU3-3	2.7E-12	.09	.0144	.389E-2	2.130	.0095	10	→ TC (1)
PTn	GU3-7	3.9E-07	.40	.04004	.150E-1	6.872	.16	47	→ Pt (2)
TSw1	G4-4	8.6E-13	.03	.0018	.152E-1	1.400	.040	40	→ TS (3)
TSw23	G4-7	1.3E-11	.10	.00704	.258E-2	1.907	.0070	40	→ CH (4)
CHn	GU3-14	2.7E-7	.46	.01863	.160E-1	3.872	.063	20	→ PP (5)
PPw	GU3-18	1.3E-9	.32	.02128	.314E-1	3.442	.11	10	
BFw	G4-21	2.3E-9	.24	.01459	.112E-1	4.148	.11	10	

correct alpha

Layer	ID	Ksat	THsat	THr	Beta (σ)	Van n (β)	Alpha	Bub head	layer (#)
TCw	GU3-3	2.7E-12	.09	.0144	.389E-2	2.130	.0095	10	→ TC
PTn	GU3-7	3.9E-07	.40	.04004	.150E-1	6.872	.16	47	→ Pt
TSw1	G4-4	8.6E-13	.03	.0018	.152E-1	1.400	.040	40	weighted average → TS
TSw23	G4-7	1.3E-11	.10	.00704	.258E-2	1.907	.0070	40	
CHn	GU3-14	2.7E-7	.46	.01863	.160E-1	3.872	.063	20	→ CH
PPw	GU3-18	1.3E-9	.32	.02128	.314E-1	3.442	.11	10	→ PP
BFw	G4-21	2.3E-9	.24	.01459	.112E-1	4.148	.11	10	

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~ 06 Mar 96

The bigflo simulation was then run with the correct data, (correct in6_alfa). The starting point of this new run, (simulation), was still the peak perching volume as determined earlier. The results of this new run indicated that a flux of 6.2 mm/year would produce a sustained perched water body with a volume of 528 (see note, pg 40) TJT 24 May 96 cubic meters that is located in the same region as before. The basic behavior of the water in this run seems to be relatively unchanged except for the flux needed to produce perching. The data used to produce this simulation is shown below:

layer	layer	in10_vgn	in11_ttdry	in5_ksat	in6_alfa	in7_tsat	in8_beta	Sr
1	TC	1.62	0.0018	3.86E-~~09~~ 10 (7-15-96 TJT)	0.0095	0.087	0.0218	0.0212
2	PT	2.611	0.0648	5.47E-06	0.16	0.421	0.2485	0.154
3	TS	1.73	0.0063	2.37E-09	0.018	0.139	0.0299	0.0453
4	CH	2.0866	0.0359	6.22E-08	0.063	0.319	0.0306	0.1127
5	PP	7.014	0.0201	2.58E-08	0.11	0.292	0.018	0.0688
		Table 7-7a	Sr * in7_tsat	Table 7-5a	Michael's paper		Table 7-6a	Table 7-8

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Change of "in" files

~April 1996

The results above were obtained by using mean values for the properties of the various layers, (the "in..." files). These mean values were taken from TSPA-93 and are shown on the previous page. The next step was to produce a simulation using random values within the bounds of the minimum, maximum, mean and coefficient of variation. The random values were to be determined by a Latin Hypercube Sampling (LHS), routine. For this LHS routine to produce a beta distribution sampling it needs four parameters: minimum value, maximum value, "p" and "q". The minimum and maximum values are given in the TSPA-93 but "p" and "q" must be calculated. These "p" and "q" values must be greater than 0.5 in order for the LHS routine to produce reliable results. Using the input values from the TSPA-93 shown above, some of the "p" and "q" values were less than the 0.5 necessary for the LHS to produce reliable results. The problem was solved by using "entropy-fit" data from the TSPA that corresponded to the "basic" data given above. This entropy-fit data was given in the TSPA-93 because of the sparseness of the data and the fact

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that the fitting of a beta curve is quite sensative to the data end points, (TSPA-93, pg. 7-12). The entropy-fit data resides in "/home/thumper/ttolley-/bigflo/src/prop/mean_prop" is shown below.

layer	layer	in10_vgn	in11_ttdry	in5_ksat	in6_alfa	in7_tsat	in8_beta	Sr
1	TC	1.6218	1.80E-02	2.04E-10	0.0095	0.087	7.91E-02	
2	PT	2.3714	6.48E-01	3.80E-06	0.16	0.421	5.56E-00	
3	TS	1.7989	6.30E-02	2.09E-10	0.018	0.139	1.36E-01	
4	CH	1.9588	3.59E-01	3.78E-09	0.063	0.319	1.33E-01	
5	PP	5.8884	2.01E-01	9.12E-09	0.11	0.292	1.60E-01	
		Table 7-7B	Sr * in7_tsat	Table 7-5B	Michael's paper	Table 7-3	Table 7-6B	Table 7-8

(The data used earlier that produced 528 cubic meters of perching with 6.2mm/year is still valid though, and will still be used as a valid simulation).

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note: The values for entropy-fit data in the TSPA-93 were given in log 10 space so when the weighted average needed to be computed, the actual values, not the log values, were averaged.

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June 13, 1995

In order to use the Latin Hypercube Sampling (LHS) program, the following data is required: minimum value ('a'), maximum value ('b'), 'p' and 'q' (parameters that determine the shape of the probabalistic distribution function graph). Values for 'a' and 'b', (in this case hydraulic conductivity, K), are given in the *Sandia Report, Total Performance Assessment Analysment for Yucca Mountain-Second Iteration (TSPA-93)*, volume 1, pg. 7-14. Values for 'p' and 'q' are not given but with the two equations given in the LHS user's manual, p23 (equations 3b & 4b), these values can be determined.

June 20, 1995

The 'p' and 'q' values, (required by the LHS program),can be obtained from the minimum, maximum, mean and coeficient of variation values given in the Sandia Report (SAND93-2675), and equations 3b & 4b from the LHS user's guide. These equations allow 'p' and 'q' to be expressed in terms of minimum, maximum, mean and coeficient of variation:

$$q = \frac{A - B(A+1)^2}{B(A+1)^3}$$

(see next page)

$$p = A*q$$

$$A = \frac{\text{(minimum value) - (mean value)}}{\text{(mean value) - (maximum value)}}$$

$$B = \frac{\text{(coef. of variation)}^2 * \text{(expected value)}^2}{\text{(maximum value - minimum value)}^2}$$

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From the LHS Usar's guide, page 23: July 31, 1995

a=minimum value
b=maximum value
E=expected value (mean)
CV=coefficient of variation
V=variance=$(CV*E)^2$
"p" and "q" are parameters that determone the shape of the probabalistic distributation function

a, b, E and CV are given in the TSPA-94; CV is calculated as shown above thus only "p" and "q" are left to be determined. This is done with equations 3b and 4b, also from page 23 of the LHS User's Guide.

eq. 3b $E = \dfrac{aq+bp}{p+q}$

eq. 4b $V = \dfrac{(b-a)^2(pq)}{(p+q)^2(p+q+1)}$

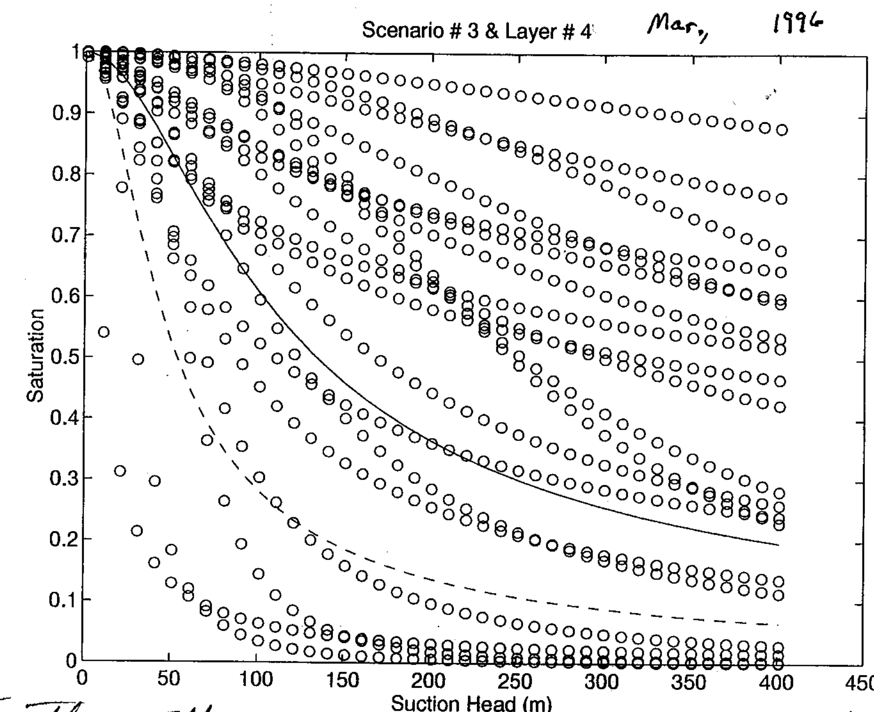
$$E = \frac{aq+bp}{p+q}$$
$$Ep + Eq = aq + bp$$
$$Ep - bp = aq - Eq$$
$$p(E-b) = q(a-E)$$
$$p = \frac{(a-E)}{(E-b)}q \qquad \text{Now let } A = \frac{(a-E)}{(E-b)}$$
$$\therefore p = Aq$$
$$V = \frac{(b-a)^2(pq)}{(p+q)^2(p+q+1)} = \frac{(b-a)^2 Aq^2}{(Aq+q)^2(Aq+q+1)}$$
$$\frac{V}{(b-a)^2} = \frac{Aq^2}{q^2(A+1)^2(Aq+q+1)} = \frac{A}{(A+1)^2(Aq+q+1)}$$
$$\text{let } \frac{V}{(b-a)^2} = B$$
$$B = \frac{A}{(A+1)^2(Aq+q+1)}$$
$$(Aq+q+1) = \frac{A}{B(A+1)^2}$$
$$q(A+1) = \frac{A-B(A+1)^2}{B(A+1)^2}$$
$$q = \frac{A-B(A+1)^2}{B(A+1)^3}$$

All terms on the right hand side of this equation are given (or easily determined from equations or substitutions given earlier in this page)

Saturation Values with Random ksat,alpha and beta

Timothy J Tolley 23 May 96

The figure below provides an example of the variability of the data when the randomly chosen variables, (ksat, alpha and beta), are used in the Van Genuchten equations. In this figure, twenty realizations, represented be the twenty curved rows of "O"s are shown. Each realization represents a situation in which all three variables, ksat, alpha and beta, are chosen randomly by the LHS (Latin Hypercube Sampling), routine based on the minimum, maximum, "p" and "q" as shown previously. For each of these twenty realizations the saturation is calculated and plotted at suction heads ranging from 0 to 400 meters. The results of this are shown in this figure below. This figure represents the Calico Hills unit (layer 4) only.



Timothy J Tolley May 23, '96

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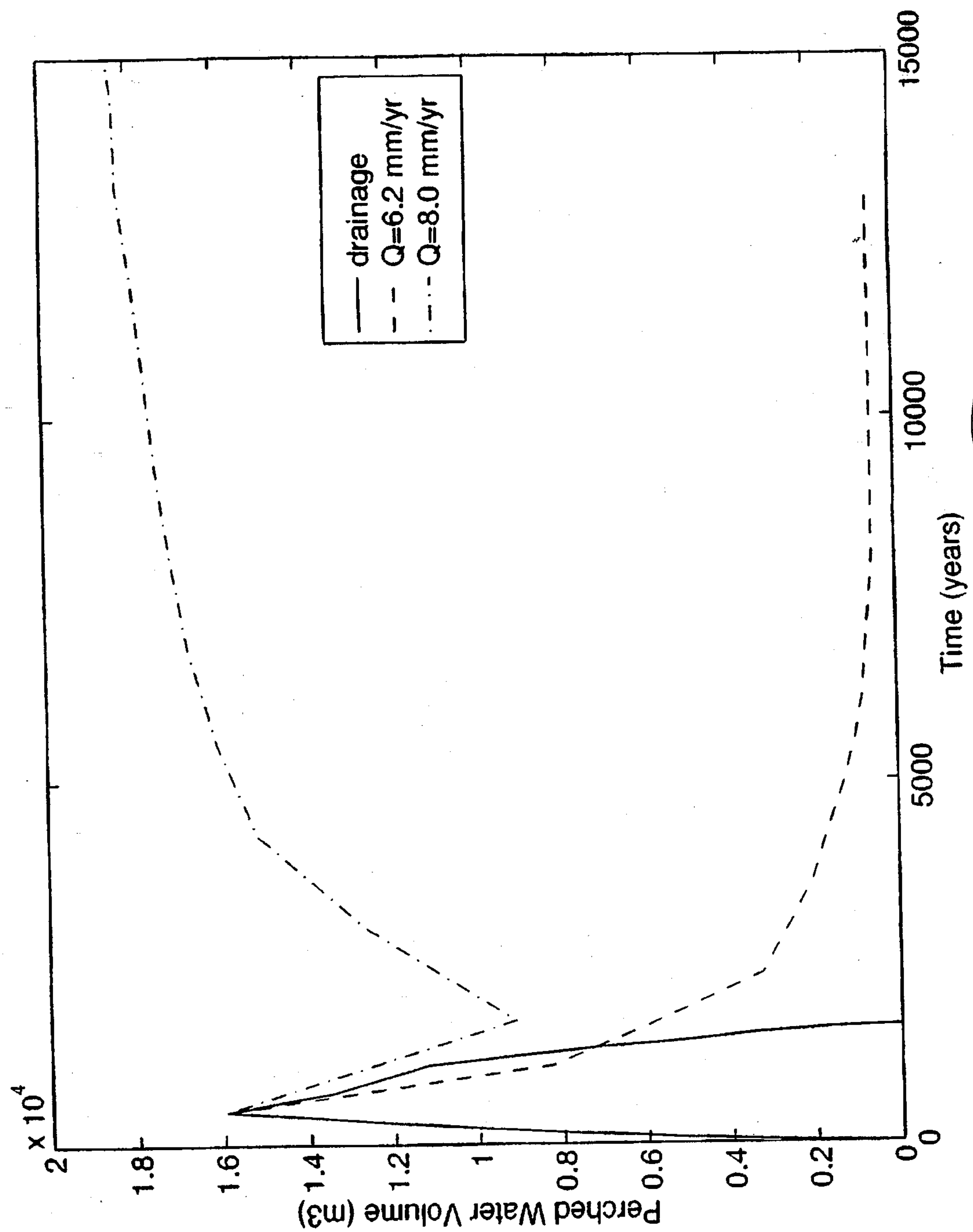
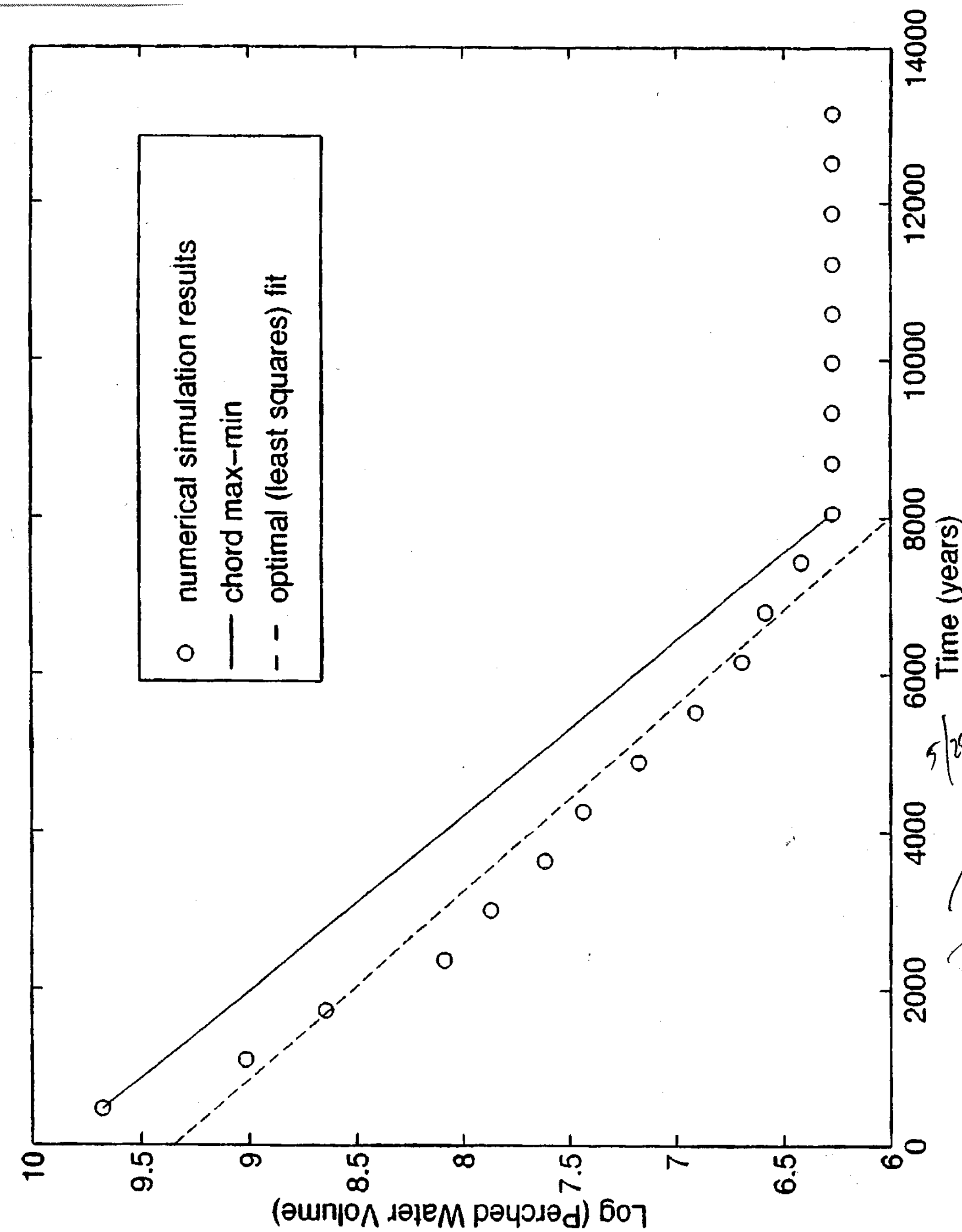
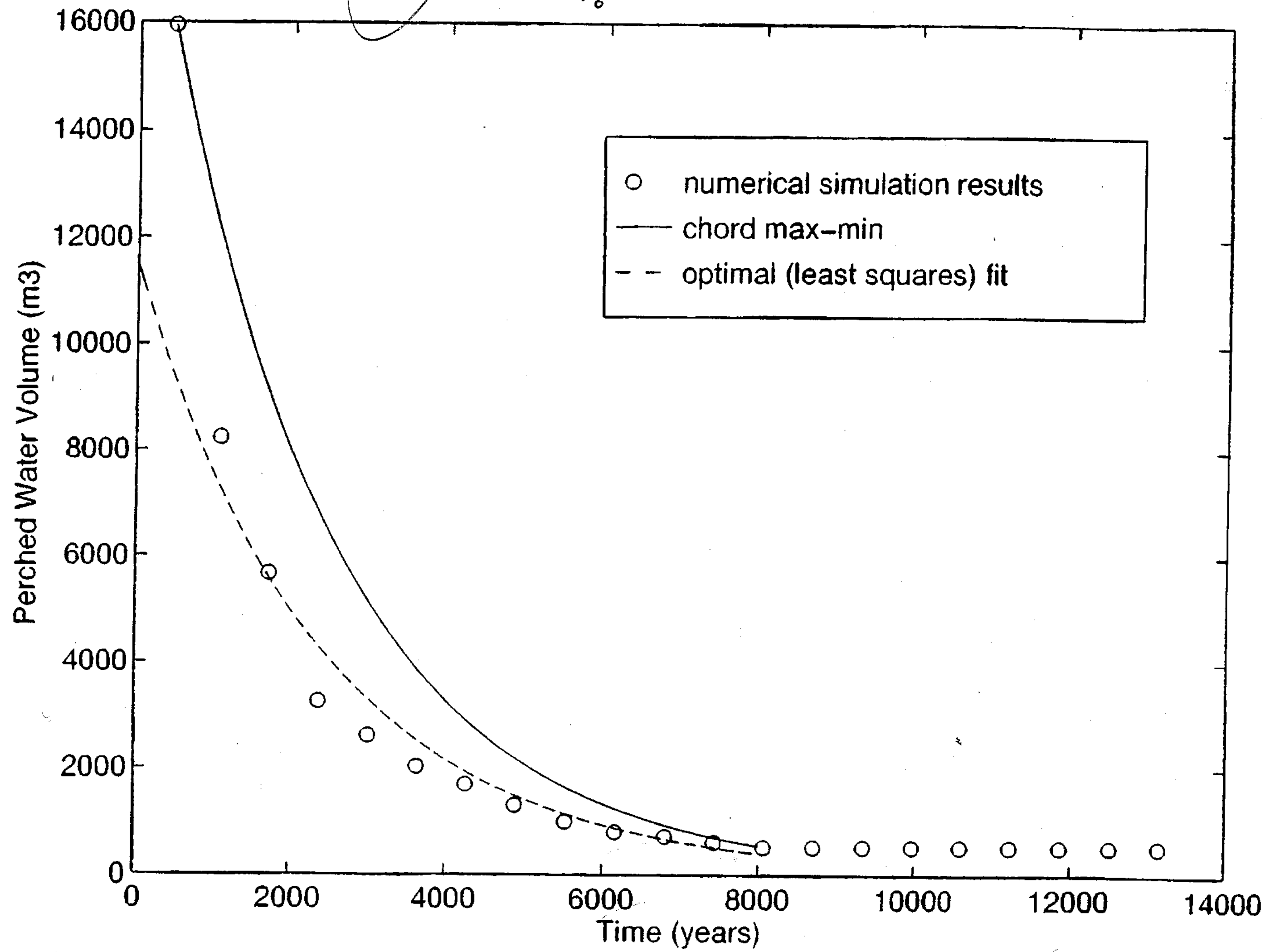

Perched Water Volume (m3)
x 10^4
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Time (years)
0
5000
10000
15000
drainage
Q=6.2 mm/yr
Q=8.0 mm/yr

24/5/96


Log (Perched Water Volume)
10
9.5
9
8.5
8
7.5
7
6.5
6
Time (years)
0
2000
4000
6000
8000
10000
12000
14000
numerical simulation results
chord max-min
optimal (least squares) fit

5/24/96



- **Simple Mass Balance of ^{14}C, Expressed in PMC**

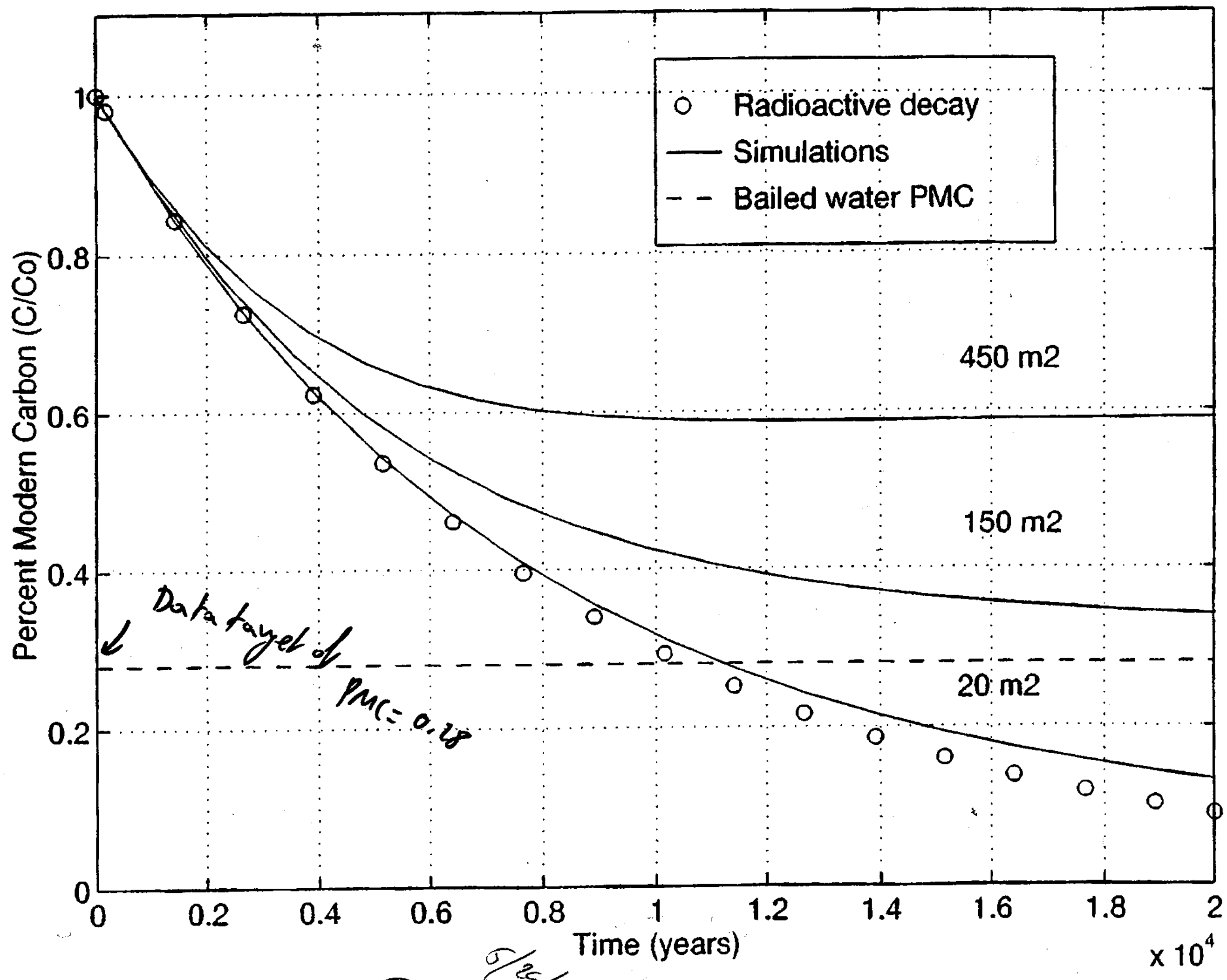
$$\frac{d(CV)}{dt} = q_i\, C_i - qC - \lambda CV$$

Leads to: $$\frac{dC}{dt} = -\frac{q_i + \lambda V(t)}{V(t)}\, C + \frac{q_i C_i}{V(t)}$$

- **Assumptions: (i) q_i is not changing with time, (ii) no contribution from episodic fast pathways (e.g., fractures), or estimates presented are the average of a matrix/fracture continuum, (iii) no daughter products contribution ($C_t = {}^{12}C + {}^{13}C + {}^{14}C$), and (iv) lumped system for transport.**

- **Integration of ODE using 4th and 5th order Runge-Kutta-Fehlberg Algorithm**

MATCAB (simple) code written to perform the ODE integration. Codes & data located under /home/sisyphus/abogtig/TCM



A Sustainable Perched-Water Body Can Be Attained With An Average Recharge Rate of 6.2 mm/yr, Following a Glacial Saturation Drainage

This is in Fair Agreement With the Work of Stothoff et al. (1996) Predicting Net Infiltration Rates of 10 mm/yr [3 ÷ 35]

A *PMC* ≡ *0.28* is Plausible for the Times and Inferred Rates Under Consideration

Timothy J Tolley 23 May 1996

Draining Simulation using Entropy-Fit Mean "in_" values

May 22, 1996

Note: These simulations were actually run of sisyphus ("/home2/sisyphus/ttolley/bigflo/run-/mean_val/runxx", "xx" indicates the run number). The input files are stored in directory "/home/sisyphus/ttolley/bigflo/src/prop/mean_prop"

Using the input values determined earlier, (and shown below), a complete draining simulation was produced.

layer	layer	in10_vgn	in11_ttdry	in5_ksat	in6_alfa	in7_tsat	in8_beta	Sr
1	TC	1.6218	1.80E-03	2.04E-11	0.0095	0.087	7.91E-03	0.0212
2	PT	2.3714	6.48E-02	3.80E-07	0.16	0.421	5.56E-01	0.154
3	TS	1.7989	6.30E-03	2.09E-11	0.018	0.139	1.36E-02	0.0453
4	CH	1.9588	3.59E-02	3.78E-10	0.063	0.319	1.33E-02	0.1127
5	PP	5.8884	2.01E-02	9.12E-10	0.11	0.292	1.60E-02	0.0688
		Table 7-7B	Sr * in7_tsat	Table 7-5B	Michael's paper	Table 7-3	Table 7-6B	Table 7-8

As was done earlier, the area of intrest was initially assigned a uniform head value throughout and the system was allowed to drain from this initial condition with no flux added. Once again the pore water, as it was pulled downwarn by gravity and channelled by the different layers with different properties, it began to form regions with saturation greater than 99.95%. The two main areas of accumulation were the right-hand side of the model and at the Ghostdance fault at the Paintbrush

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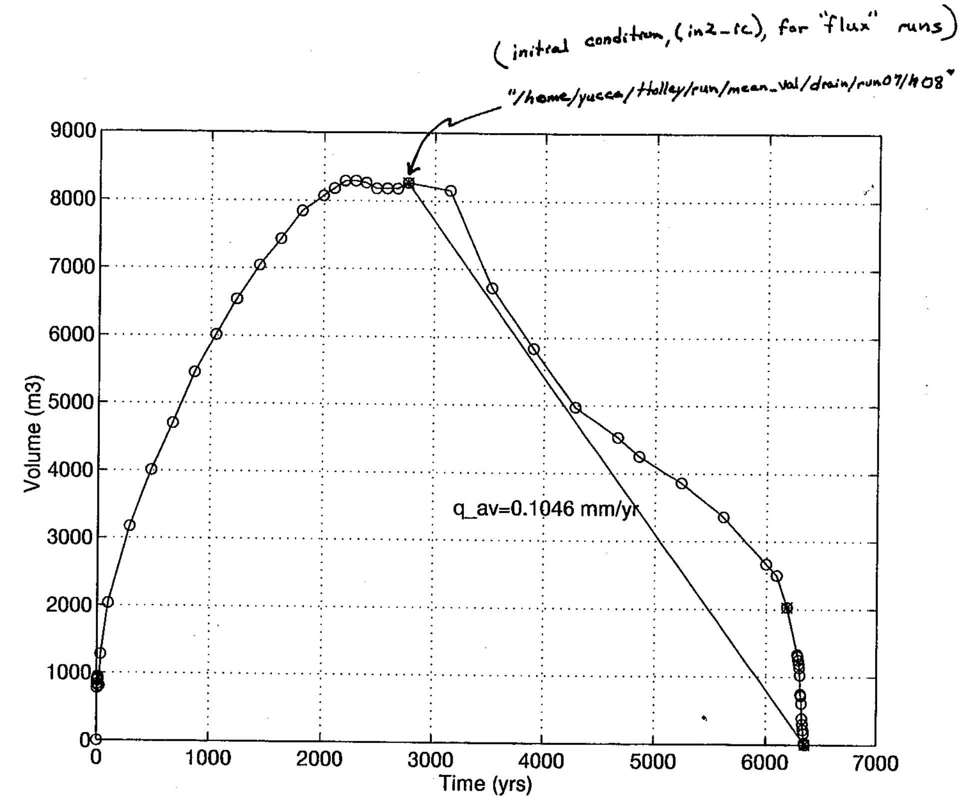
Tuff/Topopah Spring contact, (layer 2-layer 3). The accumulation at the right-hand side of the model was once again discarded from the total accumulation of perched water because it was created due to an artificial no-flow boundary of the model. The maximum perched volume occurred at about 2284 uears after the initial starting condition, (time = t^0). This perched water remained at near this approximate volume, (~8291 cubic meters), until at least 2759 years after t^0. At this time the volume began to drain and by 6374 years after t^0, the perched water body hac completely disappeared. This behavior is summarized in the table and graph below.

Timothy J Tolley 23 May 96

no flux
draining curve, mean values



Timothy J Tolley 23 May 96

Variables = Time, Total_Volume ~ May 14, 1996
(dir: /home/yucca/ttolley/tec/mean_val/drain/totvol/totalvol_drain.dat)

years	volume	
run02		
0.320000	0.	h05
run03btest		
0.320000	778.317	h01
0.640000	778.349	h02
0.960000	778.374	h03
1.28000	833.955	h04
1.60000	833.964	h05
1.92000	889.545	h06
2.24000	917.343	h07
2.56000	917.354	h08
2.88000	917.364	h09
3.20000	917.371	h10
run03		
32.0000	1278.77	h05
run04		
95.0000	2033.34	h05
run05		
285.000	3176.31	h02
475.000	4010.29	h04
665.000	4705.29	h06
855.000	5455.82	h08
1045.00	6011.81	h10
run06		
1225.00	6539.99	h02
1425.00	7040.35	h04
1615.00	7429.54	h06
1805.00	7846.48	h08
1995.00	8068.86	h10
run07		
2094.00	8180.05	h01
2189.00	8291.22	h02
2284.00	8291.25	h03
2379.00	8263.48	h04
2474.00	8180.14	h05
2569.00	8180.15	h06
2664.00	8180.16	h07
2759.00	8263.48*	h08*
3140.00	8152.26	h12
3520.00	6727.21	h16
3901.00	5837.54	h20
4281.00	4975.88	h24
4662.00	4531.09	h28
4852.00	4253.14	h30

(continued on next page)

* this is (almost) the maximum volume and is thus used for the starting point of the "flux" runs.

Timothy J Tolley 23 May 1996

~ May 14, 1996
(dir: /home/yucca/ttolley/tec/mean_val/drain/totvol/totalvol_drain.dat)

run08		
5233.00	3863.93	h04
5613.00	3363.55	h08
5994.00	2668.55	h12
6089.00	2501.69	h13
6184.00	2029.11	h14
6279.00	1333.95	h15
run08b		
6284.00	1306.13	h01
6289.00	1250.53	h02
6294.00	1194.93	h03
6299.00	1139.33	h04
6304.00	1028.16	h05
6309.00	750.281	h06
6314.00	722.479	h07
6319.00	611.321	h08
6324.00	389.022	h09
6329.00	305.657	h10
6334.00	222.294	h11
6339.00	166.718	h12
6344.00	27.7861	h13
6349.00	0.	h14
6354.00	0.	h15
6359.00	0.	h16
6364.00	0.	h17
6369.00	0.	h18
6374.00	0.	h19
6379.00	0.	h20
6374.00	0.	h16(run08)
6755.00	0.	h20(run08)

* this is (almost) the maximum volume and is thus used for the starting point of the "flux" runs.

Timothy J Tolley 23 May 96

Flux to Create Perched Water Volume of ~ 500 cubic meters

May 22, 1996

As stated previously one objective is to reproduce a perched water body that contains the same volume of water as one that has been found in the region, approximately 500 cubic meters. The assumption is once again that at some time in the past a cooler, wetter climate produced a greater saturation level and higher water table than exist at present. Under this assumption, the condition of maximum perched water obtained during the draining simulation was chosen as the initial "head" condition, (in2_ic), for the simulation in which flux is added in order to attempt to reproduce a sustained perched volume that approximates tha actual volume the perched water body found. Since the time of maximum perching for the draining simulation extends from about 2189 years after t^0 until about 2759 years after t^0, this latter time, (2759 years after t^0 and a perched volume = 8263), was chosen as the initial head condition for the following simulations in which flux is added to the model. The same input files were used for this simulation as for the last simulation, (draining with entropy-fit data). This data is repeated below.

Timothy J Tolley 23 May 96

layer	layer	in10_vgn	in11_ttdry	in5_ksat	in6_alfa	in7_tsat	in8_beta	Sr
1	TC	1.6218	1.80E-03	2.04E-11	0.0095	0.087	7.91E-03	0.0212
2	PT	2.3714	6.48E-02	3.80E-07	0.16	0.421	5.56E-01	0.154
3	TS	1.7989	6.30E-03	2.09E-11	0.018	0.139	1.36E-02	0.0453
4	CH	1.9588	3.59E-02	3.78E-10	0.063	0.319	1.33E-02	0.1127
5	PP	5.8884	2.01E-02	9.12E-10	0.11	0.292	1.60E-02	0.0688
		Table 7-7B	Sr * in7_tsat	Table 7-5B	Michael's paper	Table 7-3	Table 7-6B	Table 7-8

The only difference between this simulation and the draining simulation is that a flux was now added (uniformly) to the top of the model.

The results of this indicated that any flux less than or equal to 0.50mm/year would produce a perched water volume less than the target volume of about 500 cubic meters, if it produced a perched water volume at all. An added flux of 0.54mm/year of greater would produce a perched water volume much greater than the target volume of about 500 cubic meters. A flux of 0.51mm/year seemed to produce the closest volume to 500 cubic meters. Although it still seemed to be decreasing slightly at the end of the simulation, the change is small enough so that the volume can be considered to be stable. The results are summarized below in a table indicating the times and the respective volumes for some different added fluxes.

Timothy J Tolley 23 May 96

```
Variables = Time, Total_Volume        0.51mm/year     mean values     22 May
"/home/yucca/ttolley/bigflo/tec/mean_val/flux/0.51=flux/vol/totvol.dat"
```

years	vol
4366.00	4892.48
5972.00	3558.14
7579.00	2390.63
9186.00	1918.04
10792.0	1640.06
14407.0	1389.86
18022.0	1223.06
21637.0	1028.49
25252.0	1000.647
28867.0	806.098
32482.0	778.271
36097.0	722.665
39712.0	639.280
43327.0	611.473
46942.0	555.885

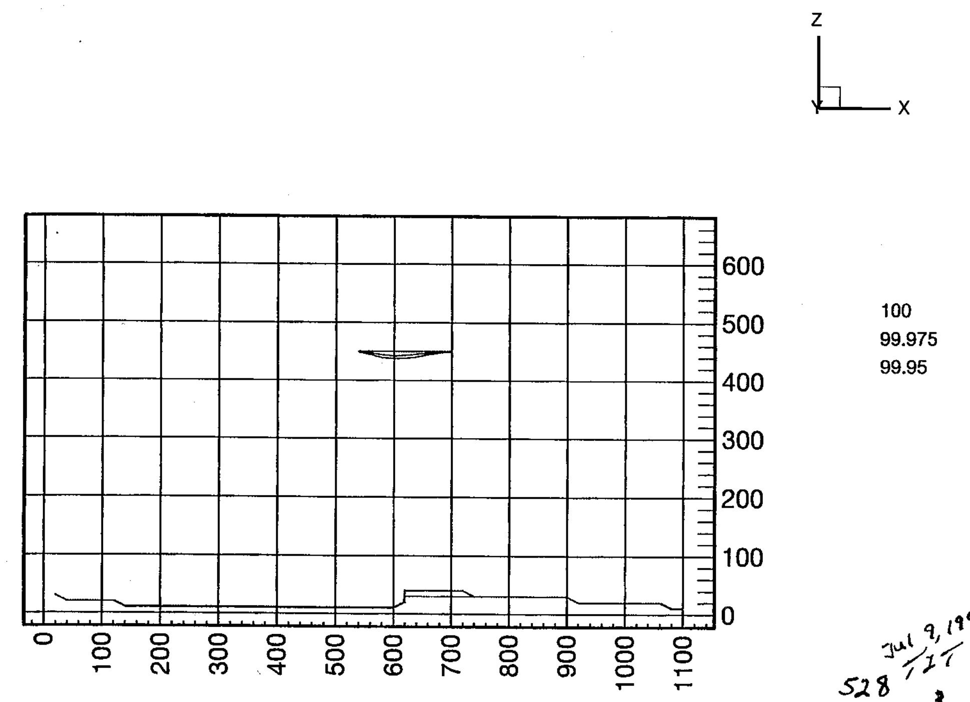
24 May 96

Note: On page 22 of this book the sustained volume reported for 6.2 mm/year flux was 528 m^3; however when it was calculated with the same "saturation criteria" as used for the mean value simulation since then, the volume was only 333.6 m^3. By "saturation criteria" I mean: 1) saturation defined as 99.95% ~~and ignoring "5" rows on left, 14 rows on right, 5 ~~columns~~ rows at bottom, 0 rows~~ (TJT 24 May 96)

2) ignoring all but the central perched region (~~ign~~ (i.e. ignore 5 left columns, 14 columns on right 5 rows at the bottom, 0 rows at top)

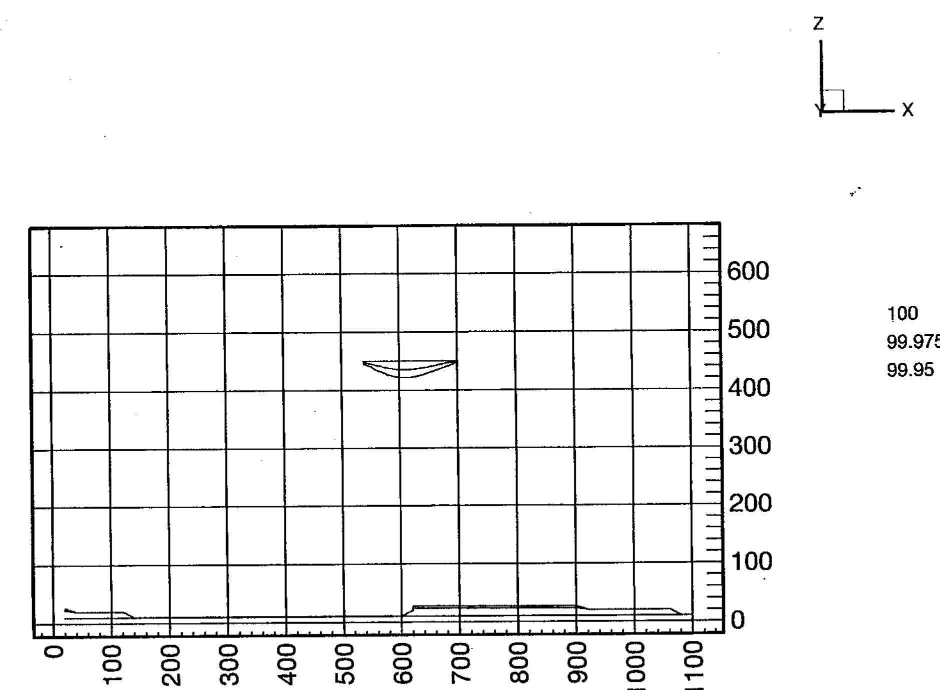
Figures showing the perched regions are on the next ~~pag~~ page.

Timothy J Tolley 24 May 96



Rflux=06.20b/h80sat old mean val 12,684 years

vol = ~~528~~ ~~333.6 m³~~ 528 ~~333.6 m³~~ (Jul 9, 1996 TJT)



0.51=flux/h15sat mean val 46942 years vol=555 m3

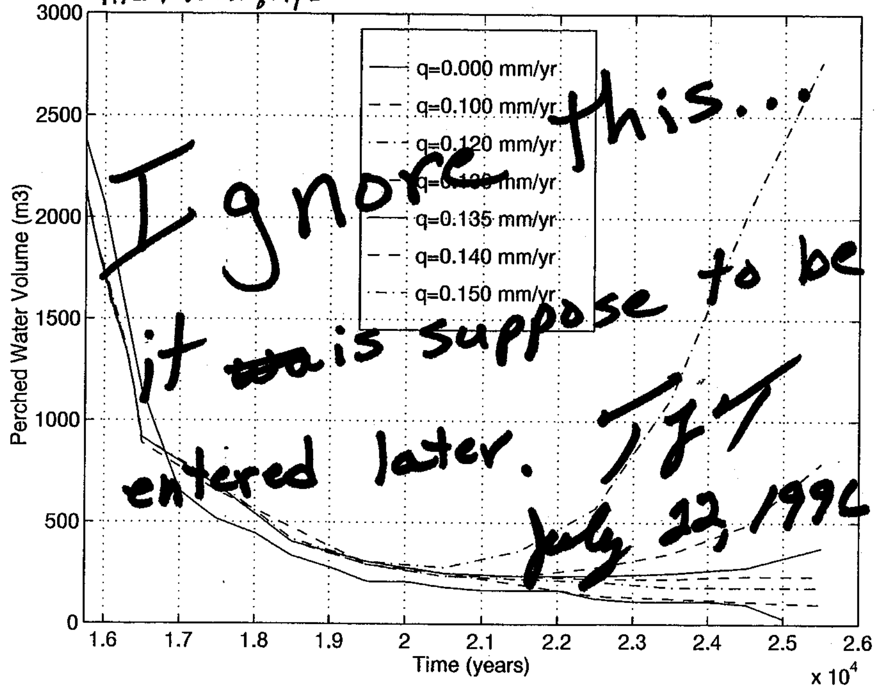
Timothy J Tolley

24 May 96

Timothy J Tolley July 22, 1996

directory: "/home/yucca/ttolley/geochem/prac"

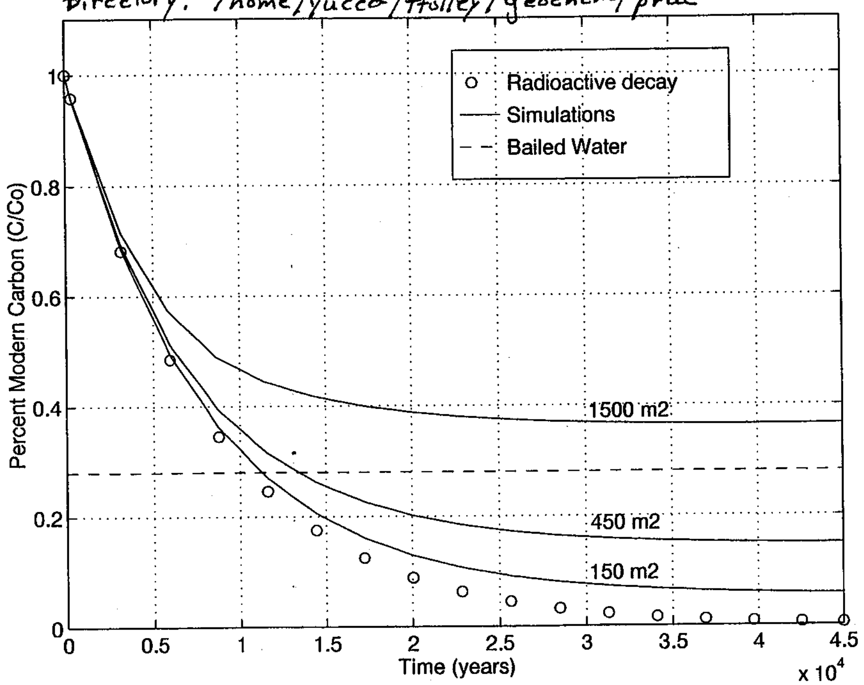
file : var_qs.ps



Ignore this... it ~~wa~~ is suppose to be entered later. TJT July 22, 1996

file ~~directory~~ : c14_age_051.ps

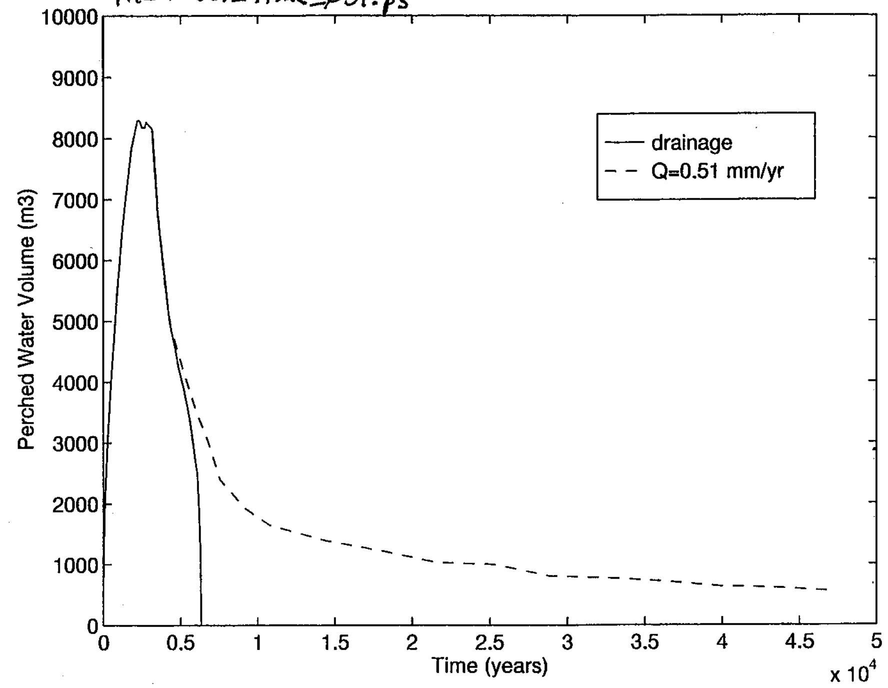
Directory: "/home/yucca/ttolley/geochem/prac"



Timothy J Tolley July 22, 1996

directory: "/home/yucca/ttolley/geochem/prac"

file: vol_time_051.ps



Timothy J Tolley July 22, 1996

ℓ CP 2/20/57

Timothy J Tolley July 23, 1996

Review 10 July 1996

Thus far two realizations have been run and have produced results. The first was using "true" mean values, (NOT entropy-fit), and this resulted in a flux of 6.2 mm/year being required to produce a sustainable perched volume of ~528 cubic meters. The next realization used "entropy-fit" mean values and resulted in a flux of 0.51 mm/year producing a sustainable perched volume of ~556 cubic meters but only after a period of ~46,000 years.

The first of these, (mean values, NOT entropy-fit), required a flux of 6.2 mm/year to produce a sustained perched volume of ~528 cubic meters. The time required to reach this volume, starting from a maximum volume of 15,949 cubic meters, (R07/h03), at 455 years, was 7155 years past the point of peak perching, (7610 years from the point of beginning to drain).

The results of the geochemistry indicate an area of infiltration of about 20 m2 to less than 150 m2 could producd the target percent modern carbon, (C/Co), of .28 in a time period of approximately 10,000 years to 20,000 years.

Thus these results indicate that this realization cannot be disqualified as a possible senario on grounds of either implausible hydrologic behavior or implausible geochemical behavior.

The second realization, (entropy-fit mean values), reached a maximum draining volume of ~8291 cubic meters after a draining period of ~2759 years, (run07/h08). From this peak volume a flux of 0.51 mm/year produced a sustained perched volume of 556 cubic meters at 44,183years after the max perching, or 46,942 years after the beginning of the draining).

The results of the geochemistry indicate an area of infiltration of about 450 m2 could producd the target percent modern carbon, (C/Co), of .28 in a time period of approximately 13,500.

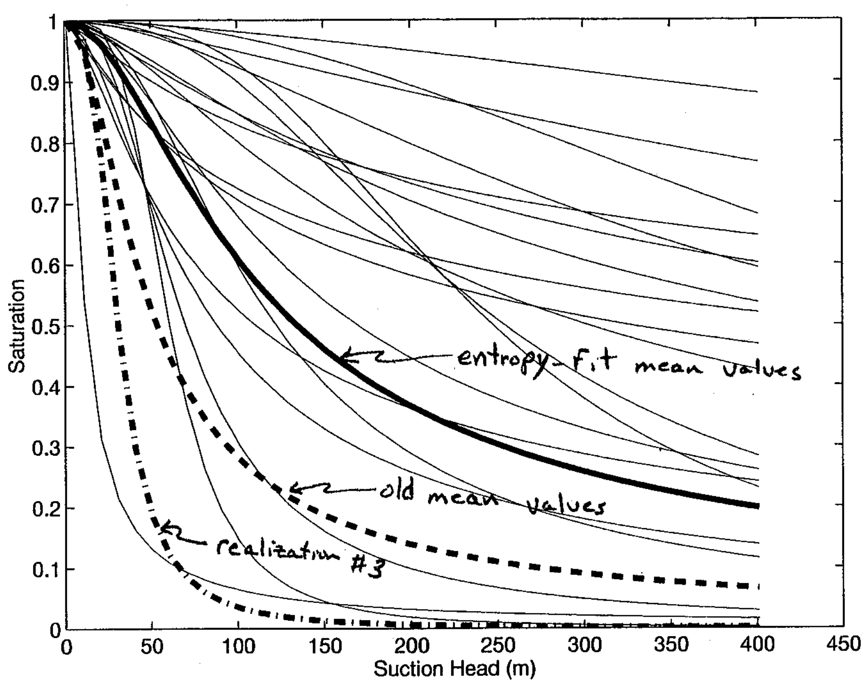
Thus these results indicate that this realization is feasible based on the geochemical behavior; however, based on the hydrologic behavior the time it takes to reach the target volume is too long to represent the roughly 18,000 years since the last period of peak precipitation.

Timothy J Tolley July 23, 1996

Random Values Produced by Latin Hypercube Sampling

Another simulation using a randomly produced set of values was run. At first the only value that was going to be produced randomly was lksat with all other values remaining entropy-fit mean values. It was also considered to use randomly produced beta value and lksat value, or even randomly produced lksat, beta, Van Genuchten n, (with all other values remaining entropy-fit mean values). So there were three choices; i) randomly produced lksat value and all other values entropy-fit mean values, ii) randomly produced lksat and beta values and all other valeues entrop-fit mean values, iii) randomly produced lksat, beta and Van Genuchten n values and all other values entropy-fit mean values. To help with the determination of which of these three would better represent the uncertainty faced in working with the data a Matlab code was written to show the variablity of the saturation and lkunsat under all three scenarios. The code is called PLOT.m and is located in directory "/home/thumper/ttolley/lhs/multi_var/plot. As expected the third scenario, (randomly produced lksat, beta and Van Genuchten n, with all other values remaining entropy-fit mean values), produced the greatest range of values of lkunsat and saturation. The figure below shows the variability of the saturation for the Calico Hills, (layer 4), at a series of suction head values when all three values were randomly produced; the figur es for the other senarios were simular except that the variability in the saturation was less for scenario two and even less for scenario one, (only lksat randomly produced). Thus the third scenario, (randomly produced lksat, beta and Van Genuchten n, with all other values remaining entropy-fit mean values), was decided upon.

Timothy J Tolley July 23, 1996



Timothy J Tolley July 23, 1996

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Random values of lksat, beta and Van Genuchten n were produced by the Latin Hypercube Sampling, (LHS), routine. Sixty random values were produced for the lksat. The first 20 values were to be used in the case of only lksat being variable and the next 20 random values were to be used in the case of random lksat and random beta values were used. The last 20 randomly produced lksat values were to be used in the case of lksat, beta and Van Genuchten all three being produced randomly, thus these were the 20 realizations that were considered. Likewise, 40 random beta values were produced; the first 20 to be used in the case of only lksat and beta values being randomly produced and the last 20, the ones which were actually used, were to be used in the case of all three, lksat, beta and Van Genuchten n, being randomly produced. Only 20 random Van Genuchten n values were produced for the case of randomly produced lksat, beta and Van Genuchten n. These randomly produced values of all three properties are shown below.

01		-12.0803	-7.27560	-10.16360	-8.72640	-8.34960	
02		-10.08530	-7.17220	-9.47810	-10.08140	-8.88240	
03		-11.8409	-6.24160	-12.3115	-10.7860	-8.43840	
04		-11.2424	-5.41440	-11.8088	-8.94320	-9.19320	
05		-11.0828	-7.12050	-11.5803	-8.56380	-8.12760	
06		-11.5217	-6.18990	-11.6717	-8.99740	-9.37080	
07		-9.12770	-5.93140	-10.7120	-10.02720	-9.01560	
08		-11.2025	-5.77630	-9.61520	-9.26840	-9.23760	
09		-11.0429	-5.51780	-10.48350	-8.72640	-9.50400	
10		-10.6439	-7.32730	-11.9002	-8.88900	-9.77040	
11		-10.8833	-6.75860	-11.7631	-9.37680	-9.10440	
12		-11.0030	-5.10420	-11.1690	-10.7860	-9.54840	
13		-11.2823	-6.81030	-10.8491	-7.80500	-9.01560	
14		-9.44690	-6.91370	-11.7631	-11.0028	-9.32640	
15		-9.92570	-6.75860	-12.0373	-8.13020	-8.43840	
16		-11.1227	-6.13820	-9.86090	-8.23860	-8.57160	
17		-11.8010	-5.77630	-11.0319	-9.75620	-10.52520	
18		-9.80600	-6.34500	-12.1744	-8.02180	-8.70480	
19		-10.48430	-7.01710	-11.9459	-9.10580	-8.70480	
20		-10.56410	-7.06880	-9.70660	-7.42560	-9.94800	
21		-9.00800	-6.70690	-9.43240	-9.59360	-8.21640	
22		-8.72870	-6.50010	-9.34100	-10.9486	-9.99240	
23		-11.3222	-5.93140	-9.79800	-10.29820	-8.39400	
24		-10.8035	-6.91370	-11.3518	-9.53940	-9.19320	
25		-11.7611	-6.44840	-10.8948	-10.24400	-8.57160	
26		-9.60650	-6.08650	-10.48350	-9.10580	-9.10440	
27		-9.56660	-6.18990	-9.84370	-9.97300	-9.28200	
28		-11.6414	-6.29330	-10.02650	-9.86460	-8.17200	
29		-10.6439	-6.65520	-11.2147	-10.35240	-10.12560	
30		-8.64890	-6.60350	-10.6206	-8.50960	-8.52720	
31		-11.6414	-6.86200	-10.20930	-9.48520	-9.90360	
32		-12.1601	-6.03480	-10.9405	-9.64780	-8.52720	
33		-11.3621	-6.70690	-11.5346	-8.02180	-10.25880	
34		-10.7636	-6.03480	-11.6260	-7.75080	-8.92680	
35		-11.4020	-5.98310	-10.30070	-8.40120	-9.10440	
36		-9.36710	-6.44840	-8.79260	-8.67220	-8.03880	
37		-10.24490	-6.39670	-10.20930	-10.51500	-9.50400	
38		-10.7237	-6.29330	-11.2147	-8.88900	-11.4132	
39		-10.8833	-6.55180	-10.9862	-7.31720	-8.61600	
40		-10.9631	-6.50010	-10.39210	-10.46080	-8.97120	
41		-10.52420	-6.24160	-11.4889	-9.43100	-8.74920	
42		-11.5217	-7.06880	-10.7120	-10.18980	-9.59280	
43	***	-9.72620	-6.65520	-10.7577	-9.05160	-8.26080	03real
44		-10.32470	-6.96540	-11.3061	-9.21420	-8.79360	
45		-10.40450	-7.48240	-10.07220	-8.78060	-10.43640	
46		-12.0005	-6.60350	-9.29530	-9.75620	-8.70480	
47		-11.7212	-5.56950	-8.97540	-8.34700	-8.88240	
48		-9.84590	-6.39670	-9.98080	-9.48520	-9.68160	
49		-11.5616	-6.24160	-9.93510	-9.37680	-8.66040	
50		-9.96560	-6.50010	-11.1233	-11.1112	-8.97120	
51		-10.36460	-5.87970	-10.6663	-10.24400	-8.08320	
52		-9.20750	-5.67290	-11.0776	-8.34700	-8.30520	
53		-11.9207	-7.79260	-10.52920	-11.3822	-8.39400	
54		-10.20500	-5.82800	-9.15820	-9.70200	-9.41520	
55		-11.4419	-6.08650	-10.34640	-10.08140	-9.37080	
56		-9.64640	-6.13820	-11.4432	-9.91880	-8.48280	
57		-10.24490	-6.34500	-11.3975	-10.56920	-8.74920	
58		-10.04540	-5.72460	-12.2658	-10.6234	-8.83800	
59		-11.1626	-6.81030	-8.65550	-9.91880	-9.72600	
60		-11.9606	-6.55180	-10.8491	-9.26840	-8.26080	
		layer 1	layer 2	layer 3	layer 4	layer 5	

directory: "/home/thumper/ttolley/lhs/multi_var/lksat" file: lksat.dat
These are the 60 random log ksat values (from entropy fit data) that are used to get a random value simulation.The first 20 were to be used if only lksat was generated randomly, (to be used with mean beta and Van Genuchten n values).
Lines 21 to 40 were to be used if only lksat and beta were to be generated randomly, (and the mean Van Genuchten n was used). The last 20 lines were to be used if all three were generated randomly.(and this was the case).

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directory: "/home/thumper/ttolley/lhs/multi_var/lbeta" file:beta.dat
These are the random log beta values (from entropy-fit data), that are used for a simulation of random values. The first 20 realizations were to be used if only lksat and beta values were generated randomly and the mean Van Genuchten n value was used. The last 20 realizations were to be used if all three values, (lksat, beta, Van Genuchten n), values were used ... and this was the case.

layer1	layer2	layer3	layer4	layer5	
-1.87740	-0.381770	-1.03787	-2.36675	-2.06482	
-1.73196	-0.587360	-1.22803	-2.70767	-1.71256	
-1.78652	-9.75043E-03	-1.63212	-1.00307	-1.78054	
-0.886282	9.79395E-02	-2.22637	-2.53721	-1.81762	
-1.21364	-0.646100	-1.70343	-1.85537	-1.78672	
-2.19572	-0.460090	-1.96490	-2.84972	-1.95976	
-2.30484	-0.440510	-2.05998	-1.51445	-2.03392	
-1.37732	-2.93304E-02	-1.34688	-1.88378	-2.06482	
-2.00476	9.82958E-03	-2.51161	-1.99742	-1.64458	
-1.89564	-9.78603E-02	-2.15506	-1.37240	-1.68784	
-2.25028	-0.195760	-0.990331	-1.11671	-1.53952	
-2.35940	-0.411140	-1.46573	-1.31558	-1.98448	
-2.65948	-0.137020	-0.871481	-2.42357	-1.72492	
-3.04140	0.156679	-1.84605	-2.22470	-1.92886	
-0.995402	-0.274080	-1.89359	-0.576921	-2.00920	
-1.86836	-0.234920	-1.15672	-2.16788	-1.74346	
-2.11388	0.186049	-2.27391	-1.17353	-1.95358	
-2.93228	-0.254500	-2.20260	-2.25311	-2.01538	
-2.55036	4.89895E-02	-1.41819	-1.45763	-1.57660	
-2.63220	-0.538410	-2.63046	-1.20194	-1.91032	
----------	----------	----------	----------	----------	
-1.35004	-0.499250	-2.58292	-2.05424	-1.91032	
-1.51372	-0.156600	-1.32311	-1.94060	-1.93504	
-3.34148	-0.675470	-0.586241	-1.42922	-1.86706	Ø3real
-1.07724	-0.489460	-2.41653	-2.08265	-1.82380	
-1.65012	-0.685260	-1.98867	-2.39516	-1.62604	
-1.54100	-0.362190	-1.56081	-2.59403	-1.80526	
-1.92292	0.117519	-1.70343	-2.82131	-1.86088	
-3.15052	-0.332820	-2.46407	-2.28152	-1.75582	
-1.26820	-0.577570	-1.91736	-0.861021	-1.67548	
-2.79588	-0.303450	-2.36899	-1.79855	-1.65694	
-2.14116	-0.274080	-2.10752	-2.30993	-1.49626	
-1.15908	-0.166390	-1.75097	-1.57127	-1.87942	
-2.44124	-0.205550	-1.53704	-1.74173	-2.02156	
-2.49580	-4.89104E-02	-2.32145	-1.59968	-1.89796	
-2.74132	-0.430720	-2.29768	-1.94060	-1.84234	
-3.47788	-0.518830	-2.13129	-1.68491	-1.97212	
-2.03204	6.85695E-02	-1.79851	-2.13947	-1.99066	
-1.48644	-0.117440	-2.39276	-2.50880	-1.55188	
-3.17780	-6.84903E-02	-2.01244	-1.65650	-1.59514	
-2.87772	-0.323030	-2.55915	-1.74173	-2.05246	

directory: "/home/thumper/ttolley/lhs/multi_var/lvgn" file: log_vgn.dat
These are the random log vgn values (from entropy-fit data) that are used to get a random value simulation.

layer1	layer2	layer3	layer4	layer5	
0.155740	0.536760	0.147600	0.136510	0.658430	
0.242860	0.184660	0.359100	0.271320	1.00483	
0.143860	0.265140	0.267450	0.548870	0.769660	03real
0.165640	0.758080	0.295650	0.223740	0.543200	
0.304240	0.375800	0.105300	0.247530	0.821920	
0.254740	0.426100	9.12000E-02	0.334760	0.630300	
0.286420	0.144420	0.493050	0.176160	0.917730	
0.209200	0.667540	0.521250	0.414060	0.726110	
0.181480	0.939160	0.182850	0.310970	0.499650	
0.189400	0.285260	0.415500	8.89300E-02	0.882890	
0.225040	0.335560	0.246300	0.485430	0.673850	
0.262660	0.587060	0.168750	1.04790E-01	0.743530	
0.175540	0.164540	0.133500	0.445780	0.839340	
0.133960	0.234960	8.41500E-02	0.207880	1.13548	
0.230980	0.214840	0.204000	0.382340	0.604170	
0.195340	9.41200E-02	0.316800	0.287180	0.473520	
0.274540	0.506580	0.232200	0.184090	1.05709	
0.205240	0.114240	0.196950	0.160300	0.421260	
0.157720	0.345620	0.380250	0.128580	0.935150	
0.219100	0.456280	0.253350	0.612310	1.09193	

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As mentioned earlier, the LHS routine requires a "p" and "q" parameter and it was shown how to derive these on pages 25 and 26 of this book. The routines that perform the computations are located in directory "/home/thumper/ttolley/lhs/multi_var/pq". These are Matlab files and are named: pq_beta.m, pq_ksat.m and -pq_vgn.m. The minimum, maximum, "p" and "q" values used for the LHS routine are listed below:

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dir:"/home/thumper/ttolley/lhs/multi_var/pq" May 28, 1996
file:"lhs_input"

log ksat (in5_ksat)

layer#	min	max	p	q
1	-12.20	-8.21	1.3380	2.1976
2	-8.93	-3.76	11.5012	12.1885
3	-12.54	-7.97	1.9693	2.8692
4	-11.87	-6.45	3.0419	3.6875
5	-12.39	-7.95	5.5718	1.8129

log beta (in8_beta)

layer#	min	max	p	q
1	-3.587	-0.859	1.5824	1.3245
2	-0.744	0.235	1.4976	1.5007
3	-2.678	-0.301	1.3103	2.5348
4	-3.077	-0.236	2.3331	3.1859
5	-2.071	-1.453	1.0201	1.5715

log vgn (in10_vgn)

layer#	min	max	p	q
1	0.130	0.328	1.2597	1.8581
2	0.074	1.080	1.1509	2.6956
3	0.063	0.768	1.3389	3.5773
4	0.081	0.874	1.1457	3.1602
5	0.369	1.240	1.5471	1.8133

note: This is the data that is input into the LHS routine to produce the random values (using the beta function of LHS). These values were determined from the TSPA-93, Table 7-5b, Table 7-6b, Table 7-7b. The values for unit 4 are a weighted value of units 5 and 6 of the TSPA tables. The weighing is based of the thicknesses of the units, (table 7-2, pg 7-9), and the true values are used in the averaging calculation, NOT the log values. The weighted values are converted to log values.

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Realization #3 (03real)

The next step was to repeat the entire procedure for the third realization. As mentioned earlier twenty of the variables "Van Genuchten n" (in10_vgn), Ksat (in5_ksat), and beta (in8_beta) were generated randomly using the Latin Hypercube Sampling (LHS) method. The third of these random samples was chosen for the next realization. Changing these three variables resulted in the change of the Gardner alpha (in6_alfa). The input data for this realization are listed below:

lay	in10_vgn	in11_ttdry	in5_ksat	in6_alfa	in7_tsat	in8_beta
1	1.3927E+00	0.0018	1.87850E-10	0.0065	0.087	4.5553E-04
2	1.8414E+00	0.0648	2.21208E-07	0.2500	0.421	2.1112E-01
3	1.8512E+00	0.0063	1.74703E-11	0.4100	0.139	2.5927E-01
4	3.5389E+00	0.0359	8.87973E-10	0.1000	0.319	3.7220E-02
5	5.8838E+00	0.0201	5.48530E-09	0.0010	0.292	1.3581E-02

Once again a draining simulation was run with no flux added. This produced the draining data shown below. Because of the properties of top layer and the assumed initial head level of -10 meters, (Tiva Canyon), this layer was saturated at the very beginning of the simulation and then began to drain. This is the reason for the high initial saturated volume. After this condition disappeared and the saturated volume reached a low of about 926 cubic meters at 10 years, the volume began to accumulate again as the water drained from some locations and a become trapped in other locations. The maximum volume of 3676 cubic merters, (r08/h06), was attained at about 8,000 years after the draining began. At about 25,000 years the saturated region had completely dissipated, (r09/h33). (The nature of this realization was very "jerky" as compared to the previous realizations).

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```
dir: "/home/yucca/ttolley/bigflo/tec/03real/drain"          June14 1996
file: "totvol.dat"
03real
drain (no flux)
```

years	vol	
0.0830	8297.87	
0.16700	7671.47	
0.25000	7045.07	
0.33300	7044.84	
0.41700	6418.53	
0.50000	5792.24	r01/h06
1.00	3652.36	r02/h06
10.00	926.20	r03/h09
20.00	926.19	r04/h01
30.00	1314.58	/h02
40.00	1790.39	/h03
70.00	1788.79	/h06
100.00	1788.78	/h09
400.00	2013.58	r05/h03
700.00	2827.80	/h06
1000.00	2800.00	/h09
1400.00	3078.00	r06/h04
1700.00	1814.20	/h07
2000.00	1814.20	/h10
2600.00	2008.80	r07/h06
3200.00	2147.80	/h12
3800.00	2425.80	/h18
4400.00	2481.40	/h24
5000.00	2759.40	/h30
5500.00	2954.00	r08/h01
6000.00	2981.80	/h02
6500.00	3315.40	/h03
7000.00	3426.60	/h04
7500.00	3454.40	/h05
8000.00	3676.80	/h06
8500.00	2863.40	/h07
9000.00	2418.59	r09/h01
9500.00	2474.20	/h02
10000.00	2474.19	/h03
10500.00	2474.20	/h04
11000.00	2502.00	/h05
11500.00	2502.00	/h06
12000.00	2557.60	/h07
12500.00	2696.60	/h08
13000.00	2668.80	/h09
13500.00	2641.00	/h10
14000.00	2779.99	/h11
14500.00	2946.79	/h12
15000.00	2863.40	/h13
15500.00	2529.78	/h14 *
16000.00	1584.59	/h15
16500.00	722.80	/h16 *
17000.00	444.79	/h17
17500.00	583.80	/h18
18000.00	444.80	/h19
18500.00	194.58	/h20
19000.00	222.40	/h21
19500.00	333.60	/h22
20000.00	194.60	/h23
20500.00	111.20	/h24
21000.00	166.80	/h25
21500.00	166.80	/h26
22000.00	194.60	/h27
22500.00	83.40	/h28
23000.00	83.40	/h29
23500.00	139.00	/h30
24000.00	194.60	/h31
24500.00	55.60	/h32
25000.00	0.00	/h33

* h14, h16 were initial starting volumes for "flux added" simulations

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In the previous realizations, the starting point for all simulations of a specific flux rate subsequent to the draining simulation was the point of maximum perched volume attained during draining. In this realization this procedure was also followed, however, even with very small fluxes the system would not drain, rather it would continue to increase in volume, at least for periods longer than were possible for a perched volume in the target range of ~400 cubic meters to be attained in the required ~20,000 years. For this reason a point further along in the draining simulation was chosen, actually two other points were chosen: r09/h14 with an initial volume of 2530 cubic meters and r09/h16 with an initial volume of 723 cubic meters.

The latter point was used first in order to determine whether or not this simulation would drain at all with a flux. When it was determined that the system would drain, (at least to a volume less than the target volume), with 0.10 mm/year of flux and a starting point of 723 cubic meters, the point just before an abrupt drop in perched volume was chosen as the initial starting point for the 0.10 mm/year flux simulation to compare the results. The results were quite similar in the final volume that each simulation attained. The final volume for each simulation reached a final volume of approximately 100 cubic meters by the end of the simulation.The main difference was the time that it took to reach the smaller volumes. The first simulation started at a point 1000 years later than the latter simulation and thus it took about 1000 years more for the second simulation to reach the lower volumes. It appears then that once you get away from the point of maximum perching, the system is relatively insensitive to the initial volume. The point r09/h14, with a volume of 2530 cubic meters, was chosen as the initial starting volume for the simulations where flux was added for realization #03.

Once again, several simulations with different flux rates were run to determine which would produce a sustained perched volume of near the target volume of ~400 cubic meters and the resultant data are shown on the following pages. In this realization though the volumes at the different times did NOT steadily and consistantly decrease from one time the next until it reached a point where it maintained a steady volume as has been the case in the two previous realizations. The volume went up and down with time but the overall trend of the volume was downward.

Fluxes of 0.10 mm/yr, 0.12 mm/yr, 0.130 mm/yr, 0.135 mm/yr and 0.14 mm/yr all produced volumes that fluctuated around values that were smaller than the target value of 400 cubic meters. In addition the range over which the volume for each fluctuated was quite significant relative to the magnitude of the target volume. This made it difficult to determine a specific volume at which it remained for a significant period of time. A graph of these data for the difference flux rates is shown after the data. This graph was created in Matlab and has been "smoothed out" by an averaging tecnique. Another "problem" that occurred was that at the end of the simulation the volume of some of these indicate that it may begin to increase in volume but this was difficult to determine considering the large fluctuations in the values. For fluxes greater than 0.14 mm/year, 0.15 mm/yr and 0.20 mm/yr, there was a definite increasing trend in the magnitude of the volume. For this reason these two fluxes were considered to not produce a sustained perched volume near the target volume. The flux rates of 0.12 mm/yr and 0.130 mm/yr, although they produced volumes less than the target volume, seemed to most closely represent the desired behavior and since the simulation with 0.130 mm/yr was the largest flux that did not show a strong tendency to increase in value near the end of the simulation, this flux rate was chosen to have the geochemical analysis performed upon.

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dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.10d_2530=flux/vol" 28 JUN 1996
file:"totalvol.dat"
03real
flux = 0.10 mm/yr
starting volume: 2530 m3 (r09/h14)

15600.0	2335.19	a)/h02
15700.0	2112.80	/h04
15800.0	1945.99	/h06
15900.0	1779.20	/h08
16000.0	1612.38	b)/h02
16100.0	1501.20	c)/h01
16200.0	1417.79	/h02
16300.0	1250.99	/h03
16400.0	1056.39	/h04
16500.0	722.800	/h05
17500.0	583.800	d)/h01
18500.0	222.386	/h02
19500.0	361.400	/h03
20500.0	111.200	/h04
21500.0	277.974	/h05
22500.0	83.4000	/h06
23500.0	166.800	/h07
24500.0	55.6000	/h08
25500.0	139.000	/h09

dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.12d_2530=flux/vol" 03 JUL 1996
file:"totvol.dat"
03real
flux = 0.12 mm/yr
starting volume: 2530 m3 (r09/h14)

years	vol
15600.0	2335.19
15700.0	2112.80
15800.0	1945.99
15900.0	1779.20
16000.0	1640.17
16100.0	1501.20
16200.0	1417.79
16300.0	1251.00
16400.0	1056.40
16500.0	778.376
17500.0	583.800
18500.0	222.392
19500.0	361.400
20500.0	111.200
21500.0	333.598
22500.0	83.4000
23500.0	278.000
24500.0	83.4000
25500.0	278.000

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dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.130d_2530=flux/vol" 08 JUL 1996
file:"totvol.dat"
03real
flux = 0.130 mm/yr
starting volume: 2530 m3 (r09/h14)

15600.0	2335.19
15700.0	2112.80
15800.0	1945.99
15900.0	1779.20
16000.0	1640.17
16100.0	1501.20
16200.0	1417.79
16300.0	1251.00
16400.0	1056.40
16500.0	778.380
17500.0	583.800
18500.0	222.394
19500.0	361.400
20500.0	111.200
21500.0	361.400
22500.0	83.4000
23500.0	361.391
24500.0	111.200
25500.0	361.391

dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.135d_2530=flux/vol" 08 JUL 1996
file:"totvol.dat"
03real
flux = 0.135 mm/yr
starting volume: 2530 m3 (r09/h14)

15600.0	2335.19
15700.0	2112.80
15800.0	1945.99
15900.0	1779.20
16000.0	1667.96
16100.0	1501.20
16200.0	1417.80
16300.0	1251.00
16400.0	1056.40
16500.0	778.383
17500.0	583.800
18500.0	222.398
19500.0	389.188
20500.0	111.200
21500.0	361.400
22500.0	111.200
23500.0	389.189
24500.0	166.798
25500.0	583.766

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dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.14d_2530=flux/vol" 08 JUL 1996
file:"totvol.dat"
03real
flux = 0.14 mm/yr
starting volume: 2530 m3 (r09/h14)

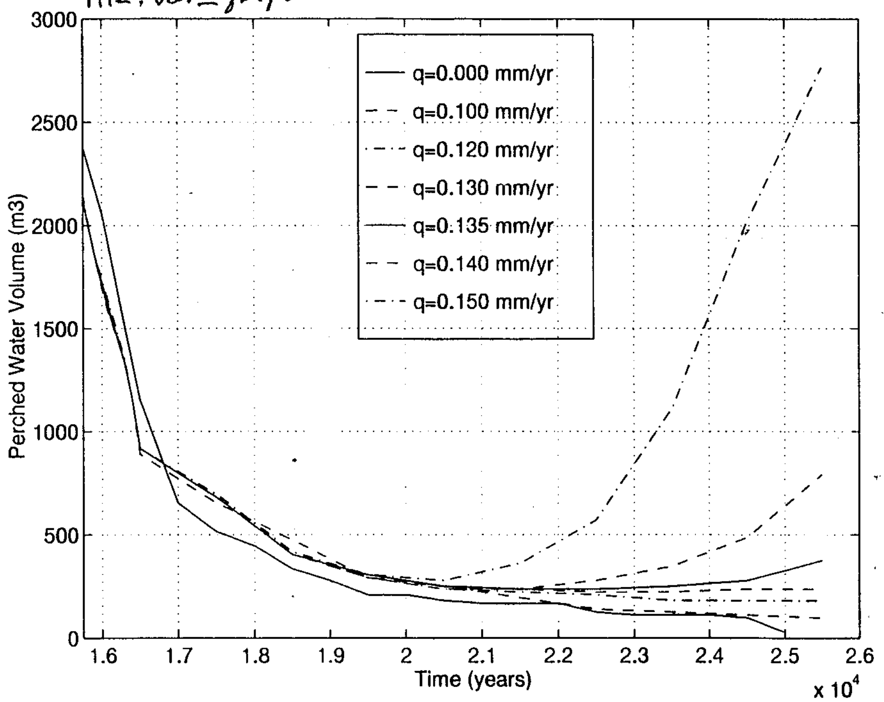
15600.0	2335.19
15700.0	2112.80
15800.0	1945.99
15900.0	1779.20
16000.0	1667.96
16100.0	1528.99
16200.0	1417.80
16300.0	1251.00
16400.0	1056.40
16500.0	778.385
17500.0	583.800
18500.0	222.398
19500.0	389.197
20500.0	111.200
21500.0	361.400
22500.0	194.586
23500.0	500.369
24500.0	472.514
25500.0	1111.90

dir:"/home/yucca/ttolley/bigflo/tec/03real/flux/sm_perch/0.15d_2530=flux/vol" 02 JUL 1996
file:"totvol.dat"
03real
flux = 0.15 mm/yr
starting volume: 2530 m3 (r09/h14)

years	vol
15600.0	2335.19
15700.0	2140.58
15800.0	1945.99
15900.0	1779.20
16000.0	1695.75
16100.0	1528.99
16200.0	1445.59
16300.0	1251.00
16400.0	1056.40
16500.0	778.389
17500.0	611.592
18500.0	222.398
19500.0	389.200
20500.0	166.792
21500.0	555.952
22500.0	583.721
23500.0	1640.02
24500.0	2390.81
25500.0	3141.34

directory: "/home/yucca/Holley/geochem/prac"

file: var_qs.ps



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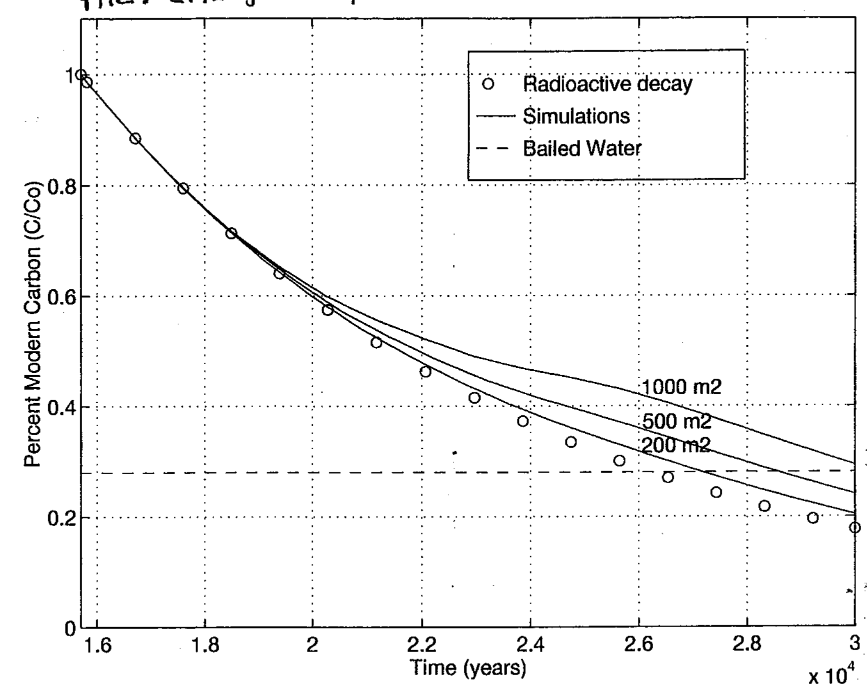
directory: "/home/yucca/Holley/geochem/prac"

file: "c14_age_013.ps



July 23, 1996

ECP 2/20/97

I have reviewed this Notebook. The first 57 pages are generally in compliance with QAP-001. Pages 95-108 provide only minimal compliance with QAP-001. On those pages, there appears not to be adequate information for another qualified person to reproduce the results.

E. C. Perry

E. Peary

2/20/97

Work recorded on Pages 95-108 was a limited exercise conducted some time ago by staff no longer at the Institute. It will stand as it is.

E. C. P

2/20/97

Pages 59 Through 98 Are Intentionally
Left Blank

TASK 3 (Part II)

&

TASK 2

Central Hypothesis

The 3D CNWRA geological model is conditioned on boreholes. What is the effect of conditioning on surface-based data? Ex: maps, satellite images etc.

Approach: Choose central block (fault-based) of CNWRA model & perform analyses on the TSw/PTn interface location.

5/20/96

All data, pre- and post-processing files are located in perlaner under directory:

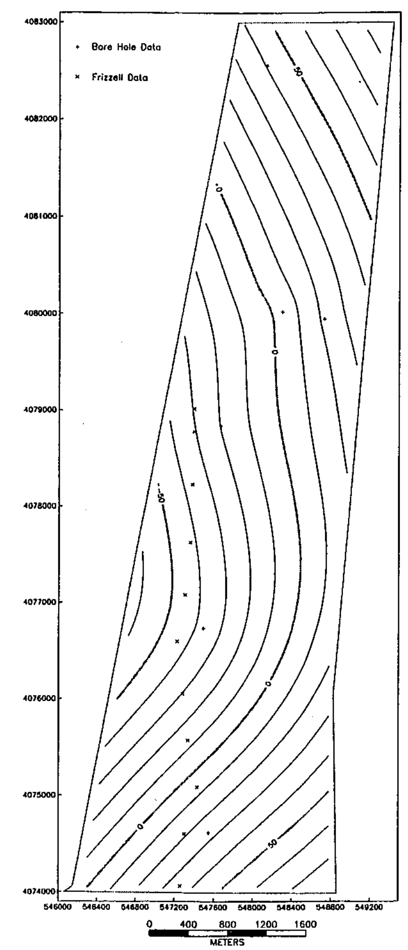
/usr4/dallen/rosskrige.

5/21/96

Summary of results so far:

bhole_TSW_diff_map.ps

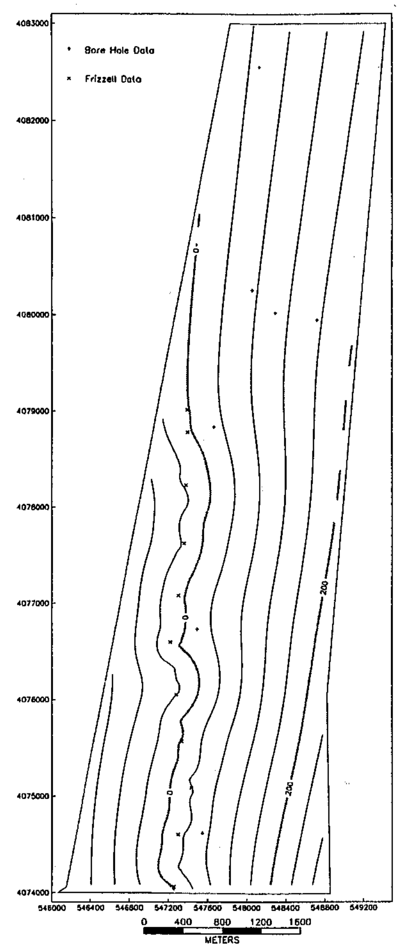
contour plot of error between bhole and horizon. in fault block 3 of 3-d model.



5/23/96

frizz_TSW_diff_map.ps

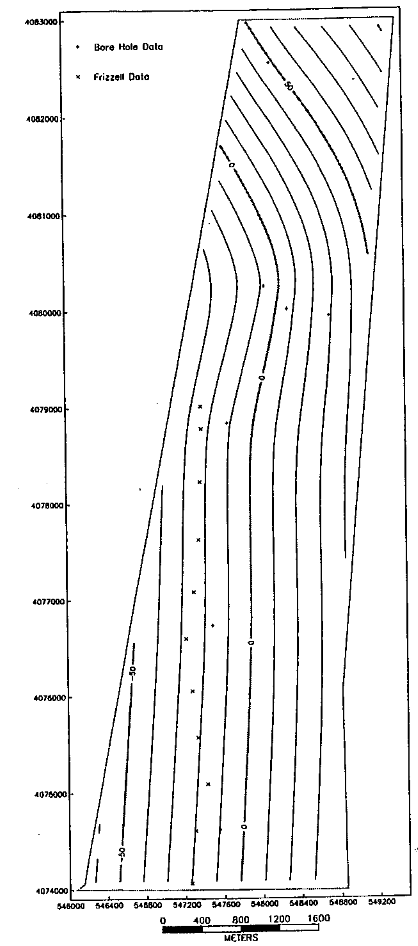
Contour plot of error between frizzell data and original horizon. Fault block 3 of 3-D model only.



5/23/96

bhole_TSw-frizz_diff_map.ps

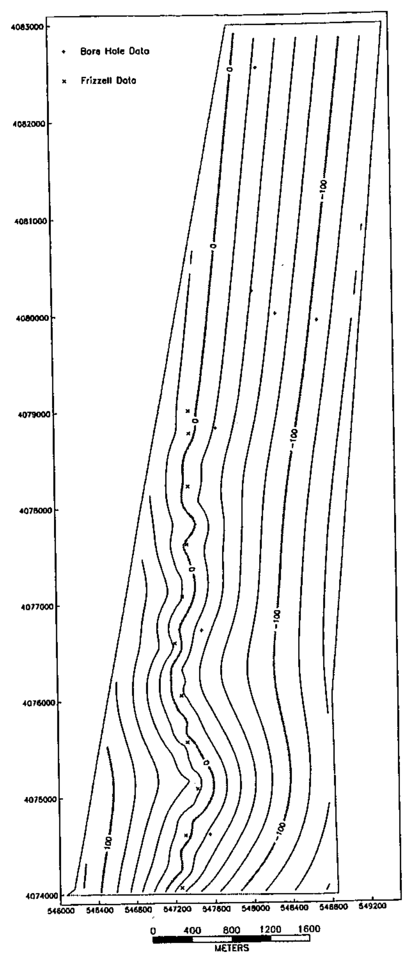
Contour plot of error between bhole and horizon corrected using frizzel data. Fault block 3 of 3-D model only.



5/23/96

frizz_TSw-bhole_diff_map.ps

Contour plot of error between frizzell data and horizon corrected using bhole data. Fault block 3 of 3-D model only.

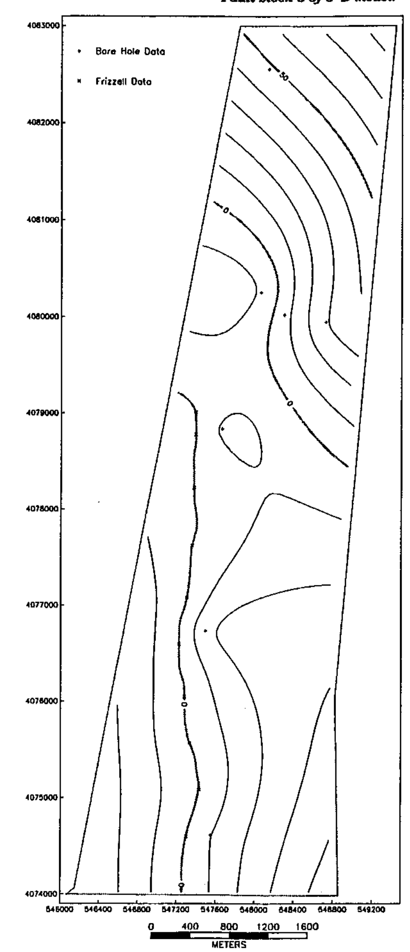


5/23/96

5/23/96

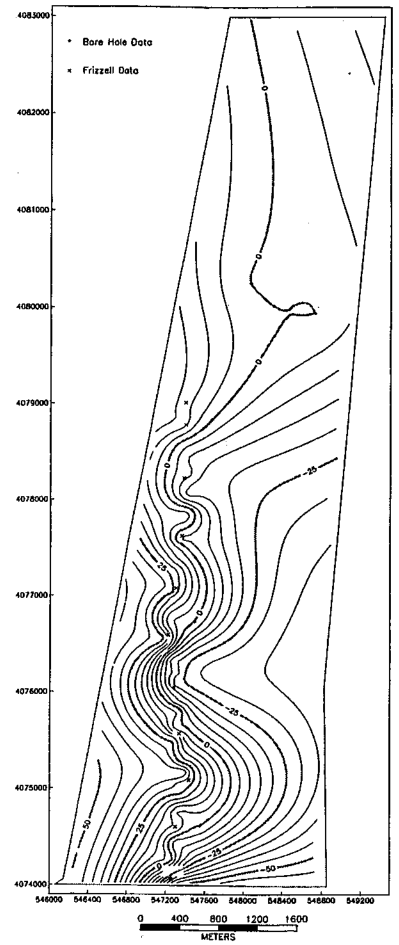
bhole_Tsw-frizz_diff_O_map.ps

Contour plot of error between bhole and horizon corrected using frizzell data and including frizzell zero poimts. Fault block 3 of 3-D model.



frizz_TSw-bhole_diff_0_map.ps

Contour plot of error between frizzell data and horizon corrected using bhole data and including bhole zero points. Fault block 3 of 3-D model only.



5/23/96


```
Statistics for difference of unit tops at TSw1 horizon

File name: bhole_TSW_diff.pdat
Comparision of boreholes vs model
Average error:         21.3477
Standard deviation:    16.3712

File name: bhole_TSw-frizz_diff.pdat
Comparision of borehole vs model corrected using frizzell
control points.
Average error:         17.3508
Standard deviation:    14.7843

File name: frizz_TSW_diff.pdat
Comparision of frizzell vs model.
Average error:         20.9815
Standard deviation:    13.7381

File name: frizz_TSw-bhole_diff.pdat
Comparision of frizzell vs model corrected using borehole
control points.
Average error:         11.1989
Standard deviation:     9.7214
```

-diff
-diff_o

-diff
-diff_o

5/24/96

This activity has produced some interesting results. In the central block of the CNWRA 3D geological model, an average error in the location of the unit tops at the TSw horizon, as observed at boreholes, has been estimated to be 21.35 m. When the geological model is conditioned on surface outcrop information, derived from maps, an improvement in the average error (17.35 m) is introduced. When borehole conditioning is effected this error becomes 11.20 m, a clear indication of the strong control that boreholes have on the model. However, interestingly enough, this improvement is not as profound as one might think, especially when compared to the effect that surface controls may have. In light of the dramatic cost differential existing between the two types of data, one may very well decide to collect much more, relatively inexpensive, surface-based data instead of borehole data. Future work, under this activity, will attempt to assign data worth attributes to these two approaches utilizing information about higher order moments of the error.

5/24/96