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Ground Water and Nuclear Waste Specialists

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COMMENTS ON VALIDATION ASPECTS OF THE YUCCA MOUNTAIN UNSATURATED ZONE TEST CASE IN PHASE 2 OF INTRAVAL - MODELING EXERCISES

By:
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November 6, 1992

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L. Lehman & Associates has undertaken a number of modeling exercises utilizing information provided to the Working Group towards the first step of developing and calibrating models of the near-surface tuff sequence. Additional published data were utilized as well to help fill in data gaps and to provide additional confidence in results. We modeled the data set utilizing 1-D, 2-D and fracture type mathematical models. We also utilized models which calculated runoff and infiltration in order to verify boundary conditions.

We conclude that neither the 1-D nor 2-D models did as good a job of matching the water content data as did our fracture model. Further, we believe the problem is not well posed as a validation exercise because the solutions are non-unique. More constraints are needed either to boundary or initial conditions to further compare results. Additionally, we conclude that more than one performance measure must be utilized to determine if any given model is a valid representation. For example, comparison to the tritium data could be extremely useful in this INTRAVAL problem. The following discussion summarizes the results of each model activity.

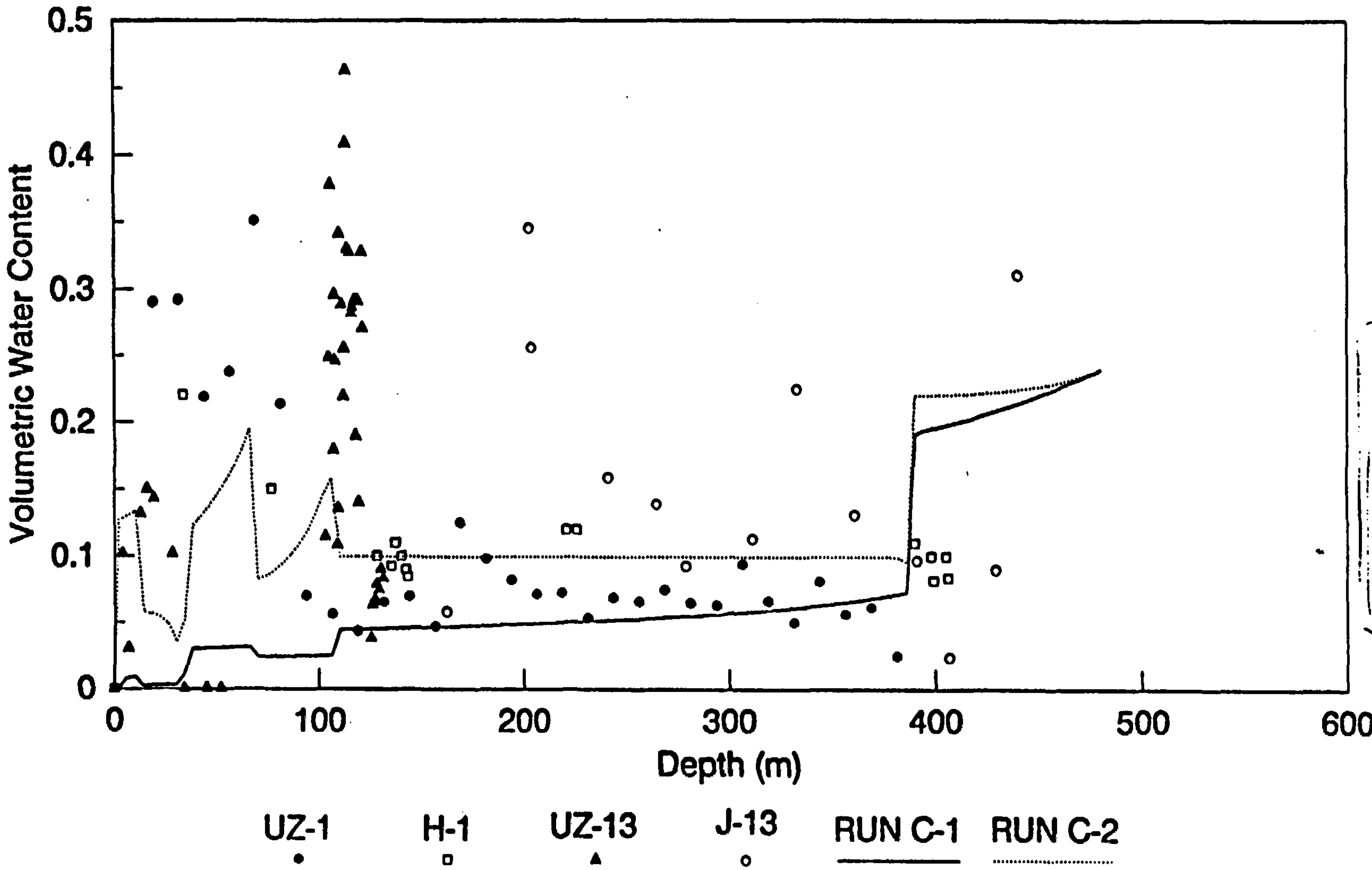
One Dimensional Model

The one dimensional VTOUGH simulations consist of seven hydrologic units based on the composite data provided by the USGS and use three different infiltration scenarios. The properties and geometry of the model are given in Table 1. Hydrologic units were inferred from the data based on qualitative grouping of similar valued measured properties. Conductivities are estimated as the geometric mean of measured conductivities from inferred units. Porosity and other properties are taken as the arithmetic mean. Parameters used in the VTOUGH Sandia function to represent the water retention characteristics were fitted to the available data by minimizing the sum of the squared error between the function and the data.

Figure 1 shows the modeled water content profiles for this model with infiltrations of 0 mm/yr (solid line) and 0.0126 mm/yr (dotted line) compared with data from drill

1. **Comparison of Measured and Modeled**

Volumetric Water Contents



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holes UZ-1, H-1, J-13, and UZ-13. This upper level of 0.0126 mm/yr is near the maximum infiltration the model will allow without creating zones of positive pressure and saturation within the low conductivity units, a condition not seen in any boreholes at Yucca Mountain.

Significant differences exist between the modeled and measured profiles for both infiltration rates. While water contents within the Topopah, from about 110 m to 390 m down, seem to match reasonably well, the upper units with very high measured water contents are much dryer in the model.

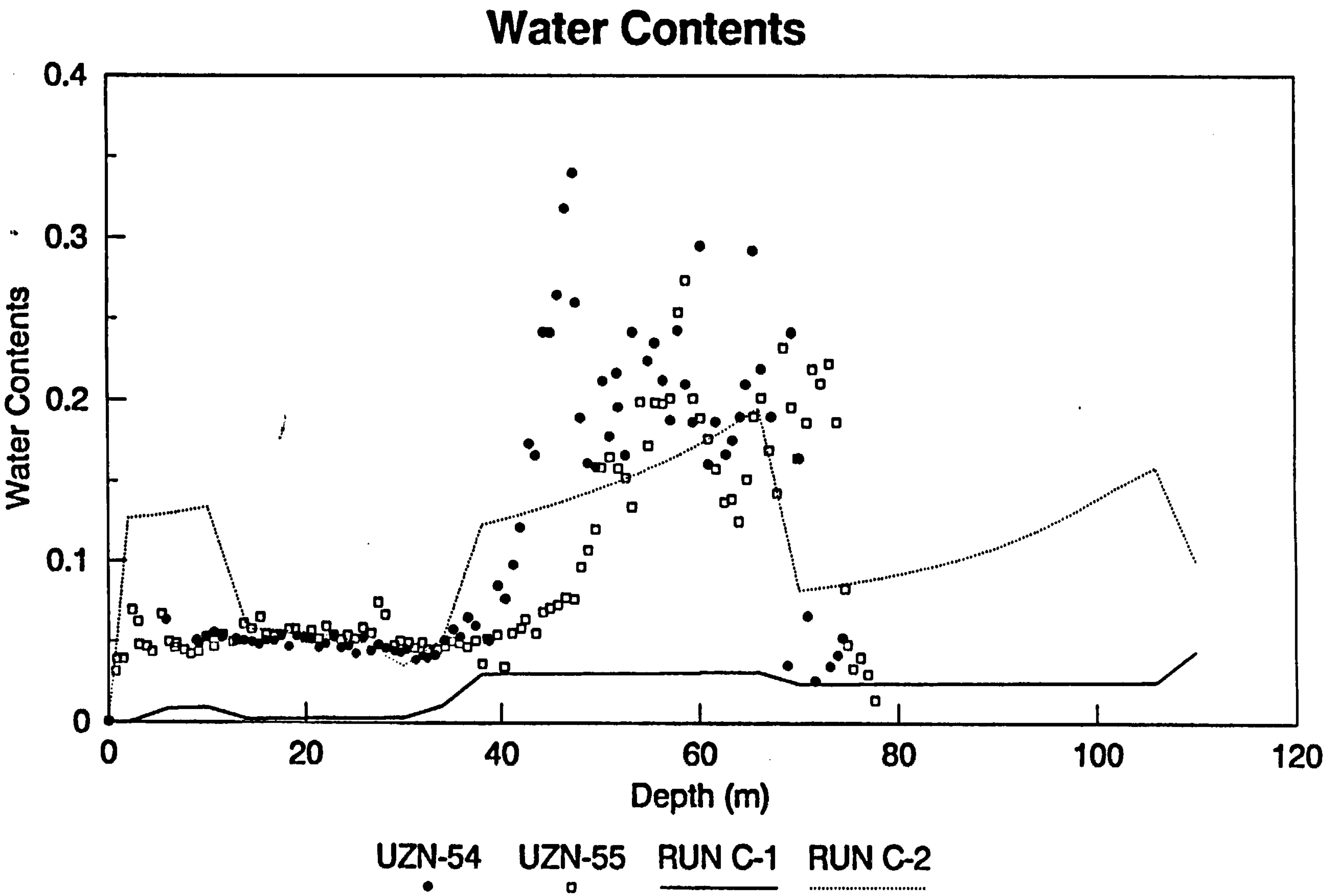
Figure 2 is a plot of the water content data with depth for the shallow boreholes UZN-54 and UZN-55 only. This figure shows a similar discrepancy between the modeled water contents and the actual borehole data. Water contents within the high permeability zone modeled as unit 4, are lower in the model than those measured.

Figure 3 shows the same model configuration but with a "pluvial" infiltration input. Based on Spaulding's (1983) rat midden study and scaled to the maximum infiltration the 1-D column will allow and be consistent with present day measurements, an infiltration signal beginning at 45,000 years ago of 0.012 mm/yr was linearly ramped to 0.054 mm/yr at 18,000 years ago, and then ramped back to the present day, 1-D estimate of 0.01 mm/yr as shown in Figure 3a. The initial condition was that of column equilibrium with 0.01 mm/yr. Again the model is much to dry in the upper highly permeable zone. The same is true when the model is compared to the shallow holes UZN-54 and 55 (Figure 4).

This 1-D model was one of three model configurations we ran, each with a different number of hydrologic units ranging from 4 to 11 units. All of our 1-D modeling did a poor job of matching the observed water content profiles and additional units did not significantly improve the fit. The wet conditions within the upper high conductivity unit, co-existing with the unsaturated conditions in the low conductivity units such as the Topopah, cannot be modeled with 1-dimensional geometry and infiltration realistically. By introducing a slug of infiltration at the surface and halting the simulation before the slug reaches the Topopah, one may achieve very wet conditions in the high conductivity zone without saturating the Topopah. We feel this is not a realistic representation of recharge at Yucca Mountain where recharge is probably slowly decreasing with time and no mechanisms exist to justify this "large slug" Model.

The fit was also found to be relatively insensitive to changes in the matrix characteristic curves. More likely, the discrepancy between the model and the data is due to two or three dimensional effects not accounted for in the 1-D model. Lateral flow or flow within fractures could produce the wet conditions in the area observed while allowing the unsaturated conditions observed in the Topopah.

2. Comparison of Measured and Modeled



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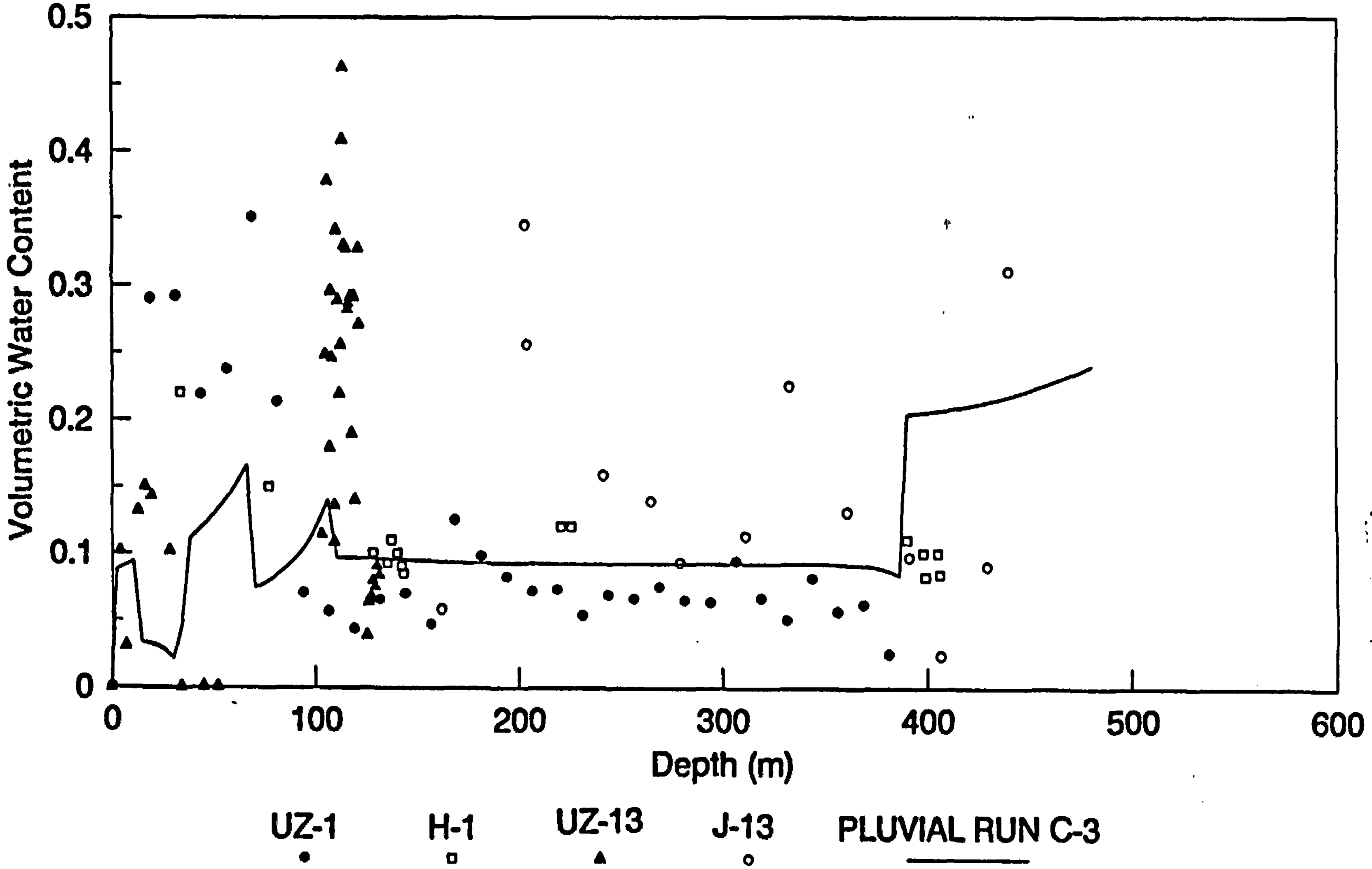
3. Comparison of Measured and Modeled

Volumetric Water Contents



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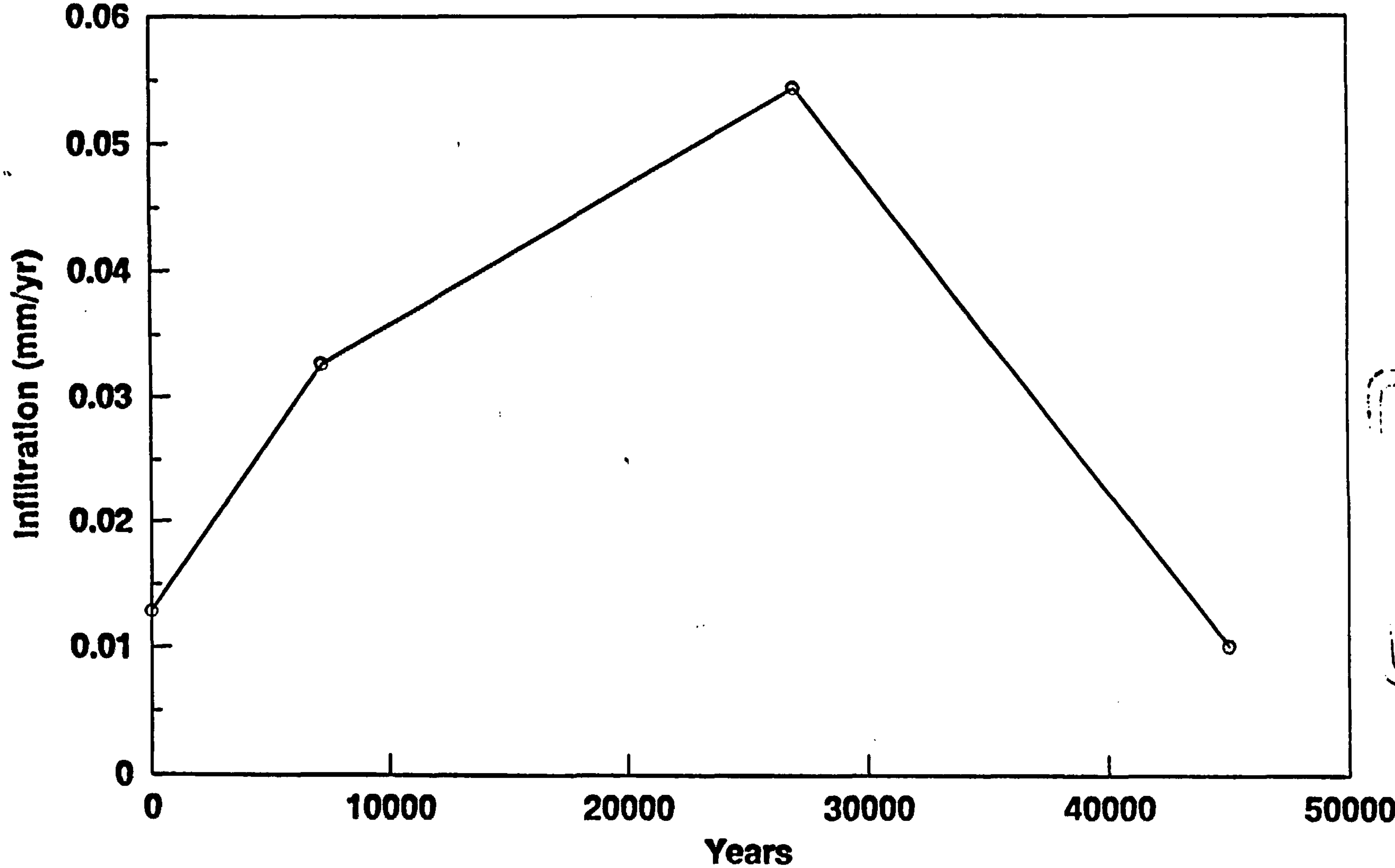
3A.

Pluvial Infiltration History

Estimated From Spaulding (1983)



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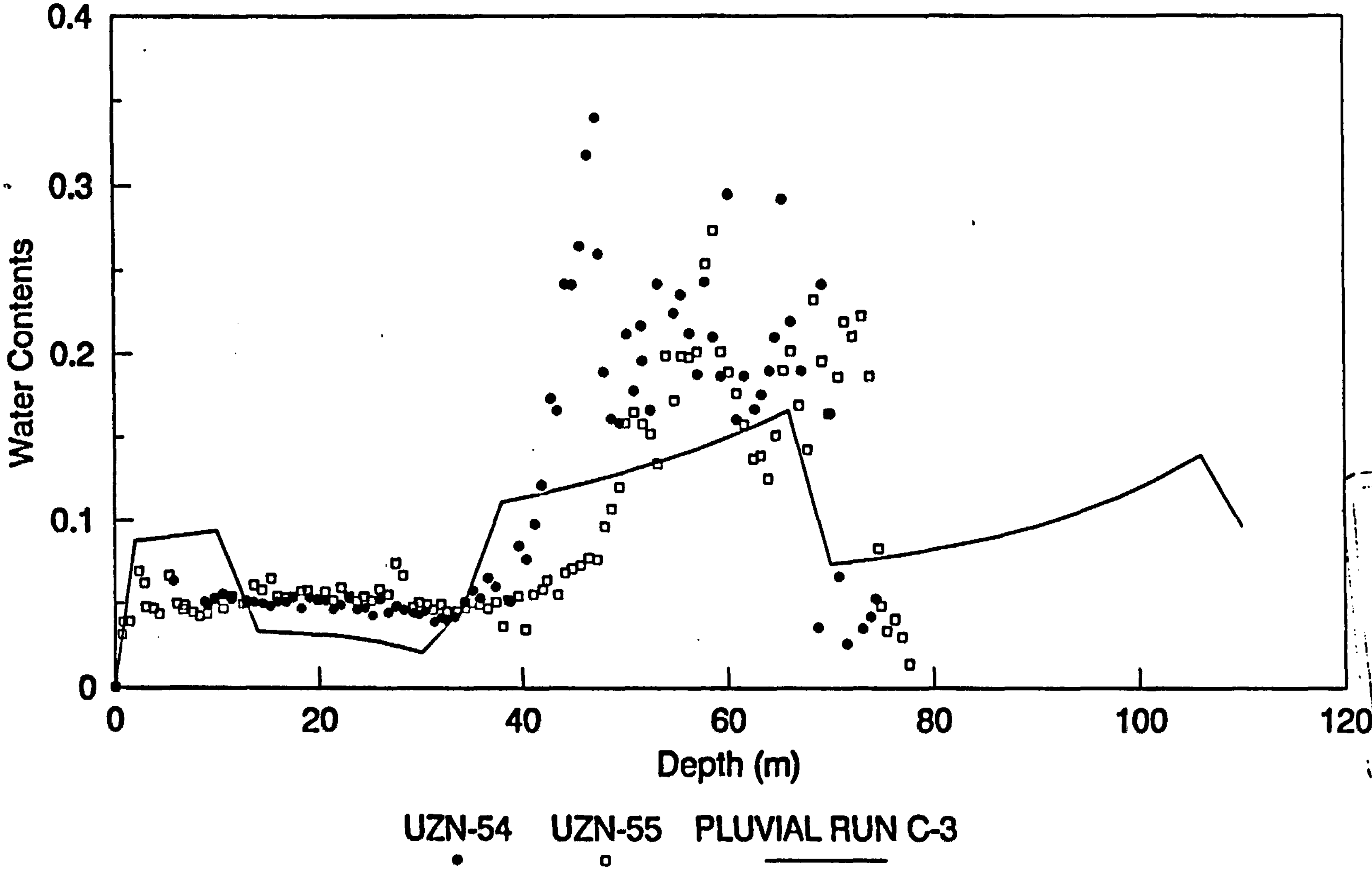
4. Comparison of Measured and Modeled

Water Contents



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To explore this possibility we first tried a two-dimensional model, then since we needed some estimate of the recharge mechanisms and amounts of recharge available to fractures and fault zones, we utilized a Catchment Area Runoff type model.

Two-Dimensional Model

The finite element method was used to solve the two-dimensional form of the Richards equation. The solution allowed for heterogeneous porous media conditions. A computer program implementing the finite element solution, called TWOD (J.L. Nieber, H. Munir, and M. Friedel, A Finite Element Model of Unsaturated Flow Using Simplex Elements, US Bureau of Mines, In press) was applied in the analysis.

A two-dimensional vertical section of the Yucca Mountain site was used as a model of the repository. The vertical section was conceptualized to contain seven distinct porous media units (i.e. the same units as in the 1-D model). The porous media properties in these units were represented by the van Genuchten equation for both the fluid retention and the hydraulic conductivity.

The vertical section was taken to be 750 meters wide and 488 meters deep with a water table as the lower boundary. The left boundary was taken to be a faulted zone (supposedly beneath the Solitario Canyon) and a line of symmetry was selected at a distance of 375 meters to the right of the fault. Therefore we did not model the full 750 meters, but assumed symmetry on either side of the midline. The line of symmetry is taken to be an impermeable boundary.

It was assumed that water infiltrated at a mean rate of 0.1 mm/year through the top boundary of the region, while water infiltrated through the length of the fault boundary on the left at two rates; 1.0 mm/year, and 0.1 mm/year. The source of water for the fault boundary is assumed to be water derived from depression focused recharge into the alluvium of the Solitario Canyon.

The finite element grid for the model domain is attached as Figure 5. It consisted of 720 nodes and 1330 linear triangular elements. In the simulations presented, the initial condition for all runs was assumed to be that of static equilibrium (i.e. no flow). Simulations were performed for times up to 200,000 years at which point the flow in the domain for all cases was at steady state. Qualitative comparisons of these results can be made to the measured water contents or saturations at selected boreholes.

Two water content profiles are given in Figure 6, one for each of the fault flux rates. These profiles are for a vertical transect taken along the line of symmetry of the two-dimensional domain. Like the 1-D simulations they still underestimate the measured water contents in the upper units.

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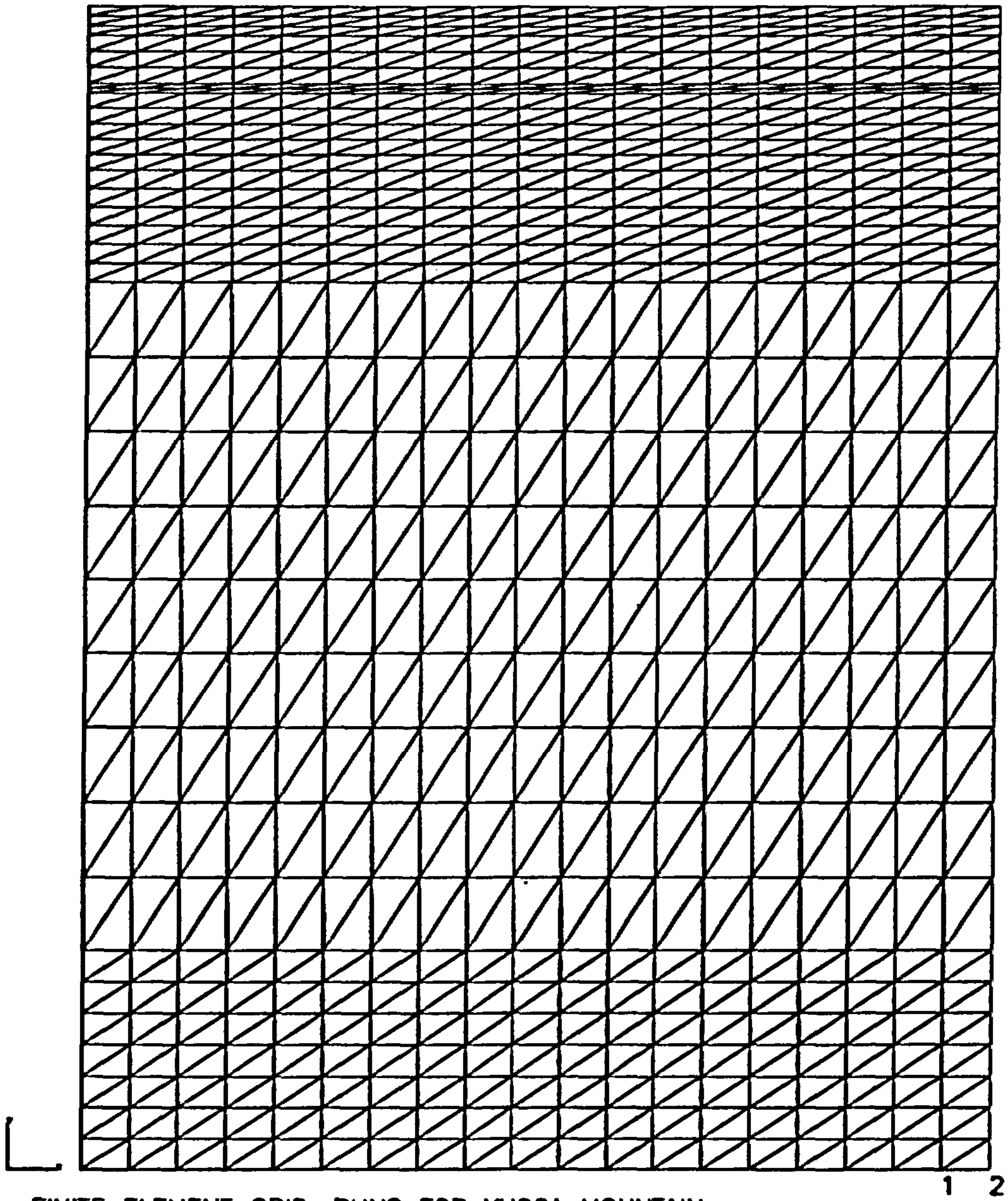
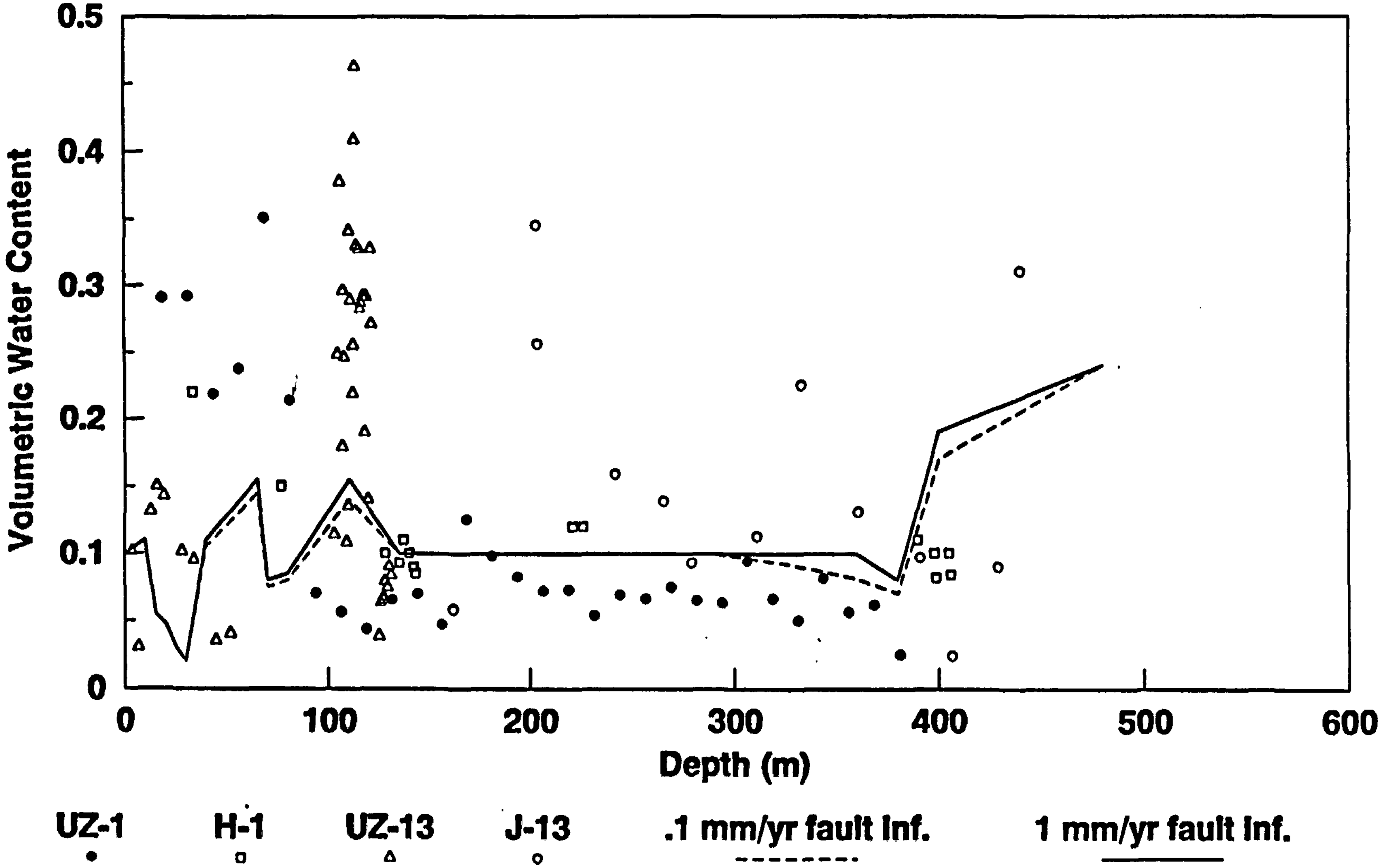


5. FINITE ELEMENT GRID: RUNS FOR YUCCA MOUNTAIN
DISTANCE BETWEEN 1-2 IS 19.74 UNITS

6. **Comparison of Measured and Modeled**

Volumetric Water Contents for 2-D Model



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Depression Focused Recharge (DFR) Model

The Depression Focused Recharge Model of Nieber et al, was used to estimate recharge available to fractures and fault areas which lie near canyon or channel bottoms and are covered with alluvium.

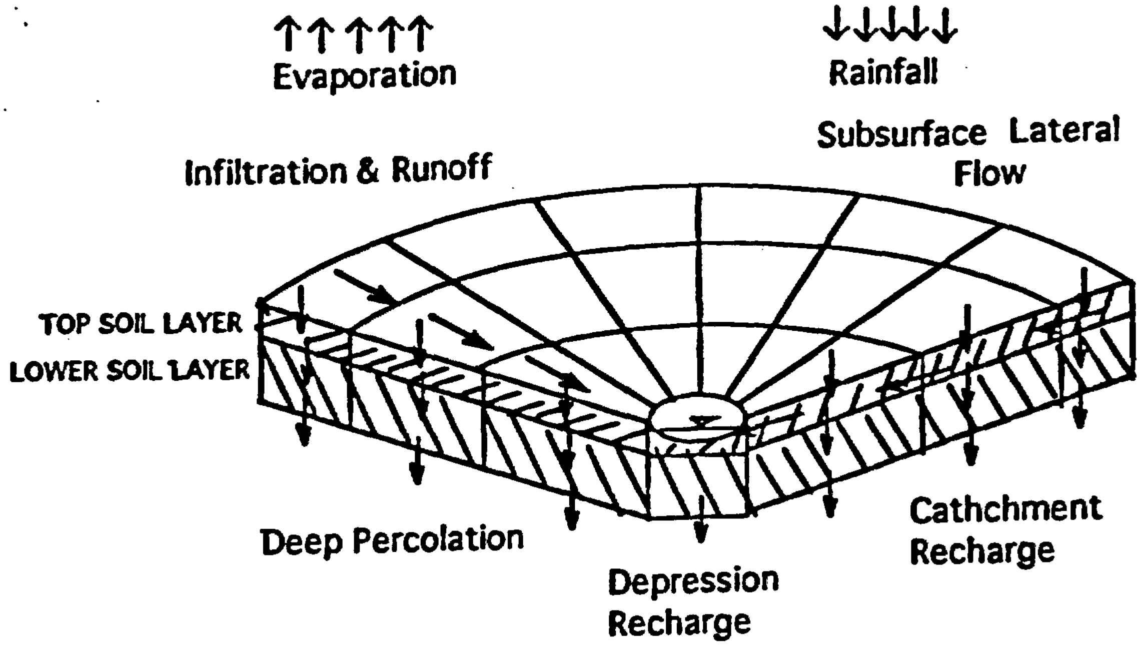
The model performs a full water balance of the hydrologic cycle of a small catchment containing a topographic depression using stochastically generated weather variables, and determines the spatial and temporal structure of groundwater recharge. It considers the intensity and duration of rainfall for each rain event simulated, calculating runoff evaporation and percolation for the catchment and depression. It takes into account the soil or rock hydrologic properties of the catchment and depression in calculating percolation which escapes evaporation (recharge).

Weather data from the Tonopah, Nevada weather station was used to generate 20 years of rainfall and solar radiation using the CLIGEN model (Nicks, 1989). Precipitation at Tonopah averages approximately 130 mm/yr, slightly less than estimated for Yucca Mountain. The model generates climate conditions preserving the serial correlation of measured temperature, solar radiation and precipitation along with duration and intensity statistics for precipitation events.

The 20 years of climate simulation was then used by the DFR model to perform a day by day cumulative mass balance of water entering and leaving the system. The model represents the catchment-depression system as a circular basin within which a depression with a outlet of fixed height exists (Figure 7). The climate simulation is applied uniformly over this circular geometry.

The catchment and depression geometry was based on the Solitario Canyon (Figure 8). The catchment boundary was estimated from the topography and the depression was chosen as the area of low relief at the canyon bottom. Two simulations were run using the same climate data with conductivity of the catchment based on the upper unit of the composite data and conductivity of the depression based on alluvium properties from Tyler (1985). Both simulations were modeled as a single layer, with deterministic soil properties, and with outlet height 10 cm. The 10 cm outlet height represents a rough estimate of water depth during a large precipitation event. Table 2 shows parameters used for the two runs. The two runs were designed to give a high estimate of recharge (Run 1) and a low estimate (Run 2). Run 1 used a lower value of conductivity for the catchment rock and a higher value of conductivity for the depression alluvium. Run 2 incorporated 1 mm of microdepression storage per rainfall event while Run 1 had none. This resulted in a value of depression recharge 3 times higher for Run 1.

Figure 9 shows the model mass balance for the entire basin for model run 2, the more conservative of two runs with regard to recharge estimate. The total recharge in both simulations occurs only in the depression due to the relatively low



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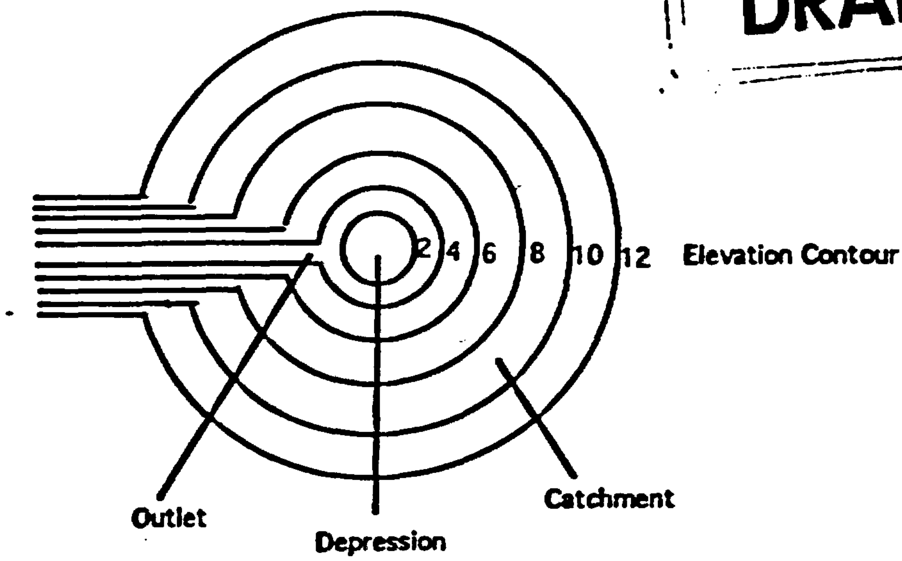

7. Diagram showing simplified representation of catchment used in the DFR model.

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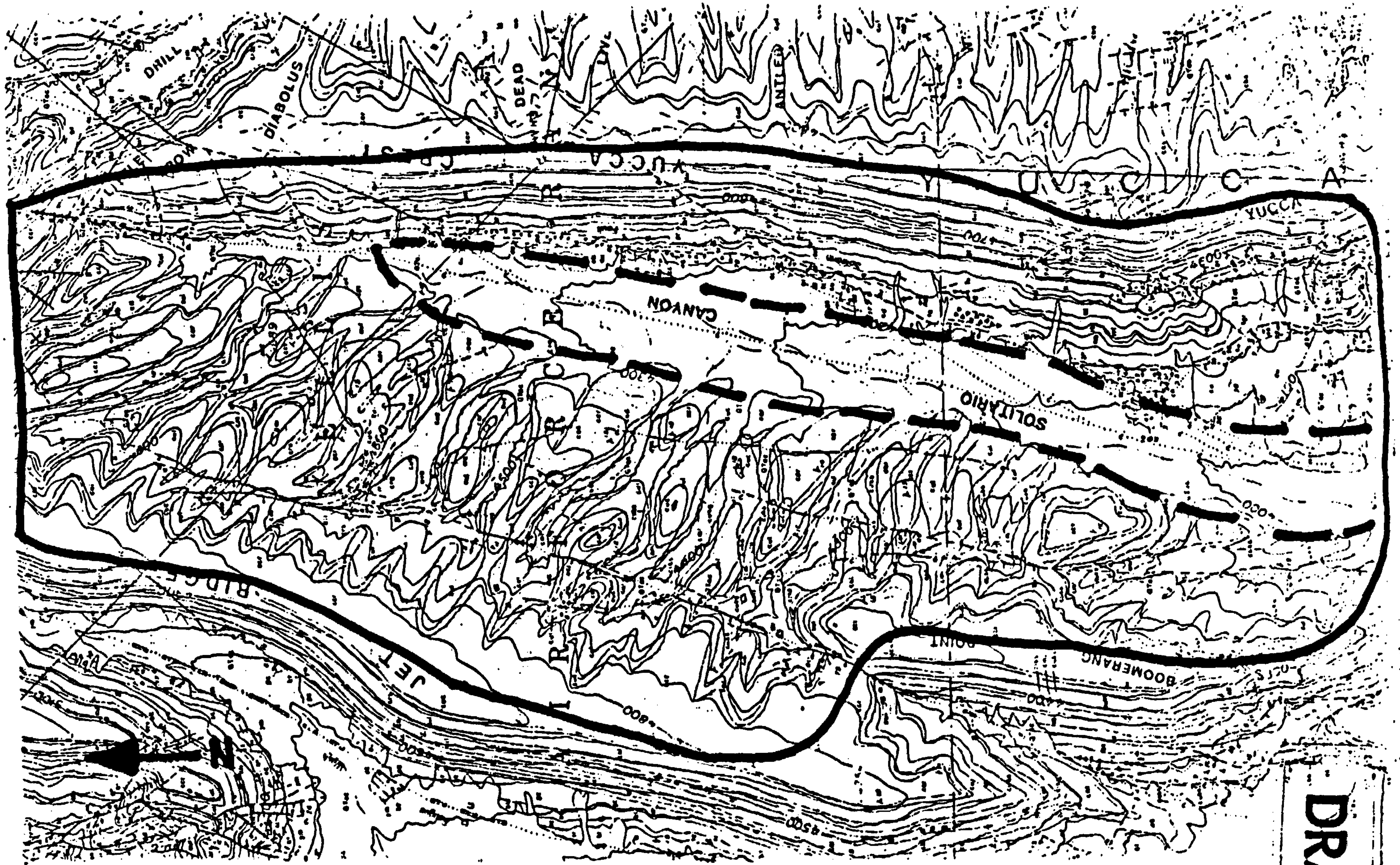

8. Map showing estimated catchment area (solid line), and area modeled as a depression (dashed line).

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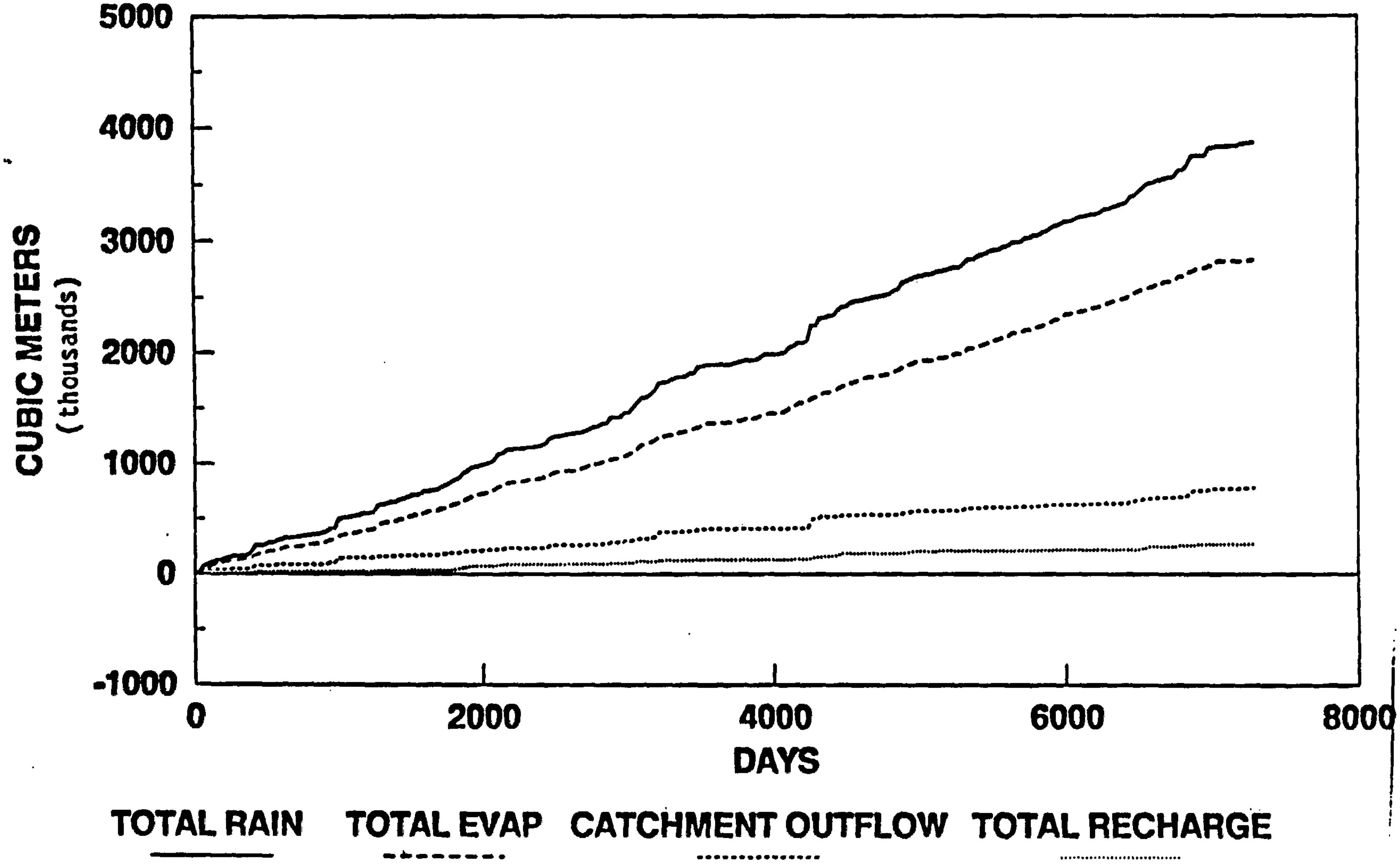
9. # Total Mass Balance
from DFR Model



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conductivity of the "exposed" rock unit in the upper catchment. Figure 10 shows the Run 2 mass balance for the depression alone. The amount of recharge for the runs totaled 12.1 cm/yr for Run 2 and 30.8 cm/yr for Run 1. These high recharge rates reflect the large proportion of runoff from the catchment rock and the high conductivity of the depression alluvium. This recharge is focused in the low alluviated area of the canyon, where fractures and faults are likely to exist.

Recharge rates of 12 to 30 cm/yr are considerably higher than estimates based on one-dimensional modeling and are specified for a particular morphology rather than a hypothetical uniform application. Hockett et al, (1991) have shown infiltration rates of 5 cm could be achieved under pluvial conditions in bare infiltration plots. We think this is a much more realistic approach to estimating recharge on the site because it allows consideration of ground surface material, topography, and climate data.

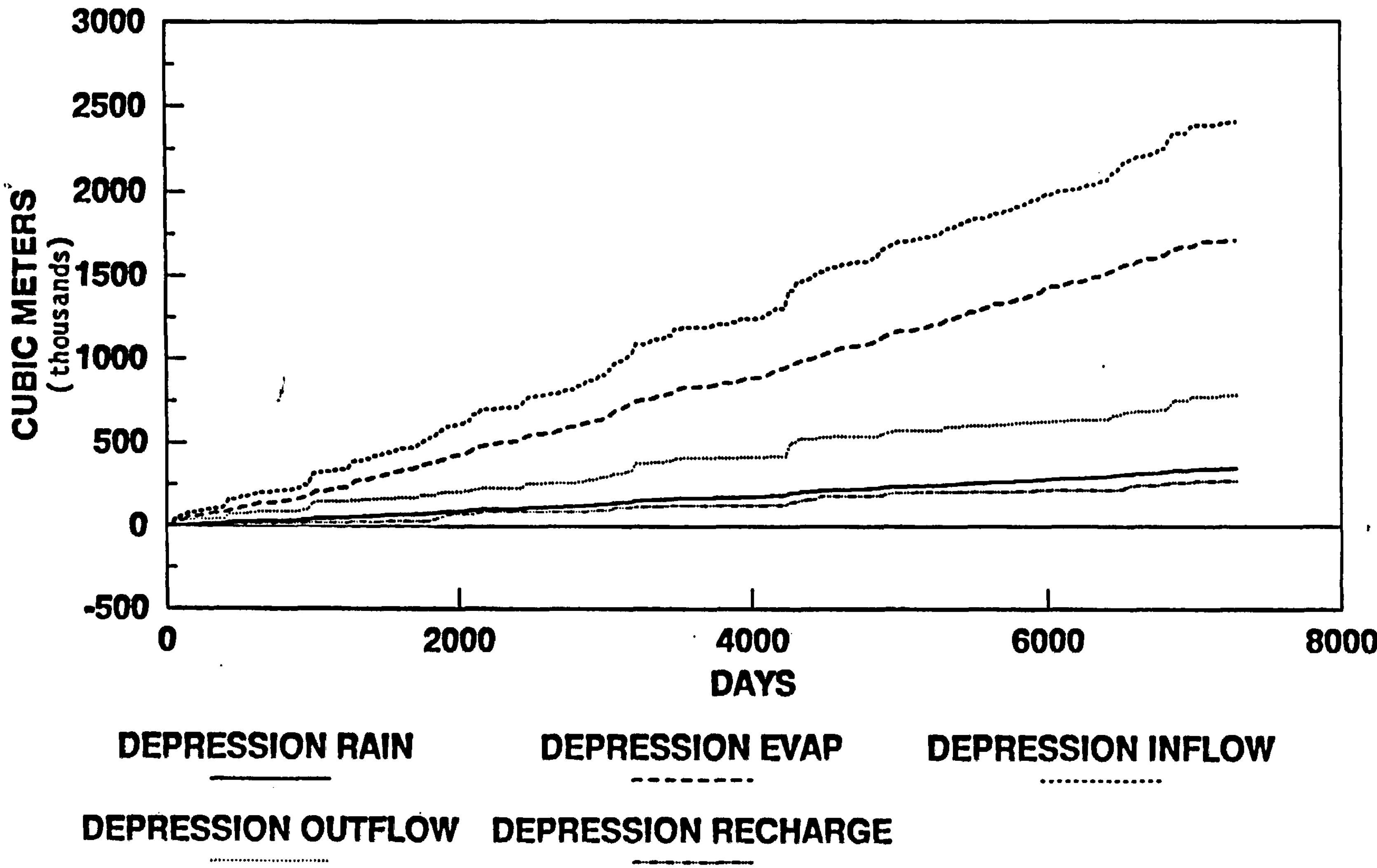
These high rates of recharge have not been previously utilized with our, or any other, one dimensional modeling efforts that have taken place for Yucca Mountain. If these estimates of potential recharge are within an order of magnitude of the actual recharge then there must exist perched saturated zones within the alluvium filled canyons or a mechanism other than one dimensional or two-dimensional matrix flow. Since no perched saturated zones have been found in the alluvium adjacent to Yucca Mountain, it seems more likely that some mechanism of flow, such as fracture flow, is allowing recharge through the alluvium to percolate deeper. We therefore developed a fracture flow model of the site.

Fracture Model

One explanation for recharge rates higher than that allowed by the rock matrix, is that fracture flow plays an important role in the unsaturated zone at Yucca Mountain. To explore this possibility we have constructed a model which incorporates simplified fracture flow along with the composite data matrix properties. Information on fracture properties were estimated from work done by Spengler and Chornack (1984) and Wang and Narasimhan (1985).

The model geometry is shown in Figure 11. A vertical block of the same 7 hydrologic units used in the one dimensional simulation is connected to narrow elements which represent a discrete fracture 0.0002 meters (200 microns) wide. Hydrologic Unit 4 is not connected horizontally to the fracture elements based on the low to non-existent fracture density found in this unit by Spengler and Chornack (1984). Unit 4 does have a vertical connection to the fracture element above and below it. This column represents a simplified symmetric slice of the unsaturated zone where the width of matrix elements are a representative average half distance between fractures. Similarly, the fracture element width is a representative fracture half width or 100 microns. The symmetry used here assumes no flow boundaries along the fracture and matrix block center lines. The matrix element width represents a fracture density of about 3 vertical fractures per

10. # Depression Mass Balance
from DFR Model



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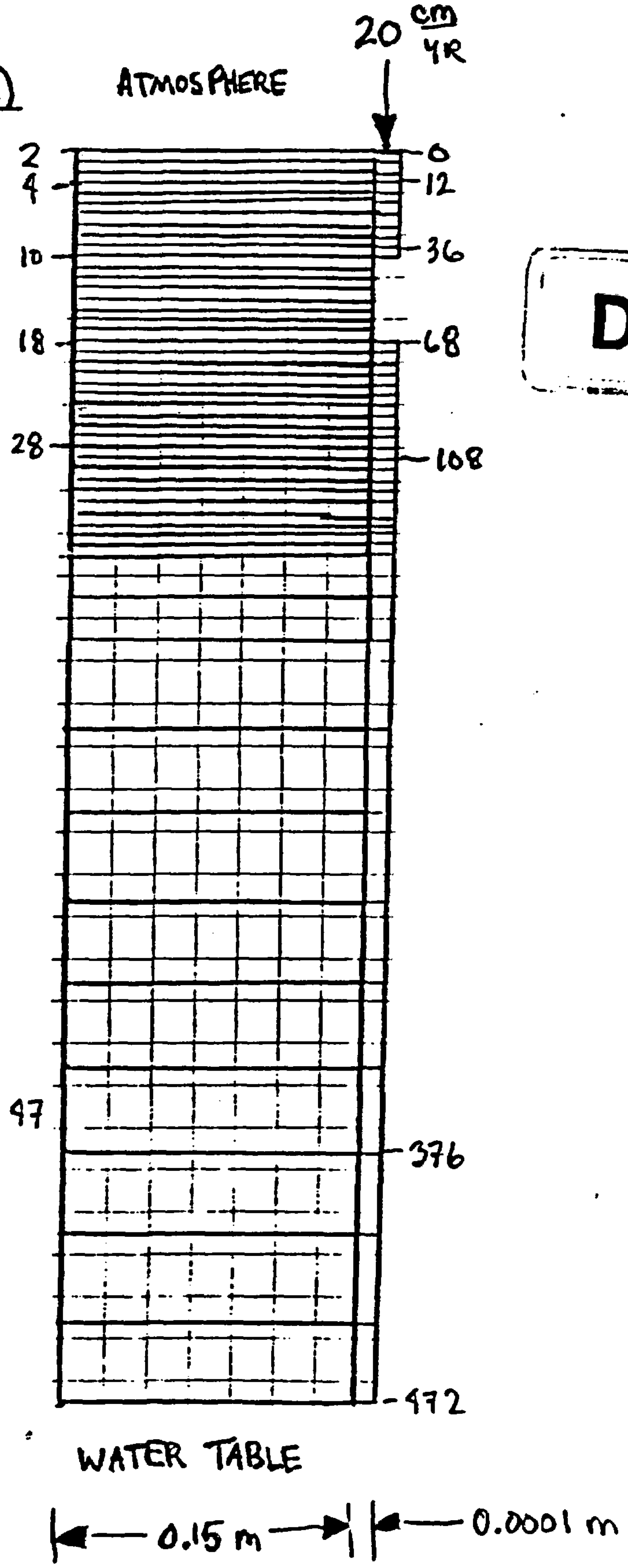
11. FRACTURE/MATRIX MODEL SKETCH

HYDROLOGIC UNIT	ELEM	DEPTH (m)
I	2-4	12
II	5-9	20
III	10	14
IV	11-18	32
V	19-28	40
VI	29-47	268
VII	48-50	96



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linear meter, probably conservative for most of the Yucca Mountain units. Table 3 shows the hydrologic properties of the model units including the fracture elements.

Based on the DFR model results, source water amounting to 20 cm/yr (an average value) over the upper surface of the column (0.1501 m^2) was applied to the top of the first fracture element representing 20 cm/yr of recharge infiltrating exclusively into the fracture at the surface. No recharge was applied to the top of the matrix elements.

Figure 12 shows the results of a VTOUGH simulation of this model configuration. The initial condition is that of 1 mm/yr fracture infiltration nearly at equilibrium with the column. Infiltration of 20 cm/yr was then applied to the fracture continuously for 65 years. The water content profile shows the largest increase in the high conductivity unit which has no fracture penetration. This is due to the difference in water retention curves between Unit 4 and the fracture. As water flows down the fracture it begins raising the saturation level of all the upper units, especially Unit 4. Little water flows into the matrix element below this unit due to its low conductivity and water cannot flow from Unit 4 into the fracture until the pressure in the matrix element reaches the pressure at which water may enter the fracture, about -20,000 Pa or -200 cm of water. This allows water to accumulate in Unit 4 until appreciable flow occurs in the lower fracture. Flow approaching that in the upper fracture and in Unit 4 began in the fracture elements below Unit 4 at about 62 years. Figure 13 compares the characteristic curve of the fracture, based on Wang and Narasimhan (1985), with the curve for Unit 4 fitted to the composite data.

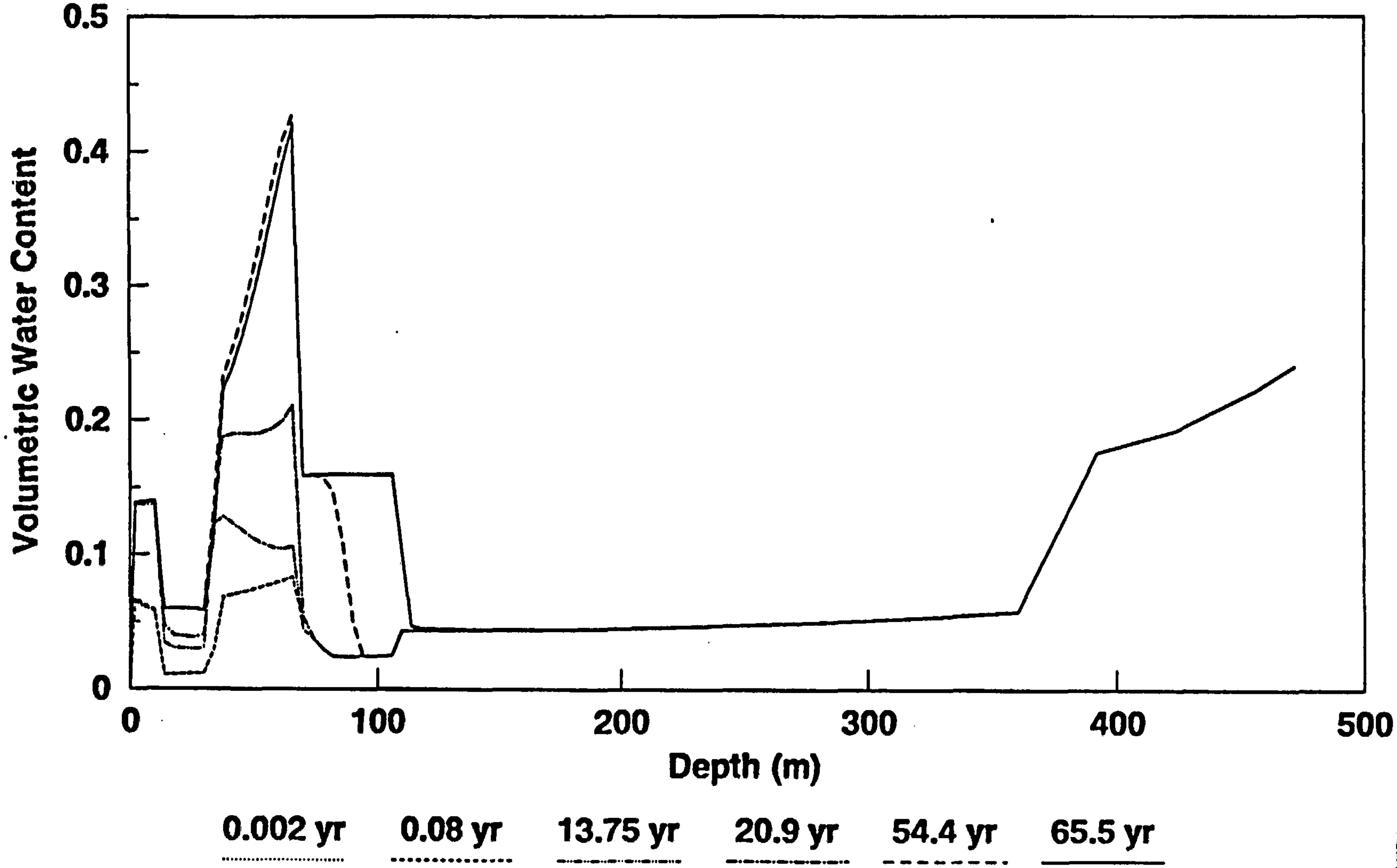
The simulation was then continued using the conditions at 65 years as the initial state, but with 0 infiltration to examine how the profile drys. Figure 14 shows the water content profile history from the initial condition through 65 years of 20 cm/yr infiltration and then through an additional 64 years without infiltration. It is interesting to note that the upper units dry considerably slower than they wet exhibiting a sort of system hysterisis. Figure 15 shows that the fracture element profile responds much more rapidly to the infiltration signal due to its higher conductivity and lower storage volume.

Figure 16 compares the fracture model water content profile to data from four deep holes. Here the very wet conditions in the upper permeable unit as well as the unsaturated conditions in the Topopah are much better represented than either the one dimensional or two-dimensional representations. Figure 17 compares water contents of the fracture model to the actual data from the shallow holes UZN-54 and 55. Here the modeled water content values agree best with the highest of the measured values.

The time periods chosen for water influx were rather arbitrary but may be reasonably consistent with conditions that may exist at the base of an alluvium deposit where large storms may cause high infiltration to be stored and gradually

12. # Modeled water content

for Single Fracture Model



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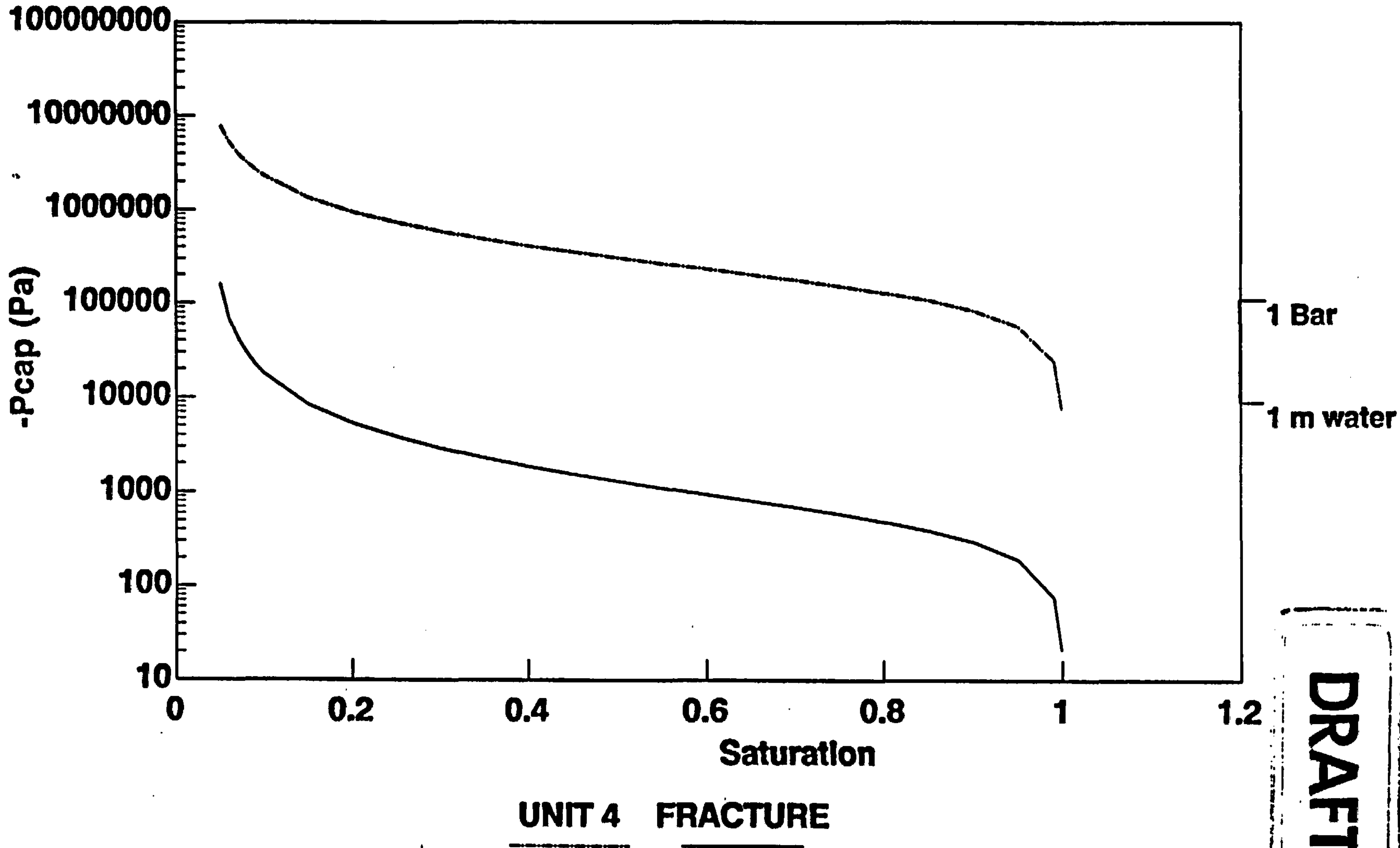
13. UNIT 4 and FRACTURE

Retention Curves



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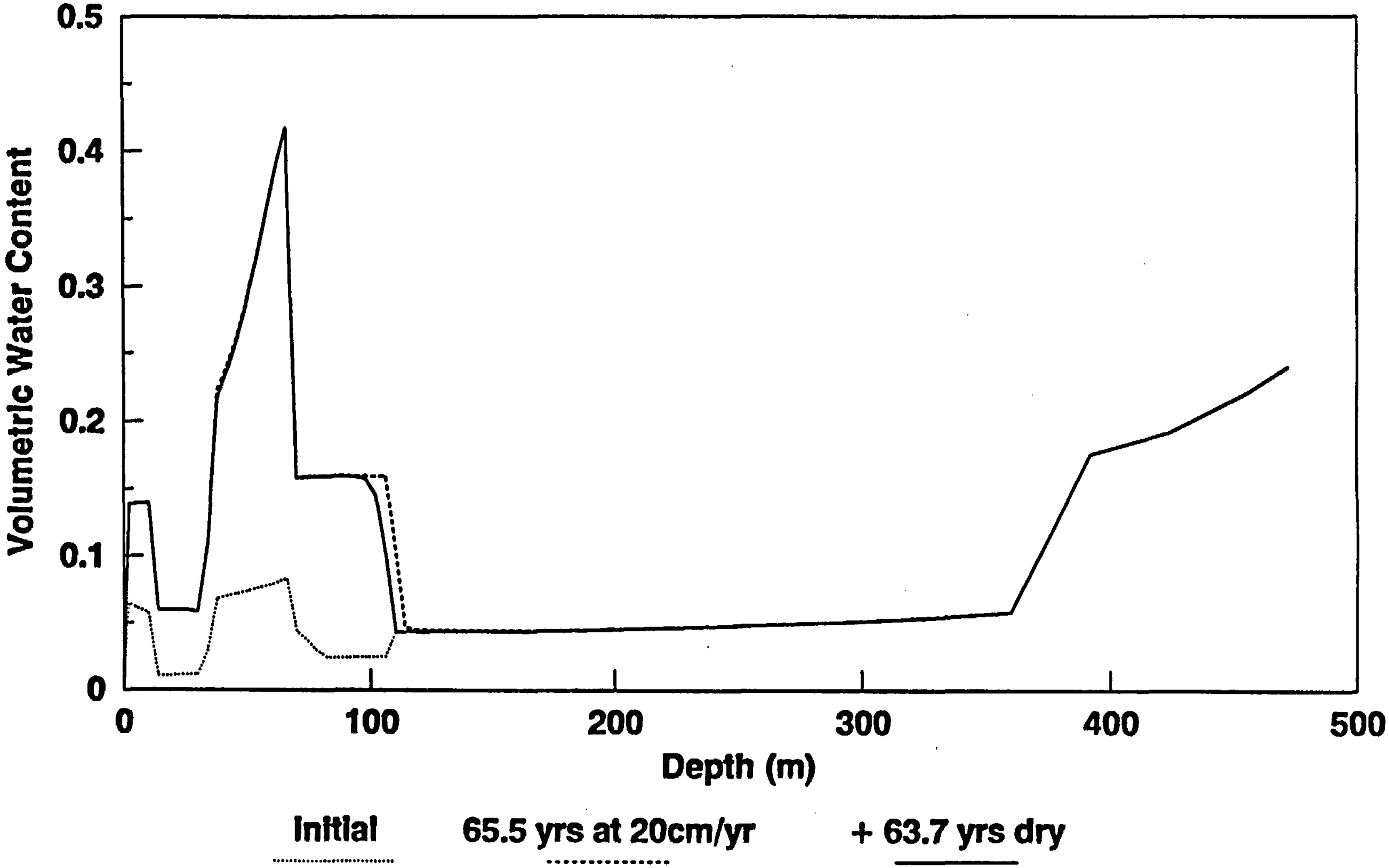
14. **Modeled water content**

for Single Fracture Model



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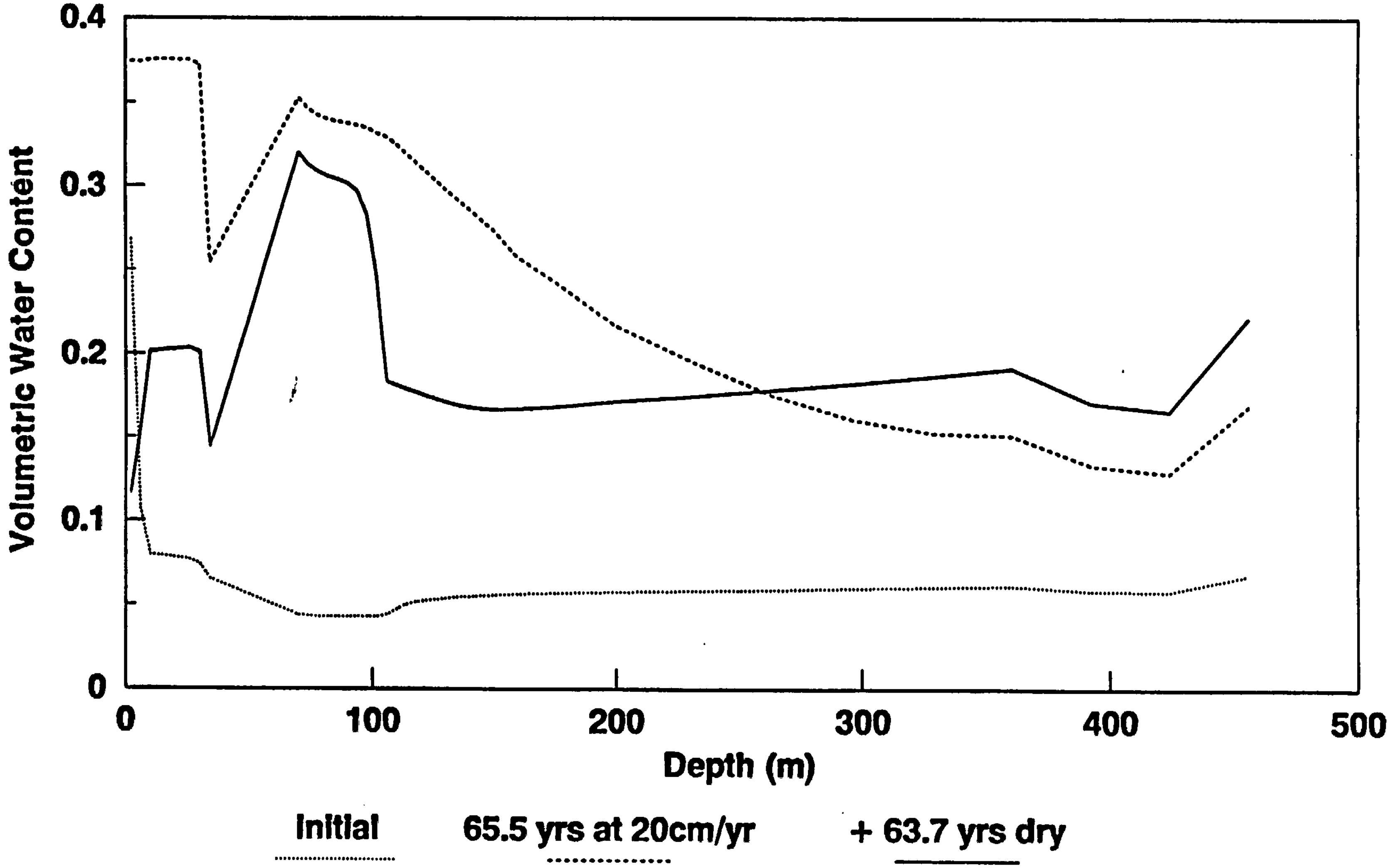
15. Modeled water content

for Fracture Elements



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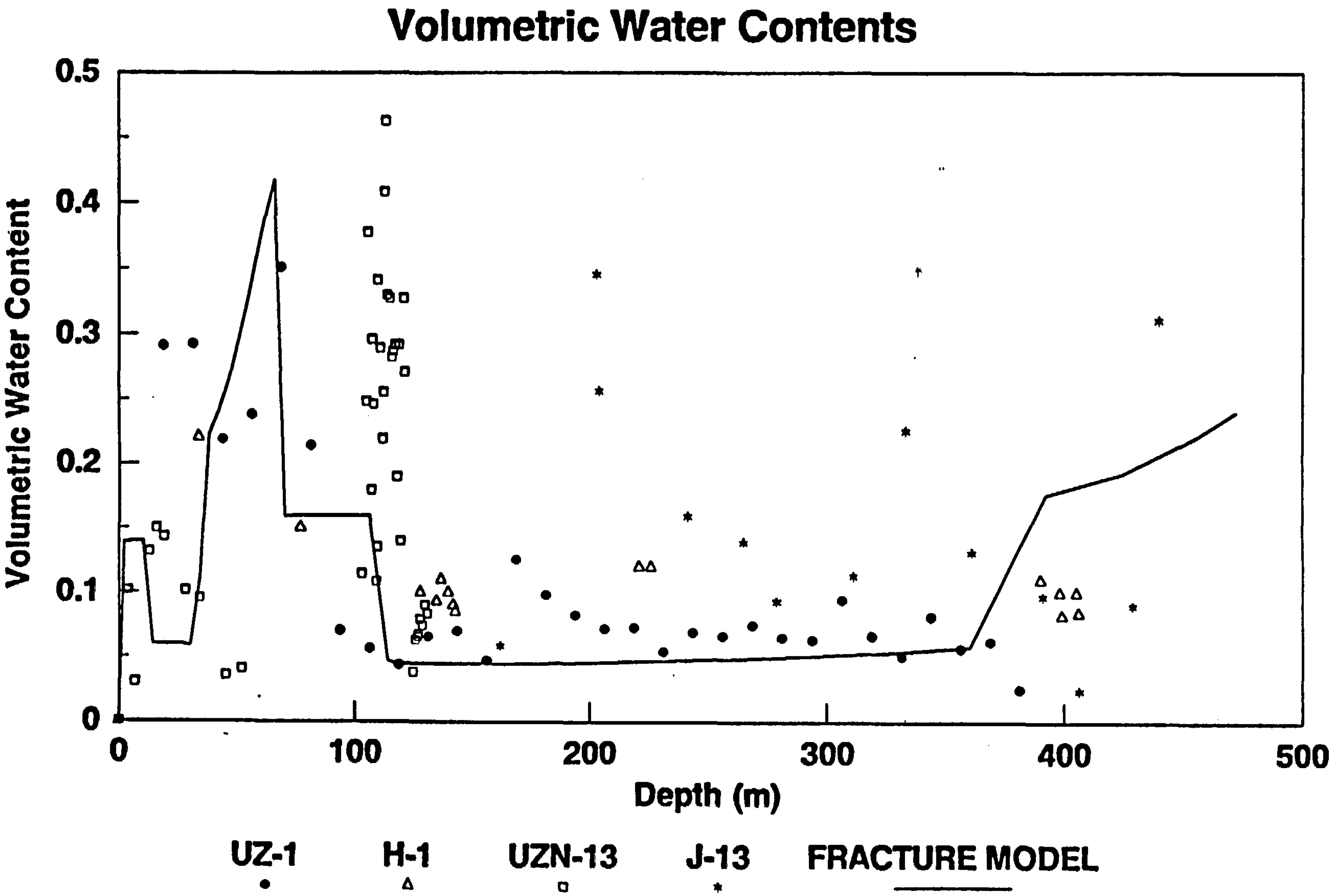
16. **Comparison of Measured and Modeled**



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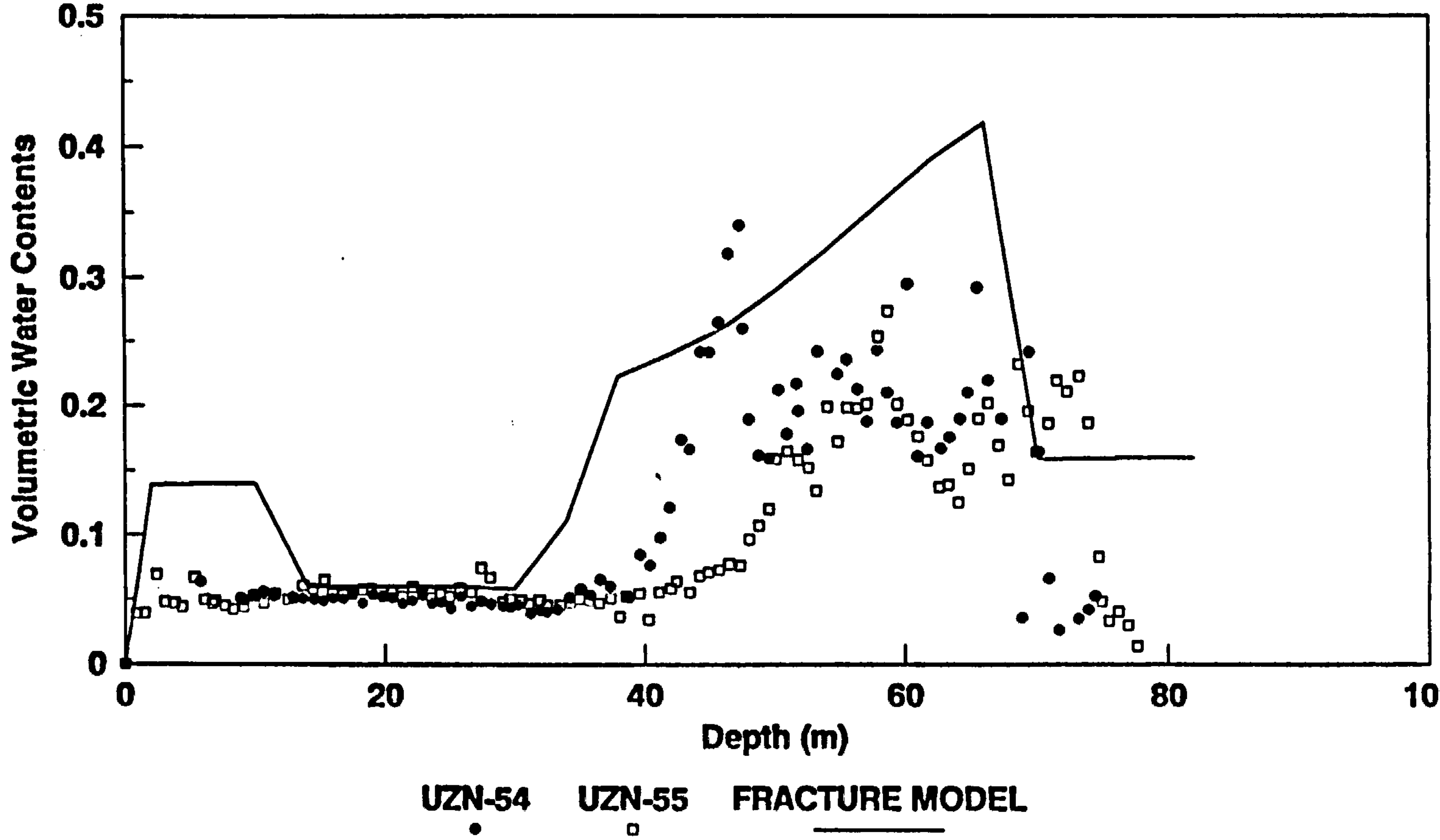
17. **Comparison of Water Content Profiles**

from Hole Data and Model



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released to underlying fractures with long periods of recharge followed by no recharge. It also serves to illustrate a mechanism that could be causing high water contents in the upper units while allowing unsaturated conditions in the low conductivity units, but operates on a somewhat different time scale. Once infiltrating water percolates deep enough to avoid evaporation it accumulates preferentially in the highly permeable, low fracture density unit and leaves there much more slowly than it enters. This phenomenon will not occur under the assumptions of the one dimensional matrix model. Rather, water tends to prefer the tightest units in the 1-D model and very low, unrealistic infiltration rates are required to avoid saturated zones in the column.

It should be noted that the fracture model lends support to Al Yang's interpretation of lateral flow of water through the mountain. Yang, in 1991, developed this hypothesis because of bomb tritium found at a depth of 46 meters, but not above that depth. This model description would allow Tritium to be present in the unit in a reasonable timeframe, i.e. within 50 years.

Conclusions

This work indicates that a conceptual model which includes fractures, higher recharge rates, and focused recharge may be required to provide an accurate picture of mechanisms operating in the unsaturated zone at Yucca Mountain.

One dimensional representations have done a poor job reproducing the state variables measured at Yucca Mountain. They also require minuscule infiltration rates which are inconsistent with our estimate of potential depression infiltration at the site and recent field work done on plots near Yucca Mountain by Hokett et al (1992) which found nearly 5 cm/yr recharge through bare alluvial plots under simulated "pluvial" conditions, but without including runon from the slope above.

The one dimensional models of this site are not consistent with the large amount of structural data available which show high fracture densities in some units along with several major faults through and adjacent to the mountain. These prevalent features likely play an important role in unsaturated flow and should be part of any site-wide model.

In performing this work it was realized that this validation problem is not well posed and that validating a model based on the data supplied would not be possible. Many important features of the problem are not well constrained, if at all. Information is unavailable regarding initial conditions of the state variables along the stratigraphic column. The boundary conditions, for example recharge amount and distribution as well as conditions along fault zones are, at best, poorly understood. This means that many solutions may exist using different combinations of initial and boundary conditions and validation of any particular model is impossible under these conditions.

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Data from deep holes UZ-1, H-1, UZ-13, and J-13 show significant variation in water content profiles across the site. This variation could be caused by wet vs dry drilling techniques or by structural or recharge variations. For instance, the J-13 water content profile may be so much higher because it is located within the 40 mile wash, widely suspected as a major recharge zone. Validation of a model based on a single borehole, UZ-16, is probably insufficient to qualify the model to represent the entire site.

For the above reasons, the measure of model accuracy being used for the INTRAVAL Unsaturated Zone problem, i.e. water content, by itself is inadequate to validate a model. Basing validation on a single state variable, water content, does little to help the non-uniqueness of solutions based on this problem formulation. An additional validation measure which relates to the time history of water flow should also be a part of any model validation effort for the Yucca Mountain site. This could include chemistry data such as tritium or carbon-14 measurements which would help constrain the time frame for infiltration and flow.

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Additional Figures

Fracture Measurements from Spengler and Chornack

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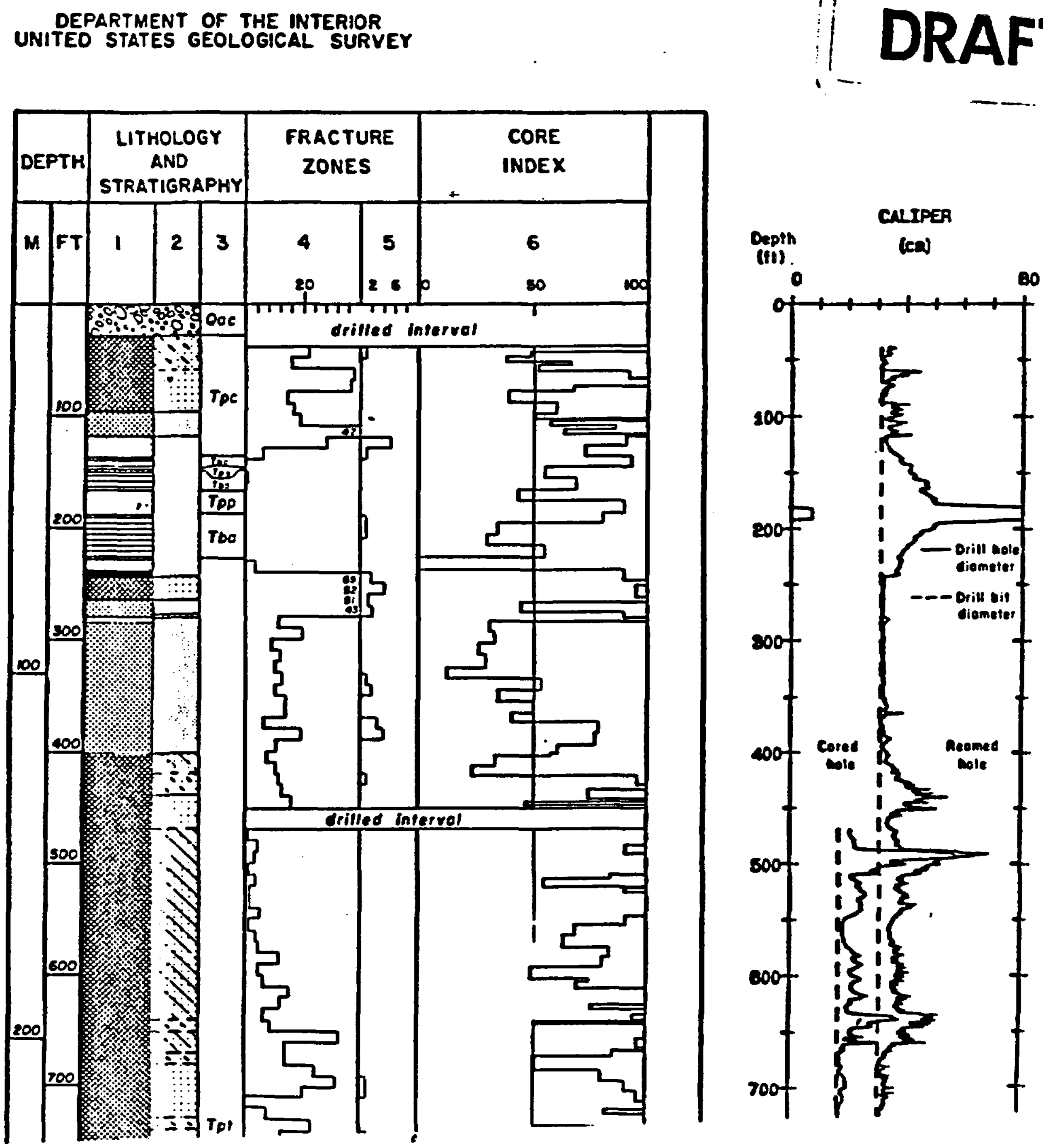

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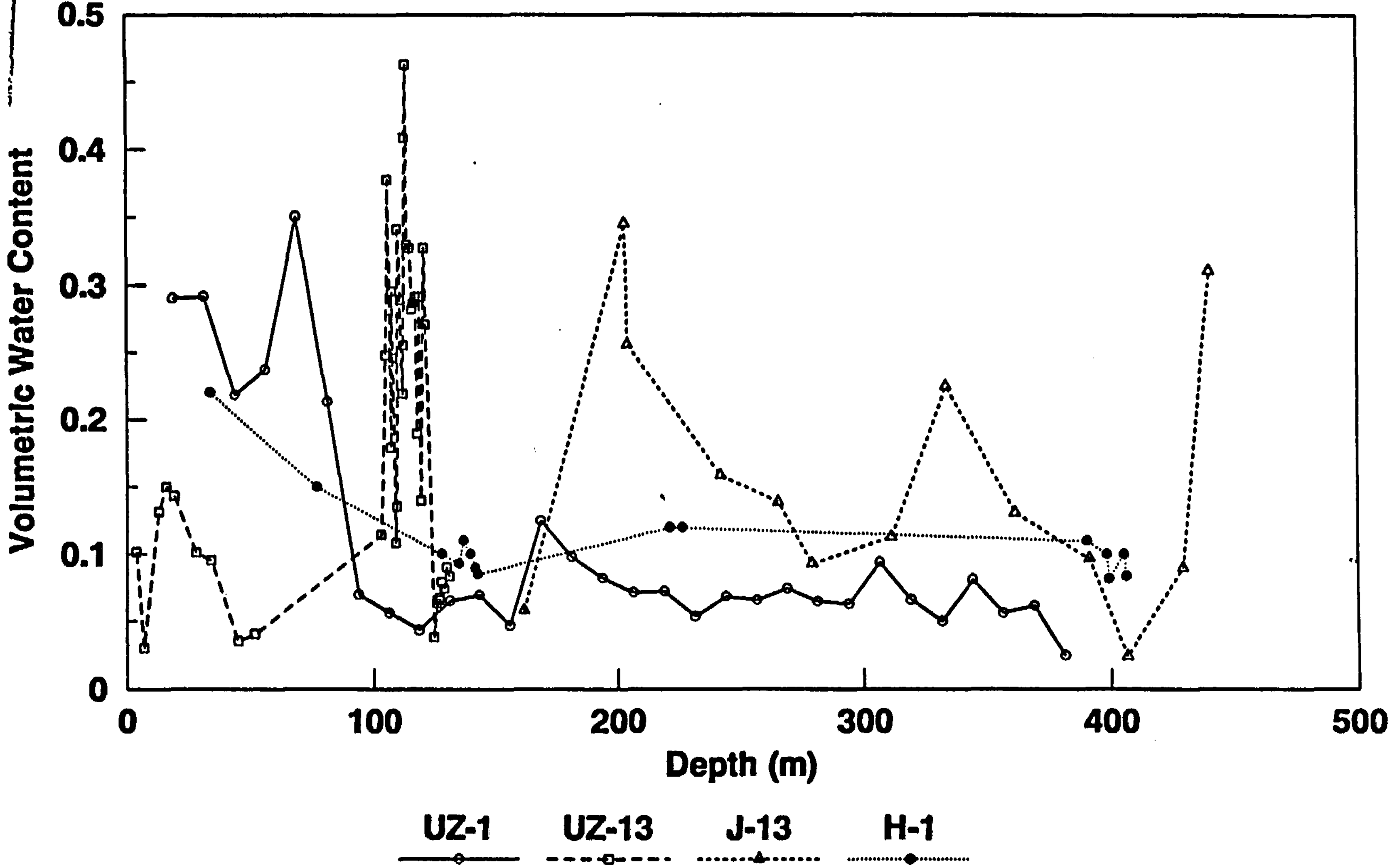
Comparison of Measured Deep Hole

Volumetric Water Contents



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Modeled Porosity
for Seven Hydrologic Unit Model

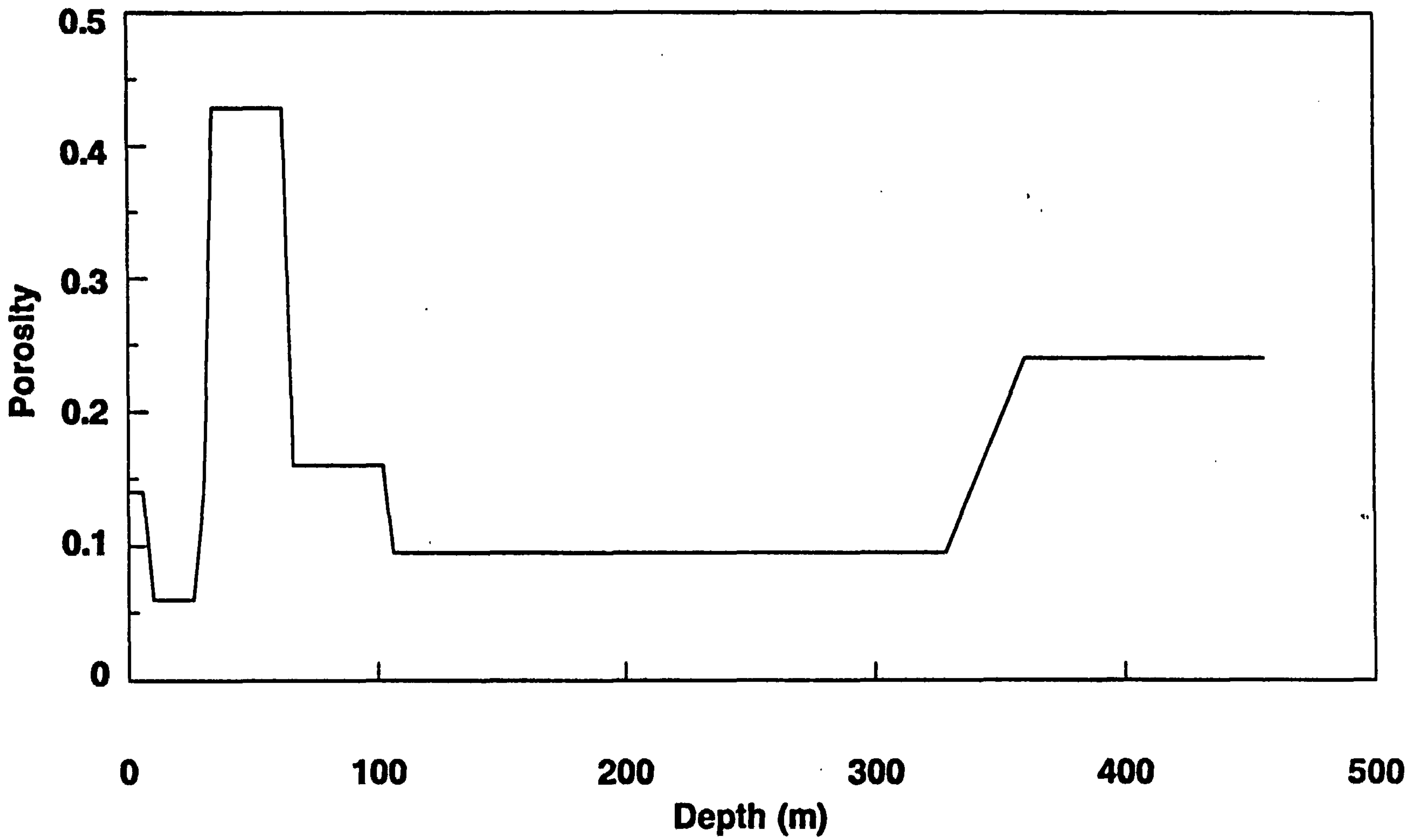

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Table 1. Hydrologic Properties and Model Geometry for Run Set C (1-D Model).

Geologic Unit	Model Unit	Element #	Thickness (m)	Mean Porosity	Geometric Mean Ksat (cm/s)	StDev Ksat (cm/s)
Tiva Canyon	I	2-4	12	0.140	2.72E-8	2.68E-9
Tiva Canyon	II	5-9	20	0.060	1.35E-9	3.45E-7
Tiva Canyon	III	10	4	0.140	7.79E-8	2.05E-7
Shardy Base, Non-welded Bedded Tuff	IV	11-18	32	0.430	2.68E-4	1.44E-3
Upper Topopah	V	19-28	40	0.160	3.91E-7	1.57E-5
Lower Topopah	VI	29-98	280	0.100	5.14E-10	8.02E-9
Calico Hills	VII	99-121	92	0.240	4.78E-9	7.03E-9

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Table 1a. Sandia Function Parameters for VTOUGH Water Retention Curves for Run Set C.

Unit	Lambda	S_{lr}	S_{ls}	$1/P_0$	P_{max}
I	0.33	0.04	1.0	7.41E-6	1.0E+9
II	0.60	0.349	1.0	3.77E-6	1.0E+9
III	0.49	0.01	1.0	4.25E-6	1.0E+9
IV	0.50	0.029	1.0	5.88E-6	1.0E+9
V	0.38	0.04	1.0	9.09E-6	1.0E+9
VI	0.24	0.04	1.0	4.54E-6	1.0E+9
VII	0.20	0.04	1.0	4.17E-6	1.0E+9

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Table 2. Depression Focus Recharge Model Parameters and Result.

Properties	Run 1	Run 2
Catchment Area (m^3)	6,157,500	6,157,500
Depression Area (m^3)	1,131,000	1,131,000
Land Slope (deg)	5.7	5.7
Albedo	0.3	0.3
Outlet Height (m)	0.1	0.1
Catchment Ksat (m/s)	1.995E-10	1.089E-8
Catchment Porosity	0.15	0.15
Catchment Soil Storage Parameter (m)	0.099	0.099
Catchment Upper Limit of Stage I Evaporation ($mm/day^{1/2}$)	5.2	5.2
Depression Ksat (m/s)	4.0E-6	1.5E-6
Depression Porosity	0.51	0.51
Depression Soil Storage Parameter (m)	0.099	0.099
Depression Upper Limit of Stage I Evaporation ($mm/day^{1/2}$)	5.2	5.2
Microdepression Storage (m)	0.0	0.001
Depression Recharge (m/yr)	0.308	0.121

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Table 3. Hydrologic Properties and Model Geometry for Fracture Model.

Unit	Element #	Thickness (m)	Mean Porosity	Geometric Mean Ksat (cm/s)	StDev Ksat (cm/s)
I	2-4	12	0.140	2.72E-8	2.68E-9
II	5-9	20	0.060	1.35E-9	3.45E-7
III	10	4	0.140	7.79E-8	2.05E-7
IV	11-18	32	0.430	2.68E-4	1.44E-3
V	19-28	40	0.160	3.91E-7	1.57E-5
VI	29-47	268	0.100	5.14E-10	8.02E-9
VII	48-50	96	0.240	4.78E-9	7.03E-9
FRAC	102-150	472	0.990	8.17E-1	----

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Table 3a. Sandia Function Parameters for VTOUGH Water Retention Curves for Fracture Model.

Unit	Lambda	S_{lr}	S_{ls}	$1/P_0$ (1/Pa)	P_{max} (Pa)
I	0.33	0.04	1.0	7.41E-6	1.0E+9
II	0.60	0.349	1.0	3.77E-6	1.0E+9
III	0.49	0.01	1.0	4.25E-6	1.0E+9
IV	0.50	0.029	1.0	5.88E-6	1.0E+9
V	0.38	0.04	1.0	9.09E-6	1.0E+9
VI	0.24	0.04	1.0	4.54E-6	1.0E+9
VII	0.20	0.04	1.0	4.17E-6	1.0E+9
FRAC	0.45	0.04	1.0	0.001667	1.0E+9