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Validation of the TRACR3D Code for Soil Water Flow Under Saturated/Unsaturated Conditions in Three Experiments

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by

B. Perkins, B. Travis, and G. DePoorter

ABSTRACT

Validation of the TRACR3D code in a one-dimensional form was obtained for flow of soil water in three experiments. In the first experiment, a pulse of water entered a crushed-tuff soil and initially moved under conditions of saturated flow, quickly followed by unsaturated flow. In the second experiment, steady-state unsaturated flow took place. In the final experiment, two slugs of water entered crushed tuff under field conditions. In all three experiments, experimentally measured data for volumetric water content agreed, within experimental errors, with the volumetric water content predicted by the code simulations.

The experiments and simulations indicated the need for accurate knowledge of boundary and initial conditions, amount and duration of moisture input, and relevant material properties as input into the computer code.

During the validation experiments, limitations on monitoring of water movement in waste burial sites were also noted.

I. INTRODUCTION

One of the mechanisms for mobilization and transport from landfills is for soil water to leach soluble elements from the waste and the leachate to move either as mass flow with the soil water or through the soil water by diffusion.

To predict how well a disposal site may be able to contain toxic materials, simulations of the movement of these waste components are necessary. The TRACR3D computer code (Travis 1984) has been developed at Los Alamos to simulate transport of solutes through unsaturated as well as saturated soils and rock. The model computes water and/or air flow under soil moisture conditions ranging from fully saturated to completely dry. Material properties can vary spatially. A variety of boundary and source/sink conditions are possible. The model also simulates transport of sorbable species. Transport mechanisms include advection, diffusion, and dispersion. Sorption can be either equilibrium or kinetic and saturable or not. Decay chains and leaching sources are allowed. The TRACR3D model has been used to study migration of species from underground nuclear explosions, high-level radioactive underground waste storage, and low-level radioactive shallow waste burial.

Any mathematical model, to be useful, must be verified and validated. Verification means comparison with analytic solutions. A number of verification examples for TRACR3D are given in Travis (1984). Validation means comparison of the model with experimental data. A few validation examples for TRACR3D are discussed by Travis (1984).

Laboratory experiments are usually well controlled but do not allow all length and time scales to be tested. Field experiments allow a wider range of length and time scales but are frequently subject to uncertainty regarding the spatial distribution of material properties. The Los Alamos caisson experiments allow testing of larger length and time scales than laboratory experiments allow but without the uncertainties of large-scale field experiments.

The purpose of this report is to describe additional validation of the TRACR3D code. The code calculations are compared with measurements made in both caisson and field experiments for infiltration of water into partially saturated soils of crushed Bandelier tuff. These measurements provide only flow validation and are part of a series of experiments which will provide data for validation of both flow and transport in partially saturated, unconsolidated media.

II. VALIDATION

A. Caisson A Water Pulse

The purpose of the first experiment was to measure in a caisson the changes in volumetric water content under conditions of saturated/unsaturated flow and to compare the experimental results with the results predicted using the TRACR3D code.

1. Experimental

a. Emplacement. The experiment was run in a 304.8-cm-diameter, 609.6-cm-deep caisson (designated A), which is one of a set of six that surround a central access caisson (Fig. 1). Except for the top 25 cm, the complete assemblage is below grade. Each experimental caisson is equipped with a bottom drain that extends into the central caisson to allow for measurement of the drainage rate (Fig. 2).

Before the caisson used in this experiment was filled, the bottom drain was covered with a coarse screen. Approximately 25 cm of gravel was placed over the screen and approximately 25 cm of sand was placed over the gravel. The remainder of the caisson was filled to approximately 10 cm of the top rim with crushed, compacted tuff (Fig. 2).

The naturally occurring tuff at Los Alamos was excavated using front-end loaders, crushed by running the loaders over the tuff, and then screened by passing through a 12.7-mm screen. For maximum packing density before filling, the screened tuff was mixed in a cement truck with enough water to produce a uniform moisture of between 10 and 13% by volume in the compacted tuff. The damp tuff was then placed in layers in the caisson, and each layer was compacted with "jumping jacks" to give a layer of from 15 to 20 cm thick. Density measurements indicated that maximum density for packed tuff was achieved (DePoorter et al. 1982).

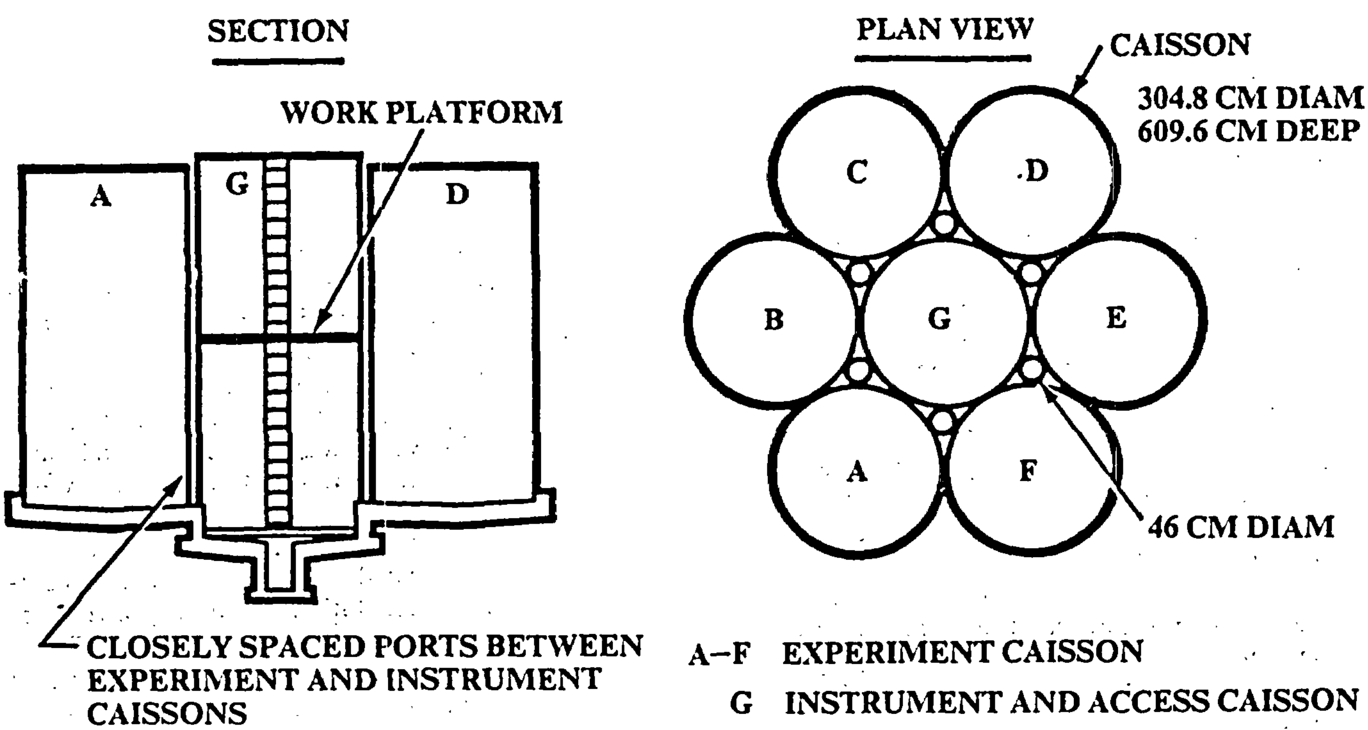

Fig. 1. Experiment Cluster.

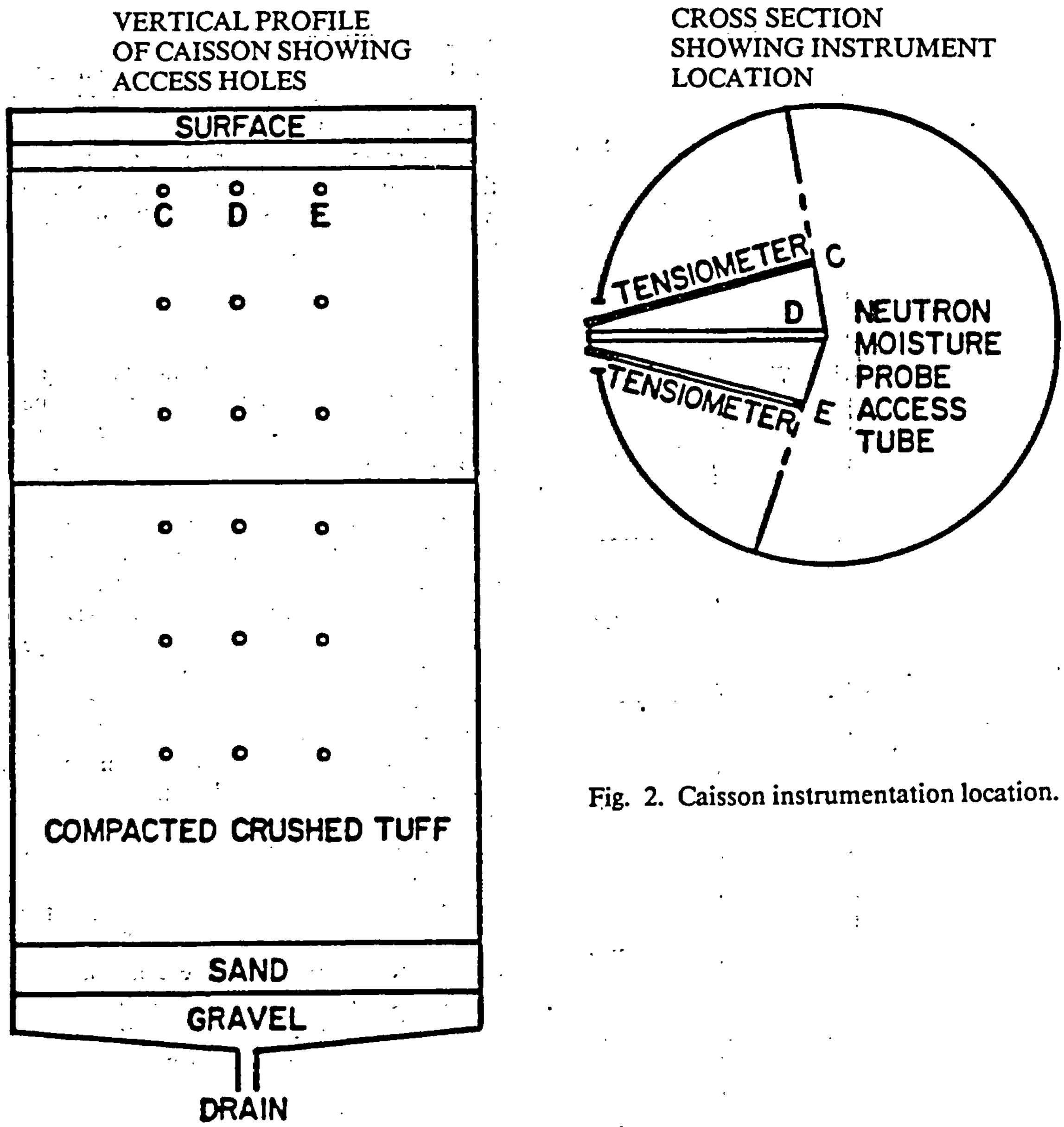

Fig. 2. Caisson instrumentation location.

After the caissons were filled, holes were made at the levels shown in Fig. 3 at the position marked D in Fig. 2 by driving a 5.08-cm-o.d. hollow stainless steel tube horizontally. Then a 5.08-cm-o.d., 0.026-cm wall-thickness aluminum tube, ~175 cm long, with an aluminum, welded end cap, was inserted to the end of the hole. These access tubes were used for inserting a neutron moisture probe. (Because of problems in driving the steel tube, the horizon marked A2 in Fig. 3 was driven only about 0.7 m; therefore, the end of the access tube is at this position.)

Tensiometers were inserted through augered holes at the same level as the neutron moisture access tubes. The location of the two tensiometers on each side of each access tube is shown in Fig. 2, at locations C and E, with a distance of 44 cm between the end of a tensiometer and the end of the access tube.

b. Material Properties of the Fill. After the tensiometers were emplaced, water was continually ponded on the surface to a depth of approximately 4 cm. Soil water content was measured by inserting the probe of a neutron moisture gauge into the end of each access tube at the seven different horizons noted as A8-A2 in Fig. 3. Ponding continued until the moisture measurements as a function of depth indicated that the caisson was as near saturation as possible, with a maximum volumetric water content of 34.6%. The caisson was then allowed to drain.

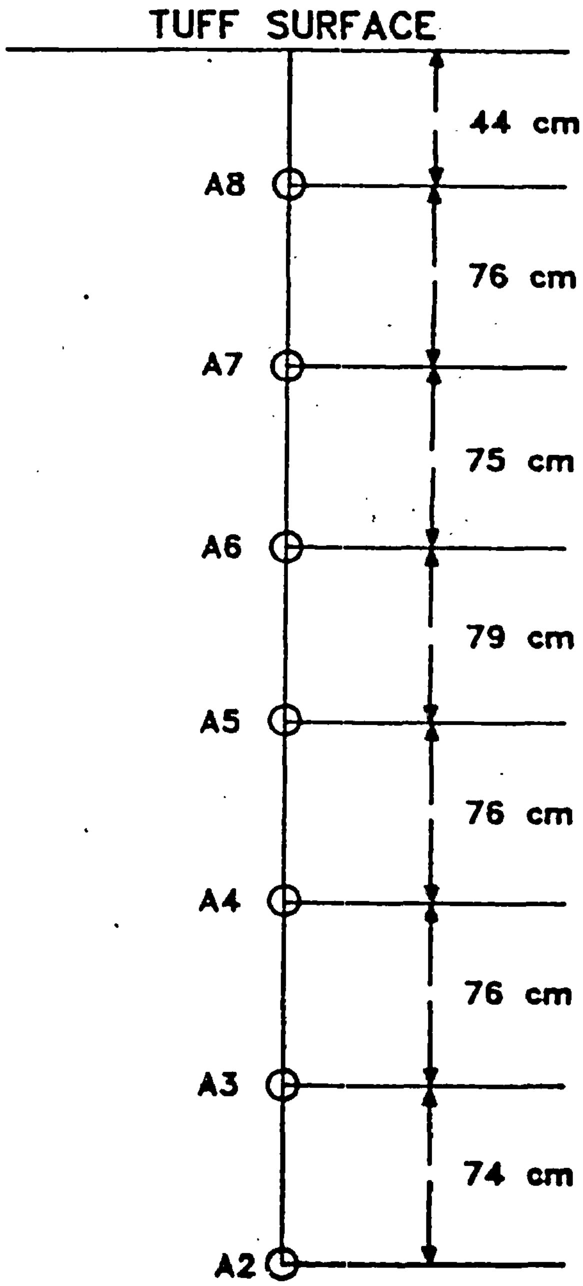

Fig. 3. Vertical position of neutron probe access tubes.

The matric potential of the compacted, crushed tuff and related material properties were obtained from experimental measurements made during this period of saturating with water and draining. For further details the reader is referred to Abeele (1984).

c. Addition of Water. To ensure that water uniformly penetrated the surface of the tuff in Caisson A, the surface was raked flat at 09:00 on September 22, 1982. Volumetric water content as a function of depth was measured to obtain initial conditions. At 10:30, water was added until the depth of water was approximately 4 in.

By 15:15 the water had completely soaked into the tuff, and volumetric water content as a function of depth was again measured. The top of the caisson was tightly sealed against further infiltration or evaporation.

d. Measurements. The rate of water outflow from the caisson, volumetric soil moisture, and tension as a function of depth were measured frequently for a period of 6 weeks (Table I). Figure 4 shows graphically the soil water content changes with time.

e. Results. The experimental volumetric soil water content data indicate that approximately 13 cm of water infiltrated. The volumetric water content decreased in amplitude rather quickly as it moved downward, and below 400 cm no change in water content could be detected experimentally.

The data indicate that although movement of soil water could not be detected below ~400 cm at any time during the experiment, drainage from the caisson required that soil water was moving below this horizon with flux in equal to flux out in those regions in which no change in soil water content was detected.

The (Table 1) data also indicate that the introduction of water at the surface was felt very quickly at the bottom of the caisson, with drainage increasing to day 12-13, after which the drainage rate remained approximately constant through day 22, when the experiment was terminated.

2. Code Simulation

a. Input Conditions. The basic equations used for the TRACR3D simulations run for the three experiments are given in Travis (1984). In these simulations the code was used in a one-dimensional geometry. For the computer TRACR3D simulations, initial and boundary conditions must be specified, as well as material properties.

In running the simulation for the pulse experiment, the initial moisture profile in the tuff fill was determined from the experimental data collected just before addition of the slug. Since the caisson had been saturated during the earlier experiments, the degree of saturation in the sand was assumed as 0.99 and in the gravel 0.05 (Table II). Free-flow (0-pressure) conditions were specified at the bottom of the column, and no flow was allowed through the sides.

TABLE I

CHANGE IN SOIL MOISTURE FOR THE ADDITION OF A 13-CM WATER PULSE

Hole A-8 (44 cm depth)

Date	Time	Volumetric Moisture (%)	Tensiometer Reading (kPa)
9/21	13:45	17.7	24.0
9/22	09:00	17.9	21.5
	15:15	29.1	7.5
9/23	09:30	26.3	9.0
9/24	09:45	24.2	10.0
9/27	09:10	22.5	14.0
9/28	08:30	21.5	13.0
9/29	08:50	21.5	14.0
9/30	09:30	21.2	14.0
10/1	10:00	21.3	15.0
10/4	10:30	20.6	16.5
10/5	09:45	19.8	17.0
10/6	10:00	20.0	17.0
10/8	09:20	19.6	18.0
10/14	11:00	19.1	21.0
10/27	04:00	17.9	24.0
11/1	NA	17.5	26.0

Hole A-7 (120 cm depth)

Date	Time	Volumetric Moisture (%)	Tensiometer[a] Reading (kPa)
9/21	13:45	18.1	24.5
			24.5
9/22	09:00	18.6	19.5
			21.0
9/22	15:15	18.6	21.0
			21.5
9/23	09:30	26.4	7.0
			7.0
9/24	09:45	25.8	7.0
			7.0
9/27	09:10	24.1	9.0
			9.5
9/28	08:30	23.5	9.5
			9.0
9/29	08:50	23.1	12.0
			10.0
9/30	09:30	22.9	11.5
			10.0
10/1	10:00	23.0	11.0
			10.5
10/4	10:30	21.5	13.0
			12.0
10/5	09:45	21.0	13.0
			12.0
10/6	10:00	20.7	13.5
			12.0
10/8	09:20	20.2	14.0
			13.5
10/14	11:00	19.7	16.0
			14.0
10/27	04:00	19.5	20.0
			18.0
11/1	NA	19.2	21.0
			19.0

TABLE I (cont)

Date	Time	Volumetric Moisture (%)	Tensiometer[a] Reading (kPa)	Date	Time	Volumetric Moisture (%)	Tensiometer[a] Reading (kPa)
	Hole A-6 (195 cm depth)				Hole A-5 (274 cm depth)		
9/21	13:45	18.1	25.0	9/21	13:45	19.1	20.0
			24.5				19.5
9/22	09:00	18.2	23.5	9/22	09:00	19.4	24.0
			23.0				23.5
9/22	15:15	18.0	23.5	9/22	15:15	19.4	24.5
			23.0				24.0
9/23	09:30	18.2	21.0	9/23	09:30	19.2	24.0
			20.0				23.5
9/24	09:45	19.8	13.5	9/24	09:45	19.4	22.0
			13.5				21.5
9/27	09:10	22.2	9.5	9/27	09:10	20.7	15.0
			9.0				15.0
9/28	08:30	21.9	9.0	9/28	08:30	20.8	12.5
			8.0				13.0
9/29	08:50	21.9	9.0	9/29	08:50	21.1	11.5
			8.5				12.0
9/30	09:30	21.8	10.0	9/30	09:30	21.6	11.5
			9.5				12.0
10/1	10:00	21.4	9.5	10/1	10:00	22.7	10.5
			9.5				10.5
10/4	10:30	21.6	10.5	10/4	10:30	22.1	10.5
			9.5				10.5
10/5	09:45	21.1	11.0	10/5	09:45	21.9	11.0
			10.0				10.0
10/6	10:00	20.9	11.0	10/6	10:00	21.8	11.0
			10.0				10.0
10/8	09:20	20.8	12.0	10/8	09:20	21.6	12.0
			11.5				11.0
10/14	11:00	20.3	13.0	10/14	11:00	21.4	12.0
			12.0				12.0
10/27	04:00	19.6	16.0	10/27	04:00	20.3	17.0
			16.0				16.0
11/1	NA	19.2	17.5	11/1	NA	20.3	18.0
			16.0				17.0

TABLE I (cont)

Date	Time	Volumetric Moisture (%)	Tensiometer[a] Reading (kPa)
		Hole A-4 (350 cm depth)	
9/21	13:45	21.1	20.0
			19.5
9/22	09:00	20.8	19.5
			19.5
9/22	15:15	20.4	20.0
			20.0
9/23	09:30	20.9	20.0
			19.0
9/24	09:45	21.0	20.0
			18.0
9/27	09:10	21.1	17.0
			16.0
9/28	08:30	20.7	16.0
			14.0
9/29	08:50	NA	14.5
			13.0
9/30	09:30	21.1	14.0
			13.5
10/1	10:00	20.7	12.5
			11.5
10/4	10:30	22.0	10.5
			10.0
10/5	09:45	21.6	11.0
			10.0
10/6	10:00	21.7	10.5
			10.0
10/8	09:20	21.7	10.0
			11.0
10/14	11:00	21.6	11.0
			10.0
10/27	04:00	21.8	15.0
			13.0
11/1	NA	21.3	15.0
			13.0

Date	Time	Volumetric Moisture (%)	Tensiometer[a] Reading (kPa)
		Hole A-3 (426 cm depth)	
9/21	13:45	22.1	15.5
			14.0
9/22	09:00	22.2	15.5
			14.0
9/22	15:15	21.9	15.0
			13.5
9/23	09:30	22.1	14.5
			13.5
9/24	09:45	22.0	15.0
			13.5
9/27	09:10	22.1	14.5
			13.5
9/28	08:30	22.0	14.0
			13.0
9/29	08:50	22.7	13.5
			12.0
9/30	09:30	22.4	13.5
			12.5
10/1	10:00	22.8	13.0
			12.5
10/4	10:30	22.8	12.0
			11.0
10/5	09:45	22.7	12.0
			10.5
10/6	10:00	22.5	10.5
			10.0
10/8	09:20	22.4	12.0
			10.0
10/14	11:00	22.9	11.0
			10.0
10/27	04:00	22.7	13.0
			12.0
11/1	NA	22.4	13.0
			12.0

TABLE I (cont)

Date	Time	Volumetric Moisture (%)	Tensiometer Reading (kPa)
Hole A-2 (500 cm depth)			
9/21	NA	NA	NA
9/22	NA	NA	NA
9/22	15:15	26.2	10.5
9/23	09:30	26.2	10.5
9/24	09:45	26.4	10.0
9/27	09:10	26.2	11.0
9/28	08:30	25.8	11.0
9/29	08:50	26.5	10.5
9/30	09:30	25.9	11.0
10/1	10:00	26.5	10.0
10/4	10:30	26.3	10.0
10/15	09:45	26.2	10.0
10/6	10:00	26.2	10.0
10/8	09:20	26.1	10.0
10/14	11:00	26.5	10.0
10/27	04:00	26.2	10.0
11/1	NA	26.4	10.0

Outflow			
Date	Time Sample Collected	Weight (g) Time (hours)	Flow mℓ/min
9/24	10:20	11 158 (43 hr)	4.32
9/28	09:25	8 386 (23 hr)	6.08
9/29	09:30	8 507.5 (24 hr)	5.91
9/30	09:30	10 262 (24 hr)	7.13
10/1	09:30	12 017 (24 hr)	8.35
10/5	10:35	18 818 (23.7 hr)	13.25
10/6	10:32	18 737 (24 hr)	13.01
10/8	09:50	20 336 (25 hr)	13.56
10/14	11:28	20 325 (25.5 hr)	13.5

[a] Two tensiometer readings at one date at the same horizon indicate data for the two tensiometers located at that horizon.

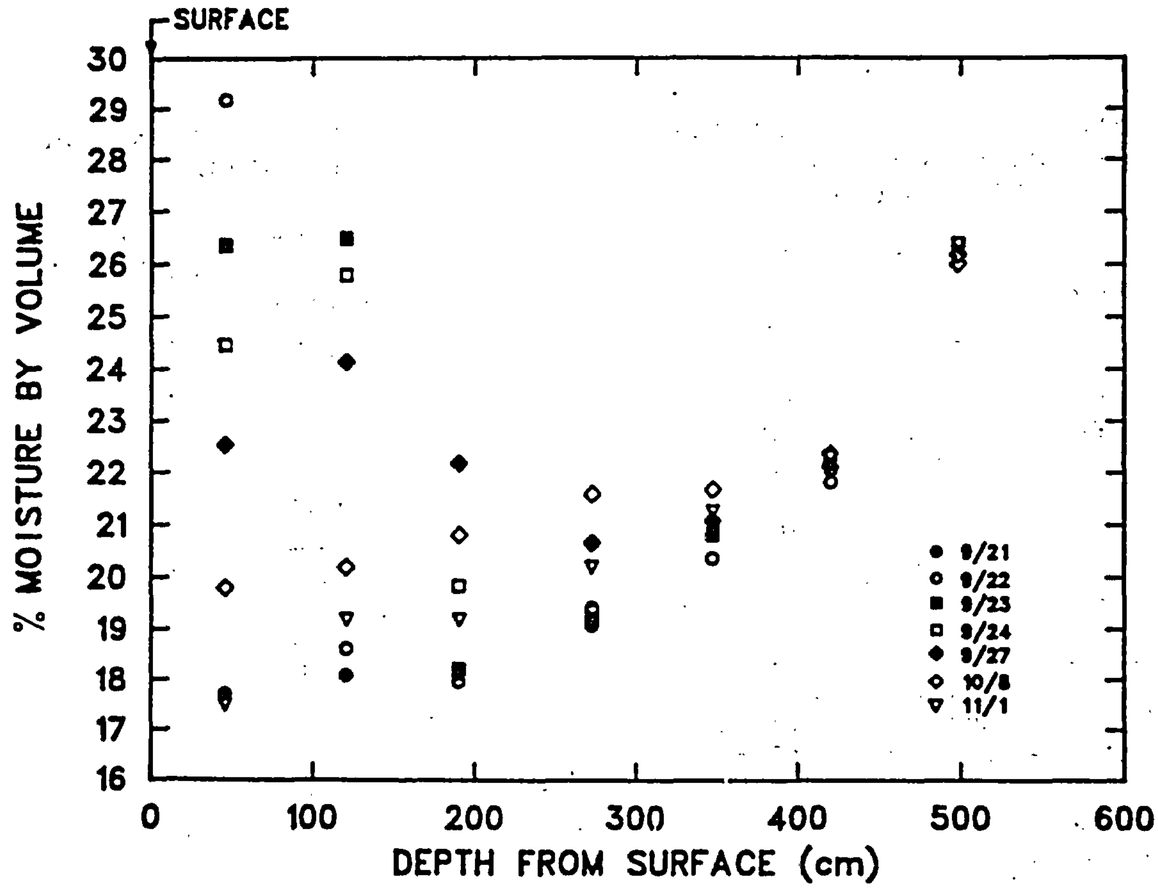

Fig. 4. Water pulse moisture as a function of depth and time.

At time 0, 13 cm of water was placed on top of the column. When this ponded water had infiltrated, the top boundary condition reverted to atmospheric conditions of no pressure, zero saturation.

Relevant material properties include porosity, saturated permeability, relative permeability vs saturation, and matric potential vs saturation and are included in Tables III and IV. Values for sand and gravel were not measured experimentally and are only estimates. Saturated permeability values for tuff were obtained from drainage experiments (Abeele 1984). Relative permeability is assumed to be given by the Brooks-Corey model (Bear 1972). (The code can, however, handle tabular relative permeability and matric potential curves.) According to the Brooks-Corey model, relative water permeability is given by

$$k_{rw} = S^{3+2/\lambda} ,$$

where S is saturation and λ is the "pore size index." For crushed tuff, λ was estimated from the matric potential curve (because Brooks-Corey also assume that matric potential ψ is given by $\psi = \psi_o S^{-1/\lambda}$, where ψ_o is the "bubbling" pressure; here a value of 0.04 bars was considered valid for the tuff). Air movement was neglected in this calculation.

b. Output. The computer simulations are given in Table V and displayed as the smooth curves in Figs. 5-18. These simulations show degree of saturation vs depth at times corresponding to the times measured experimentally.

c. Results Predicted by the Simulation. The code model predicts that for the initial given conditions once a 13-cm slug of water is added, there will be saturated flow near the soil surface just after ponding (Fig. 5). At a few centimeters below the surface, this flow becomes unsaturated, with the volumetric water content pulse having a small width at 3.2 hours. Very quickly all flow is unsaturated and the pulse width continues to broaden (Figs. 6-18), with a decrease in amplitude as the pulse moves downward. By 400 cm, the effect of the pulse becomes very small in terms of changes in volumetric water content, and below this the changes are too small to detect experimentally.

3. Comparison Code/Experimental Data

The close agreement between code prediction and experimental data in the tuff can be seen in Table V and Figs. 5-18 (in which experimental points are shown with the error bars vs the smooth simulation curves).

TABLE II

INITIAL MOISTURE CONDITIONS USED FOR INPUT FOR THE TRACR3D CODE

Depth (cm)	Volumetric Moisture (%)	Degree of Saturation*
0-80	17.9	0.517
80-152	18.6	0.538
152-228	18.2	0.526
228-308	19.4	0.56
308-388	20.8	0.60
388-468	22.2	0.64
468-550	26.0	0.75
550-575[a]	32.7[c]	0.99[c]
575-600[b]	2.2[c]	0.05[c]

*Defined as volumetric water content divided by volumetric water content at saturation—in this experiment 34.6%.

[a]Sand layer.
[b]Gravel layer.
[c]Assumed value.

TABLE IV

MATRIC POTENTIAL FOR CRUSHED TUFF

Degree of Saturation	Capillary Tension (bars)
0.20	4.0
0.25	1.3
0.30	0.70
0.35	0.46
0.40	0.38
0.45	0.30
0.50	0.22
0.55	0.17
0.60	0.14
0.65	0.125
0.70	0.09
0.75	0.07
0.80	0.055
0.85	0.045
0.90	0.04
1.00	0.00

Source: Abeele, 1984.

TABLE III

MATERIAL PROPERTIES USED IN CODE SIMULATION

Property	Tuff	Sand[b]	Gravel[b]
Porosity[a]	0.346	0.33	0.45
Saturated Permeability (10^{-5} m/s)	0.25	5.00	30.00
Pore Size Index	0.433	1.00	10.00
ψ_o (bars)	0.04	0.03	0.005

[a]Used in this context as complete saturation.
[b]Assumed value.

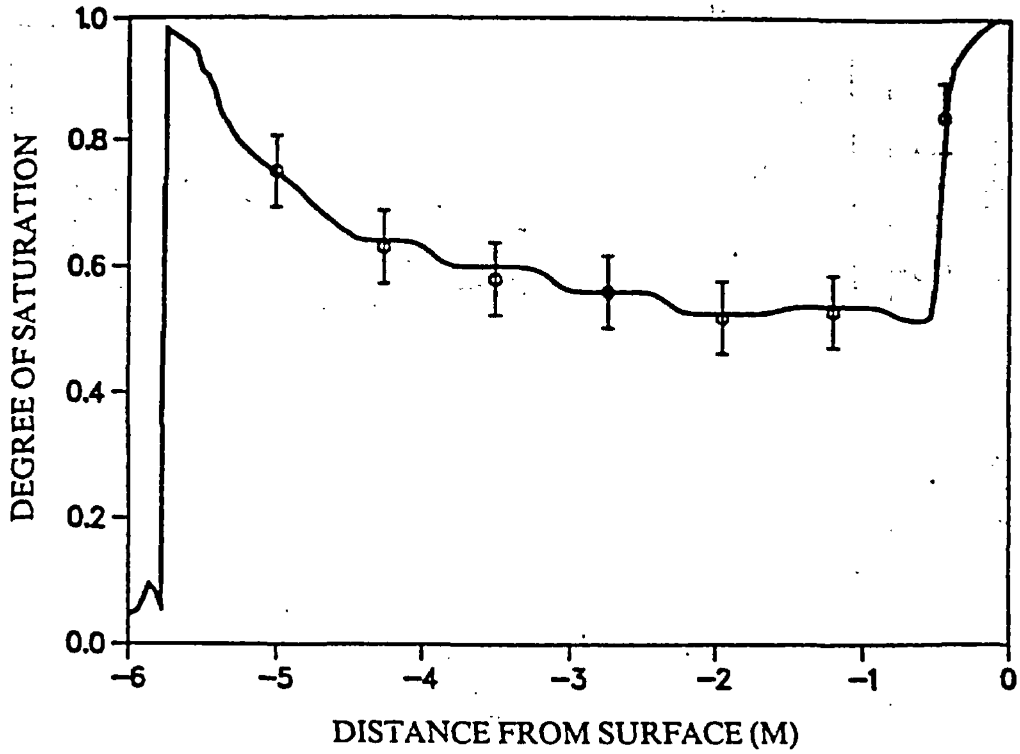

Fig. 5. 13-cm pulse, Caisson A (3.1 hr).

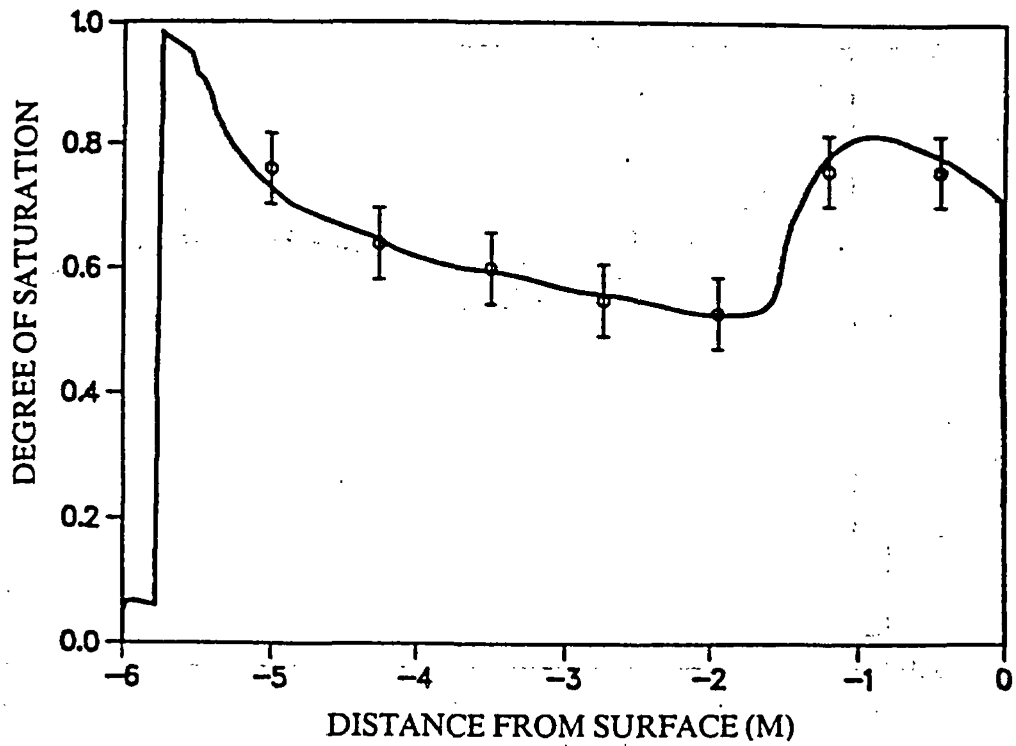

Fig. 6. 13-cm pulse, Caisson A (23.6 hr).

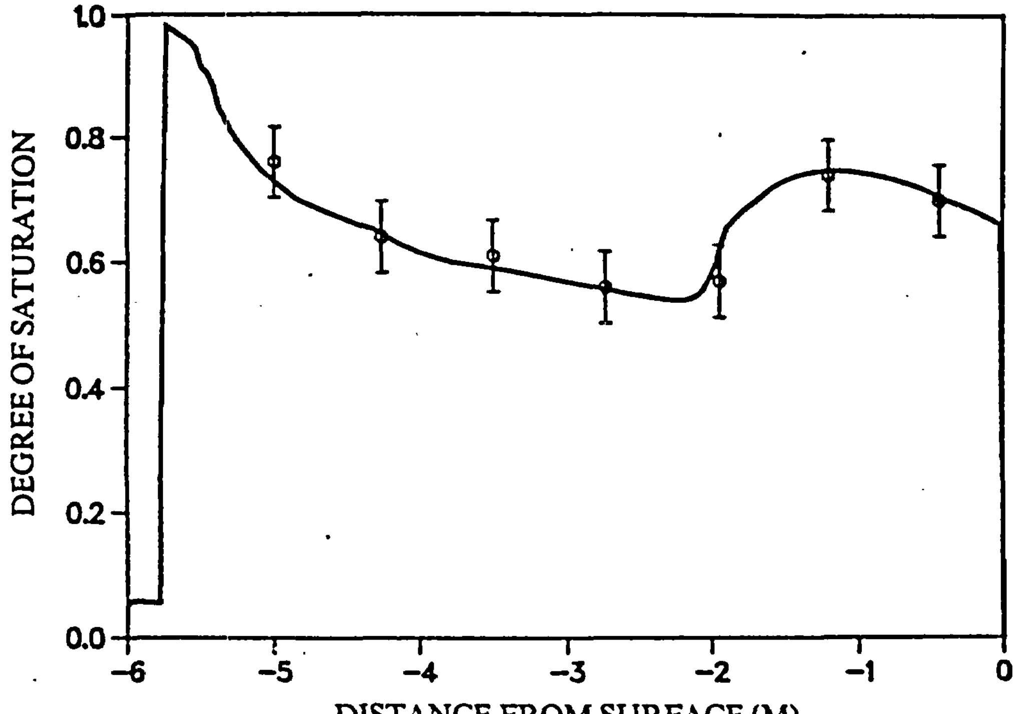

Fig. 7. 13-cm pulse, Caisson A (2.0 days).

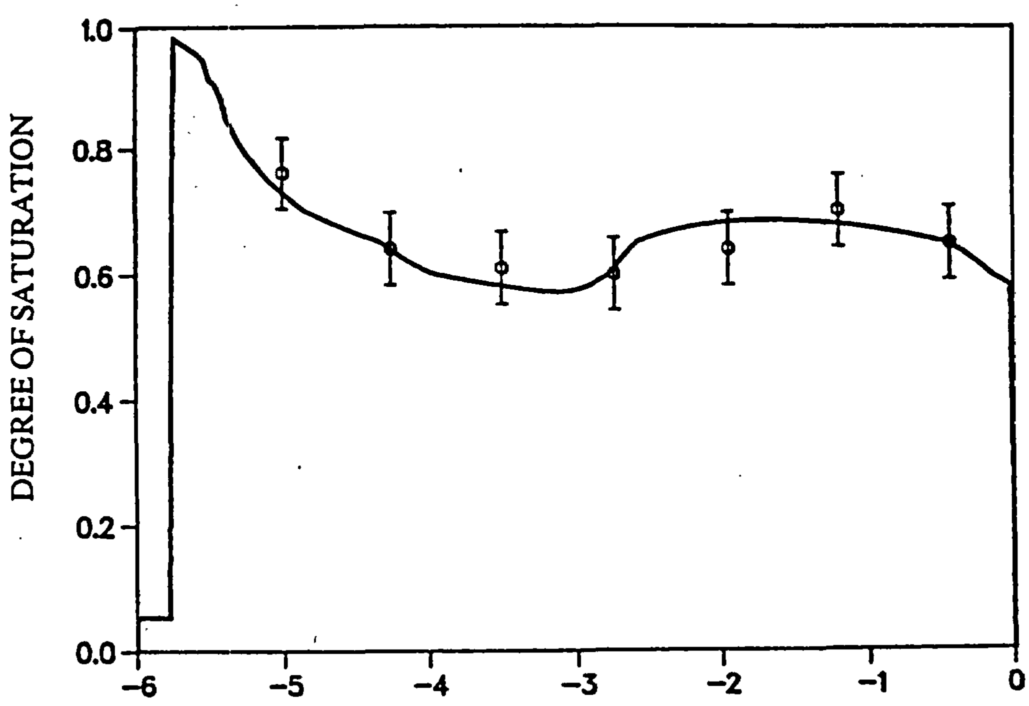

Fig. 8. 13-cm pulse, Caisson A (5.0 days).

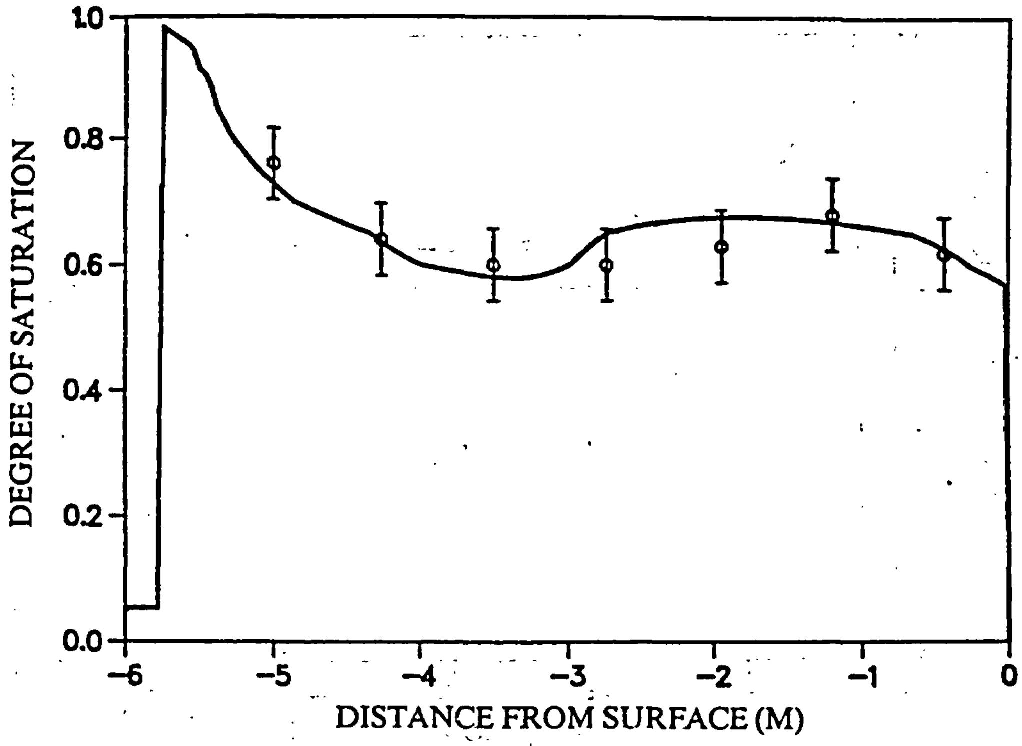

Fig. 9. 13-cm pulse, Caisson A (6.0 days).

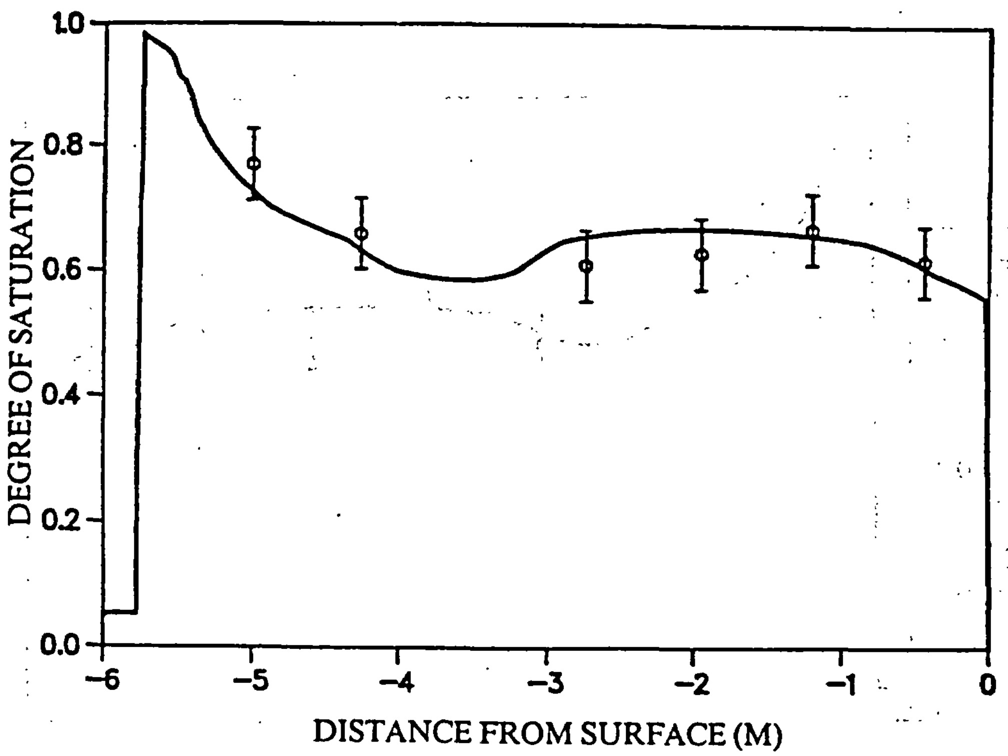

Fig. 10. 13-cm pulse, Caisson A (7.0 days).

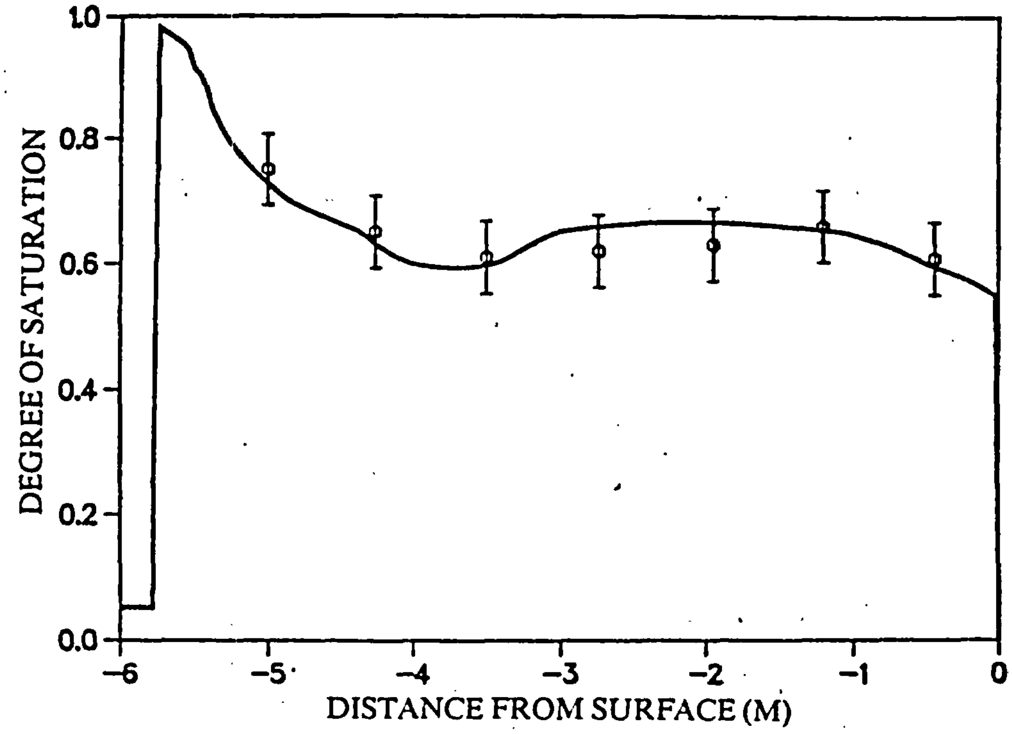

Fig. 11. 13-cm pulse, Caisson A (8.0 days).

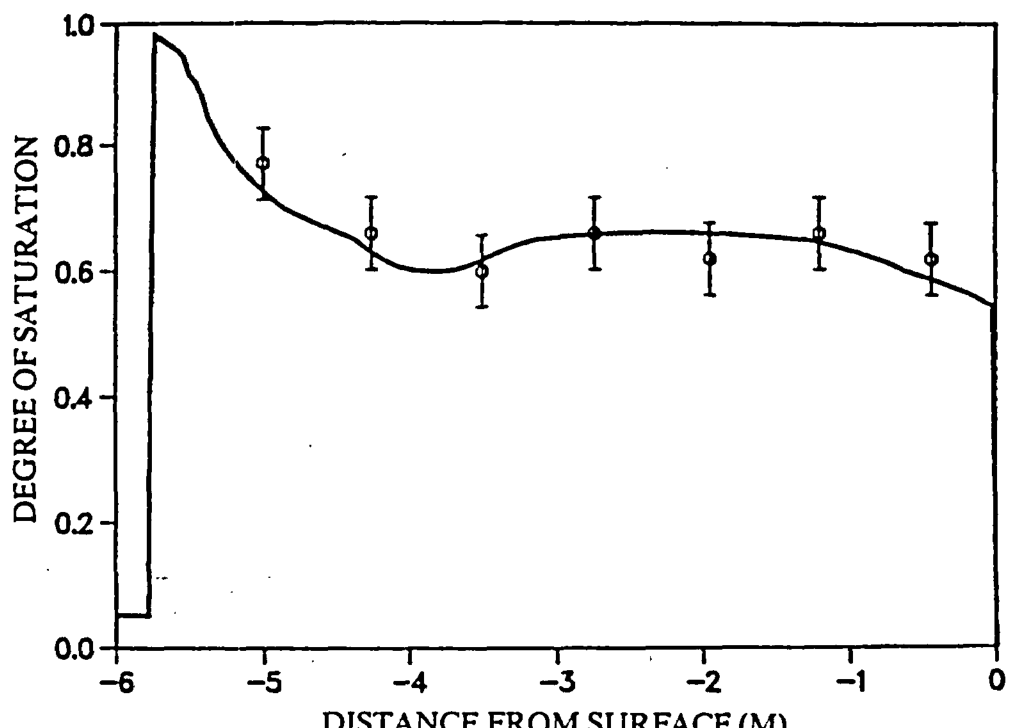

Fig. 12. 13-cm pulse, Caisson A (9.1 days).

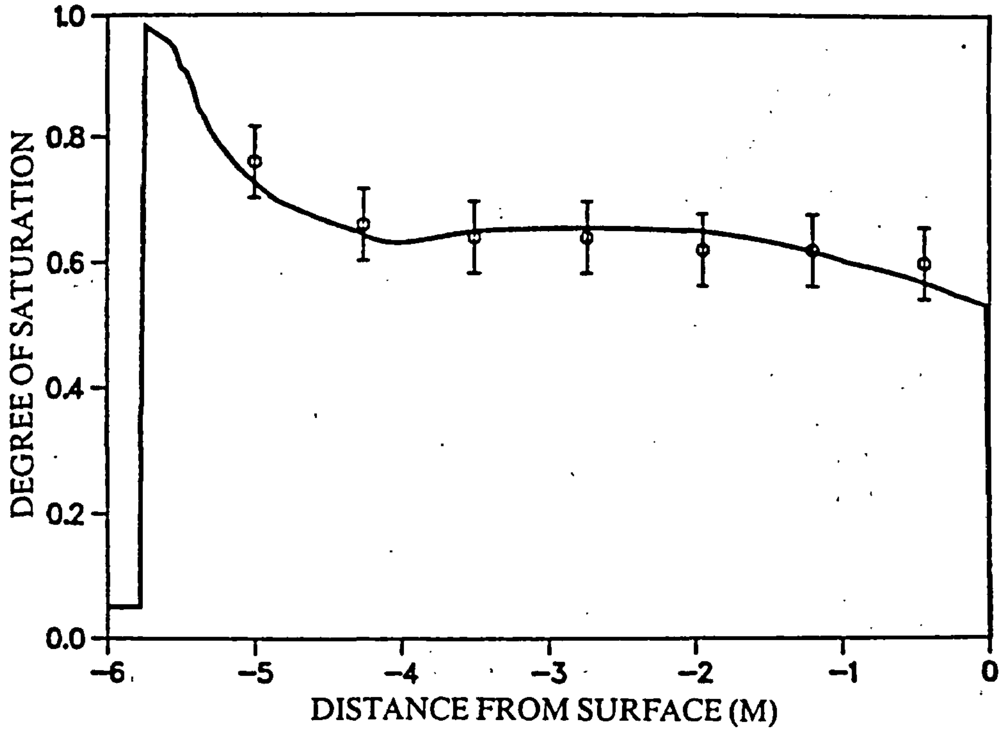

Fig. 13. 13-cm pulse, Caisson A (12.0 days).

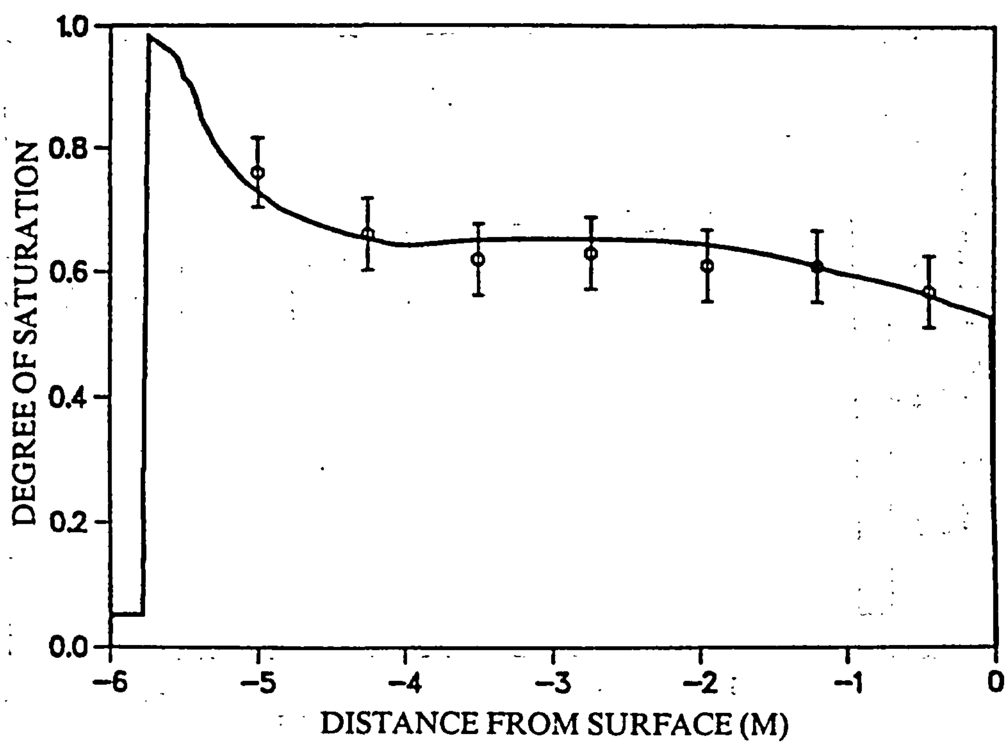

Fig. 14. 13-cm pulse, Caisson A (13.0 days).

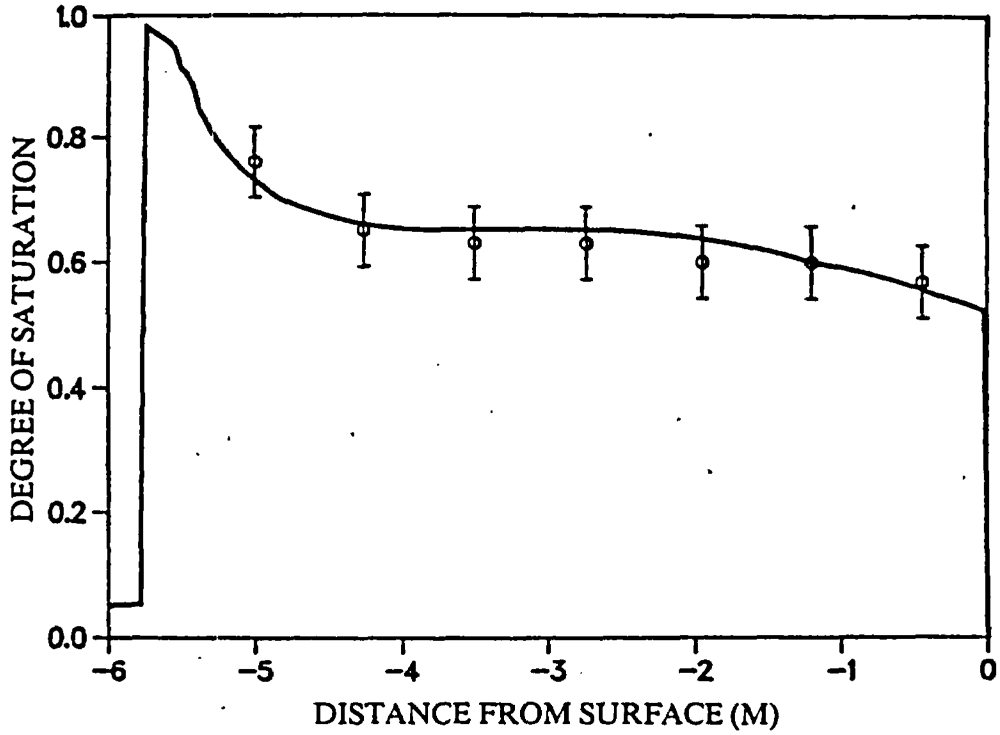

Fig. 15. 13-cm pulse, Caisson A (14.1 days).

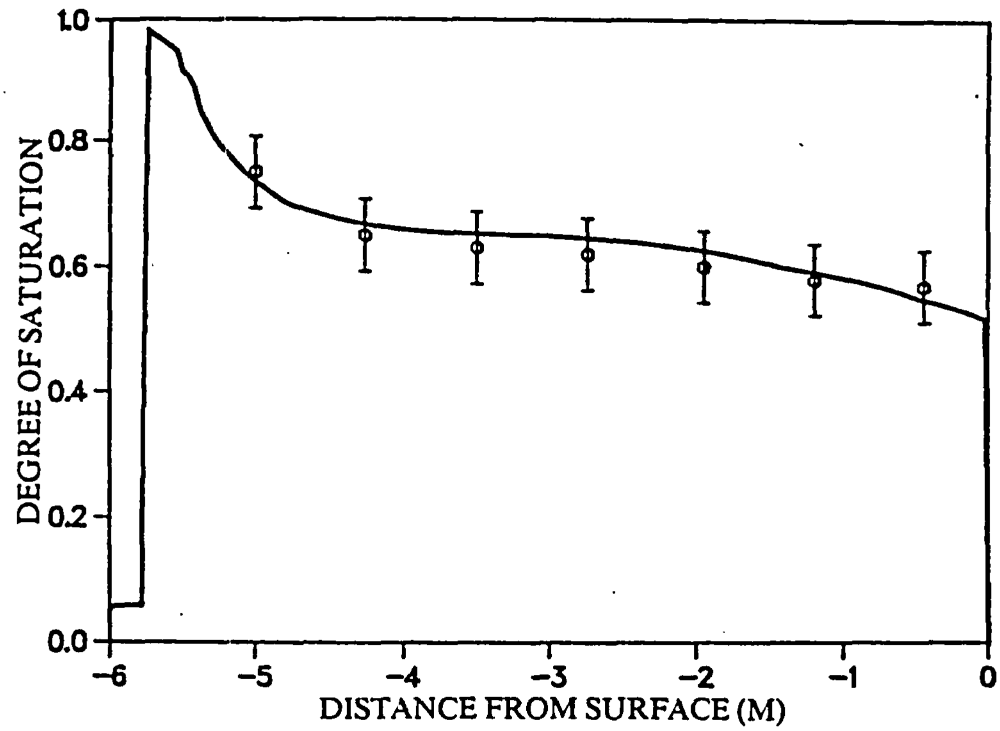

Fig. 16. 13-cm pulse, Caisson A (16.0 days).

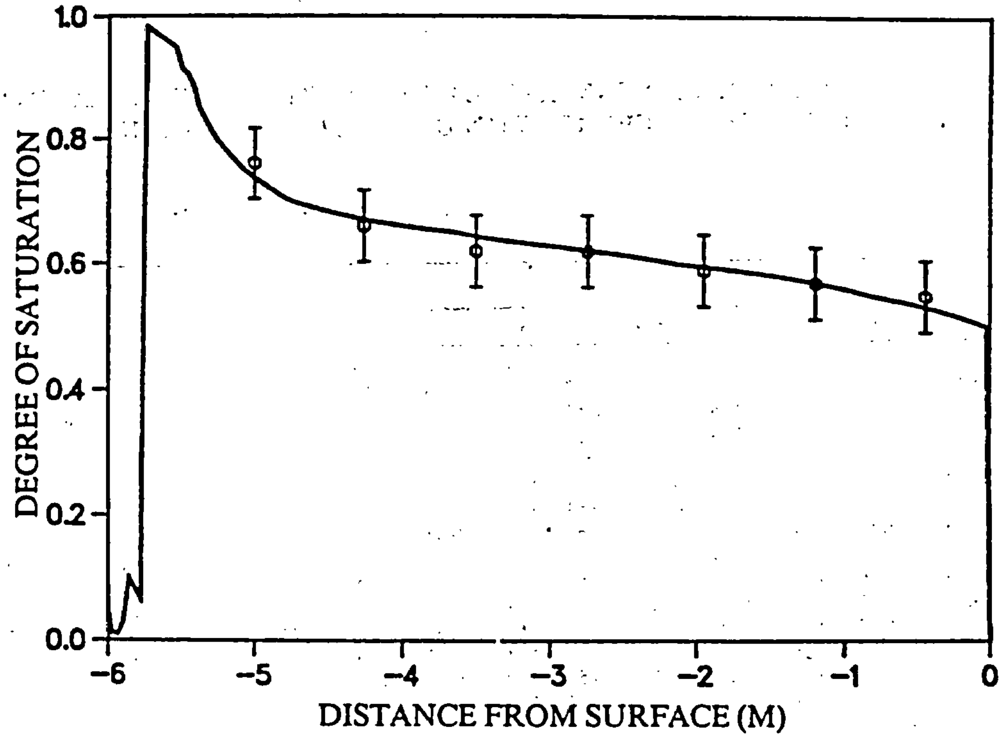

Fig. 17. 13-cm pulse, Caisson A (22.1 days).

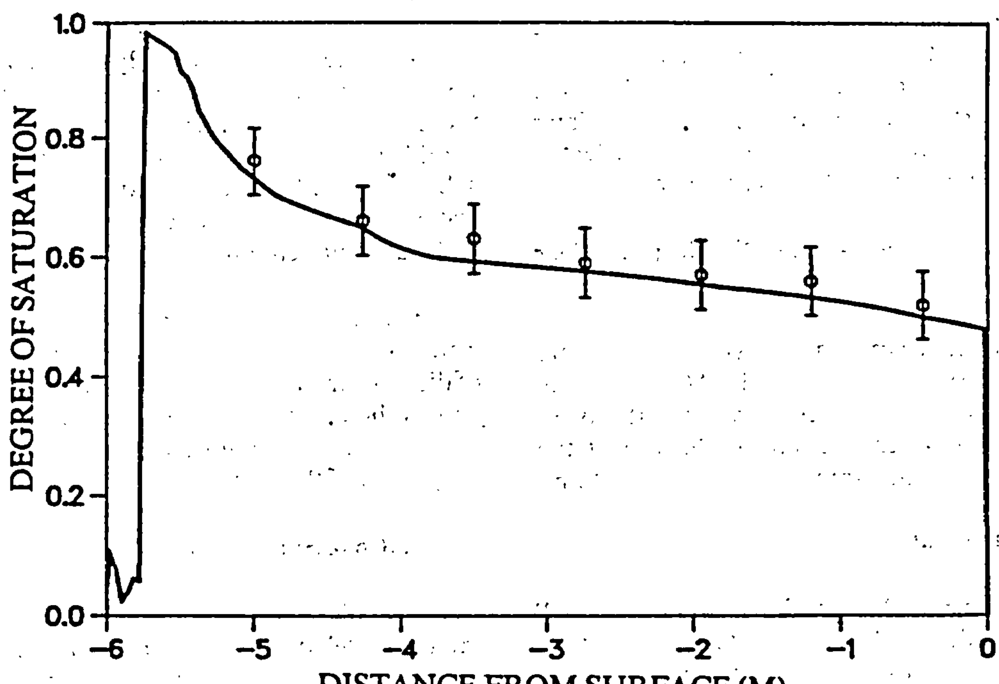

Fig. 18. 13-cm pulse, Caisson A (1.2 months).

TABLE V

COMPARISON OF EXPERIMENTAL DATA WITH CODE SIMULATION FOR PULSE EXPERIMENT (IN DEGREE OF SATURATION)

		Depth Below Soil Surface (cm)													
		44		120		195		274		350		426		500	
Date	Time	E	S	E	S	E	S	E	S	E	S	E	S	E	S
9/22	09:00	0.52	0.52	0.54	0.54	0.53	0.53	0.56	0.56	0.60	0.60	0.64	0.64	NA	0.76
9/22	15:15	0.84	0.80	0.53	0.54	0.52	0.53	0.56	0.56	0.58	0.60	0.63	0.64	0.75	0.75
9/23	09:30	0.76	0.78	0.76	0.79	0.53	0.53	0.55	0.56	0.60	0.60	0.64	0.64	0.76	0.73
9/24	09:45	0.70	0.71	0.74	0.75	0.57	0.63	0.56	0.56	0.61	0.59	0.64	0.64	0.76	0.73
9/27	09:10	0.65	0.65	0.70	0.68	0.64	0.68	0.60	0.61	0.61	0.58	0.64	0.64	0.76	0.73
9/28	08:30	0.62	0.63	0.68	0.67	0.63	0.68	0.60	0.65	0.60	0.58	0.64	0.64	0.76	0.73
9/29	08:50	0.62	0.61	0.67	0.66	0.63	0.67	0.61	0.66	NA	0.59	0.66	0.63	0.77	0.73
9/30	09:30	0.61	0.59	0.66	0.65	0.63	0.67	0.62	0.66	0.61	0.60	0.65	0.63	0.75	0.73
10/1	10:00	0.62	0.59	0.66	0.65	0.62	0.66	0.66	0.66	0.60	0.62	0.66	0.63	0.77	0.73
10/4	10:30	0.60	0.57	0.62	0.62	0.62	0.65	0.64	0.65	0.64	0.65	0.66	0.64	0.76	0.73
10/5	09:45	0.57	0.56	0.61	0.61	0.61	0.64	0.63	0.65	0.62	0.65	0.66	0.65	0.76	0.73
10/6	10:00	0.57	0.56	0.60	0.60	0.60	0.64	0.63	0.65	0.63	0.65	0.65	0.66	0.76	0.73
10/8	09:20	0.57	0.55	0.58	0.59	0.60	0.63	0.62	0.64	0.63	0.65	0.65	0.67	0.75	0.74
10/14	11:00	0.55	0.53	0.57	0.57	0.59	0.60	0.62	0.62	0.62	0.64	0.66	0.67	0.76	0.74
10/27	09:00	0.52	0.51	0.56	0.54	0.57	0.56	0.59	0.59	0.63	0.60	0.66	0.65	0.76	0.73

E indicates experimental data.
S indicates results from computer simulation.

In the simulation the sand remained at almost complete saturation, while the gravel held a small amount of water, as expected. While the code simulation did predict caisson drainage beginning within a few hours, the simulated drainage rate did not agree with the experimentally measured rate. To accurately model outflow, better numbers are needed for the hydraulic properties of the sand and gravel. Water movement in the tuff was not significantly affected by ignorance of the sand and gravel properties.

B. Caisson B Steady-State Conditions Near Saturation

A second related experiment was run to compare experimental results with the TRACR3D code predictions under unsaturated flow conditions in which the rate of water addition at the top of the caisson was equal to the drainage rate at the bottom.

1. Experimental

a. Emplacement. A second caisson, noted as B in Fig. 1, was filled and instrumented in a manner similar to caisson A. In addition, a vertical hole was drilled from the surface into the sand/gravel region to a depth of 14 cm above the bottom of the caisson, and the hole was cased with a 6.35-cm-diam aluminum access tube. The neutron moisture probe could then be used to obtain moisture readings as a function of depth.

b. Water Application. By means of a drip irrigation system, water was applied across the surface of the caisson at a uniform rate of 200 ml/min until equilibrium conditions (same flow in and out) were achieved. Under these conditions, the volumetric water content in the caisson was less than saturation, and water movement was by unsaturated flow.

c. Experimental Data. The data for volumetric water content and degree of saturation as a function of distance from the soil surface are given in Table VI and as the circles in Fig. 19. The data would suggest that there are some nonuniformities in the hydraulic properties of the material.

2. Code Simulation

A steady flux of 200 ml/min through the caisson can be modeled using the same material properties of the tuff as were used in the first experiment because the two caissons were filled using the same techniques and material.

TABLE VI

WATER CONTENT AS A FUNCTION OF DEPTH
200 mℓ/min Input/Output

Distance from Top (cm)	Volumetric Water Content (%)	Degree of Saturation
34.6	29.5	0.85
54.6	29.8	0.86
74.6	31.1	0.90
94.6	29.9	0.86
114.6	29.1	0.84
134.6	29.6	0.86
154.6	29.8	0.86
174.6	29.3	0.85
194.6	29.4	0.85
214.6	29.0	0.84
234.6	29.4	0.85
254.6	29.8	0.86
274.6	30.4	0.88
294.6	29.5	0.85
314.6	30.5	0.88
334.6	30.0	0.87
354.6	26.5	0.77
374.6	27.4	0.79
394.6	26.5	0.77
414.6	29.2	0.84
434.6	30.5	0.88
454.6	31.5	0.91

The results of this simulation are shown as the smooth curve in Fig. 19.

3. Comparison Code/Experimental Data

As Fig. 19 indicates, within the experimental errors, the code and the experimental data agree. Interface regions were not compared. The interface regions are difficult to determine experimentally because the neutron probe is an integrating instrument. In addition, properties of the sand and gravel that will affect the calculation at the sand/tuff, sand/gravel regions are not measured values.

C. Field

Although the caissons used in the two previous experiments are very large vessels, they are finite. Moreover, to complete the caisson experiments in a reasonable time frame, conditions of volumetric soil moisture near saturation were necessary.

The purpose of the final experiment was to compare the TRACR3D code simulation with a field experiment in which moisture levels were initially low and data were taken over almost a year. The field experiment was much closer to actual conditions in a burial site because the material properties of the fill had not been determined (as they were in the caisson experiments).

1. Experimental

a. Emplacement. In the field installation excavated into Bandelier tuff, 220 cm of crushed tuff is overlain by 61 cm of 7.6- to 17.8-cm-diam cobble, covered by 30 cm of 1.9- to 2.5-cm-diam gravel, and finally, at the surface, covered with 30 cm of topsoil (Fig. 20). This installation has a 366-cm-long, 6.35-cm-diameter neutron probe access tube extending down to 347 cm below the soil surface.

b. Infiltration and Moisture Data. After the experiment was emplaced, soil water content as a function of depth was measured at regular intervals over a period of almost a year (Table VII and Fig. 21).

A rain gauge at a nearby station indicated that between December 1, 1982 and February 23, 1983, ~9 cm of moisture as snow fell at the site. During Feburary the snow melted. In March ~2.5 cm of additional precipitation occurred.

The field moisture data indicate the fate of this winter precipitation. Because of low evaporation in the winter and because of the flat terrain, most of the precipitation infiltrated into the 30 cm of top soil. Because of the soil/gravel interface, buildup of soil water occurred in the topsoil until the potential at the interfaces became the same and a slug of water entered the cobble and moved downward into the underlying crushed tuff fill. The data indicate that at the top of the crushed tuff two "slugs" of water entered, creating a physical situation in the field similar to the experiment run earlier in caisson A.

Integration of the "before" and "after" water content in the crushed tuff indicates that approximately 8 cm of water entered the tuff in a fairly short interval before February 23, 1983 and another 2 cm slug of water just before March 28, 1983. Significant evaporation from the crushed tuff is prevented by the upper cobble/gravel cover. During the rest of the year, despite additional precipitation, moisture losses from evapotranspiration processes prevented significant buildup and "breakthrough" at the topsoil/gravel interface.

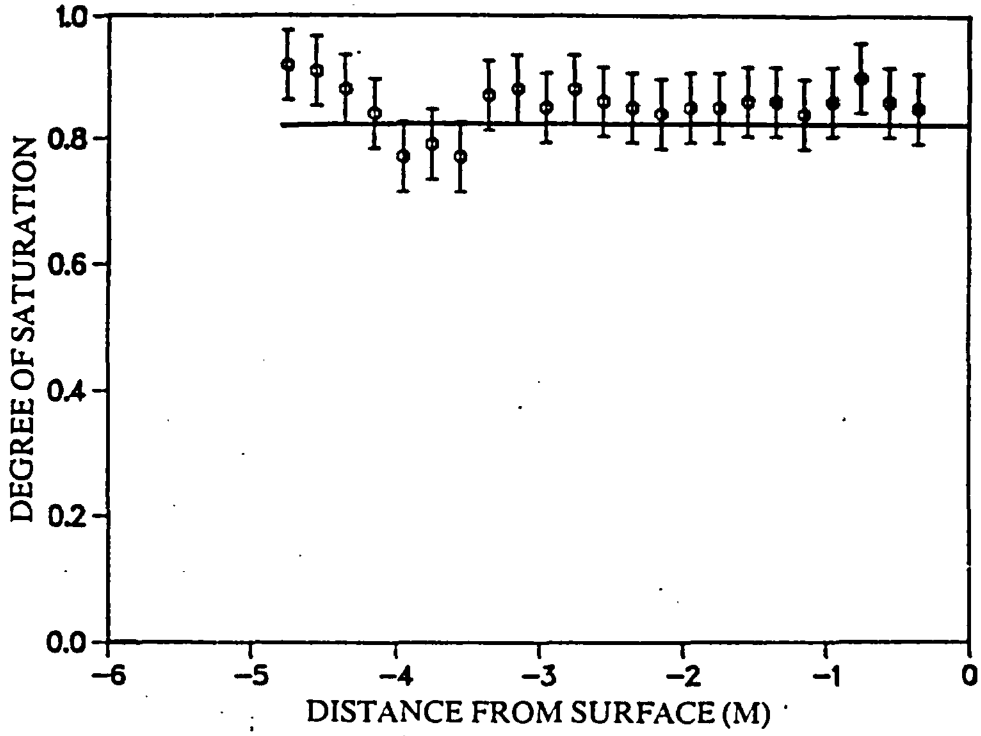

Fig. 19. 200 ml/min inflow, 45% initial saturation (18.5 days).

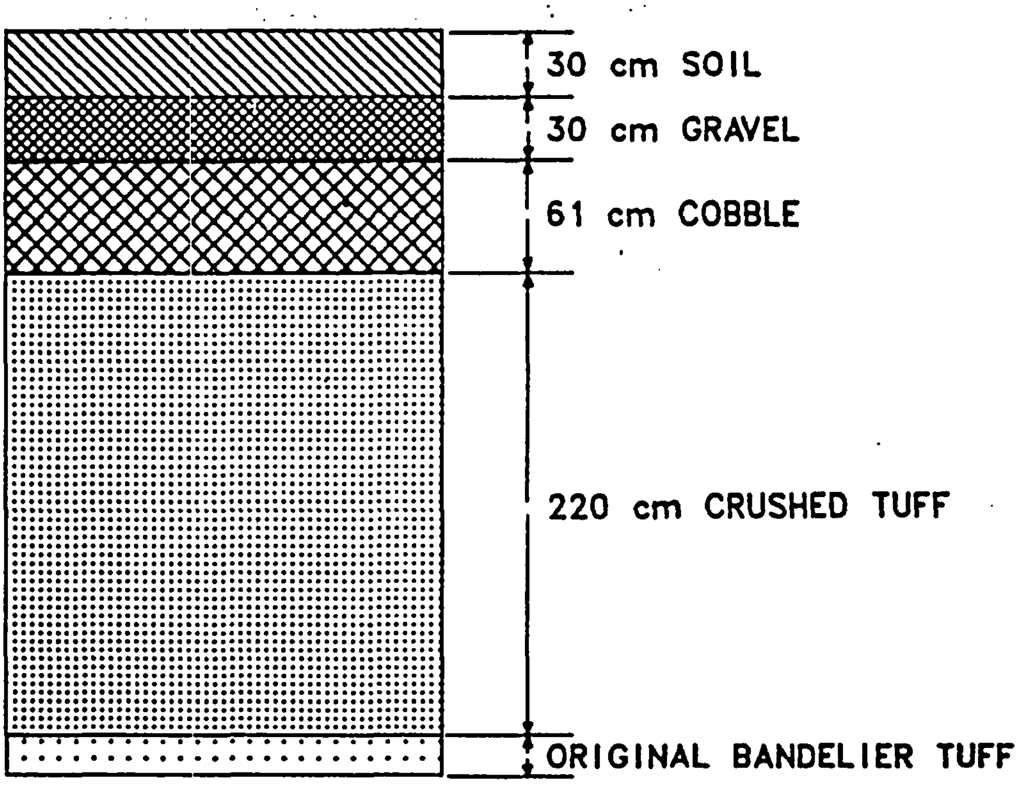

Fig. 20. Field experiment profile.

TABLE VII

MEASURED VOLUMETRIC MOISTURE FOR THE FIELD PULSE EXPERIMENT (1983)

Centimeters From Soil Surface	1/11	1/17	2/11	2/15	2/23	2/25	3/1	3/7	3/21	3/28	4/22	6/22	8/17	10/18	11/30
22.2	22.3	21.7	NA	25.7	36.0	35.0	34.2	33.4	13.9	31.1	32.6	NA	7.4	15.9	14.2
42.2	10.7	10.8	11.7	11.7	14.1	15.0	12.4	12.5	12.9	8.1	13.2	5.7	6.7	8.8	5.8
62.2	4.8	4.9	4.9	5.0	5.6	5.9	5.2	5.0	5.8	4.8	5.1	3.6	4.1	4.4	3.8
82.2	3.5	3.5	3.2	3.5	4.1	4.4	4.2	3.8	4.4	3.9	3.9	3.4	3.4	3.6	3.4
102.2	3.7	3.6	3.4	3.4	4.1	4.2	3.9	3.9	4.1	4.8	3.9	3.9	3.9	3.6	3.6
122.2	6.8	6.3	6.0	6.0	9.4	9.5	8.6	8.4	8.4	13.7	8.2	10.7	8.7	6.3	8.8
142.2	8.9	9.2	10.4	10.7	25.6	25.2	22.1	20.0	20.3	21.9	20.0	17.2	16.1	14.3	14.0
162.2	6.7	6.8	7.6	8.2	22.6	22.6	20.9	19.4	19.1	20.1	20.0	16.9	15.8	15.0	14.0
182.2	6.0	6.0	6.1	6.3	12.5	16.1	16.6	16.1	16.1	16.7	17.2	15.3	14.8	14.4	12.9
202.2	6.3	6.3	6.4	6.5	6.8	8.0	9.9	12.5	13.0	12.6	15.4	14.0	13.9	13.6	12.8
222.2	7.1	6.8	6.8	7.0	7.0	6.8	7.2	8.2	8.8	8.1	12.1	12.1	12.2	12.4	11.6
242.2	7.0	7.1	7.2	7.1	7.0	7.1	7.1	7.3	7.1	7.1	7.7	9.3	9.9	10.6	10.1
262.2	7.0	7.0	7.1	7.0	6.8	7.1	7.0	6.8	7.1	7.2	7.1	7.2	8.0	9.3	8.6
282.2	7.1	7.1	7.2	7.2	7.2	7.3	7.2	7.1	7.2	7.3	7.2	7.2	7.3	7.7	7.9
302.2	7.4	7.4	7.5	7.6	7.6	7.6	7.8	7.8	7.5	8.2	7.4	7.9	7.6	7.5	8.0
322.2	8.5	8.7	8.6	8.8	8.6	8.7	8.6	8.8	8.7	8.8	8.5	8.5	8.5	8.3	8.2
342.2	9.4	9.7	9.2	9.7	9.6	9.6	9.6	9.9	9.7	9.5	9.5	9.3	9.0	9.0	8.8

c. Experimental Results. Figure 21 indicates the downward movement of the volumetric water content pulses and the corresponding decrease in amplitude. The changes in soil moisture appear to be "damped" completely by 160 cm below the top of the crushed tuff.

The general behavior of the pulses is similar to that observed in caisson A and modeled in the first TRACR3D simulation. However, because of the initial low moisture levels and slightly smaller pulse inputs, the volumetric soil water content pulse movement is much slower, and complete damping (defined as no detectable change in volumetric water content) occurs at a higher horizon. Because the crushed-tuff fill is underlain by the undisturbed Bandelier tuff upon which the experiment was emplaced, interface effects below the crushed tuff may also be present.

2. Code Simulation

a. Input Conditions. A TRACR3D computer simulation was run using the inputs and conditions given in Table VIII. The same material properties for the tuff were used as were used in the caisson simulations, with one exception—the initial dry conditions in the crushed tuff prevented as great a compaction as in the wetter caisson fill and thus 40% was used for saturation.

b. Output. The results of the field simulations are shown as the smooth curves in Figs. 22-29.

3. Comparison Code/Field Measurements

The experimentally determined data points are included as the dots in Figs. 23-29. The experimental data are also compared with the simulations in Table IX.

As can be seen, the field and simulation agreement are not as close as in the caisson A pulse experiment. Considering the unknown material properties of the field fill and probably greater heterogeneity of the fill, the simulation results are in good agreement. The "damping" point found in the simulation (compare Fig. 22 with Fig. 29) at 160 cm is the same as was found experimentally.

Factors affecting the field measurements and code simulations will be discussed in more detail in the next section.

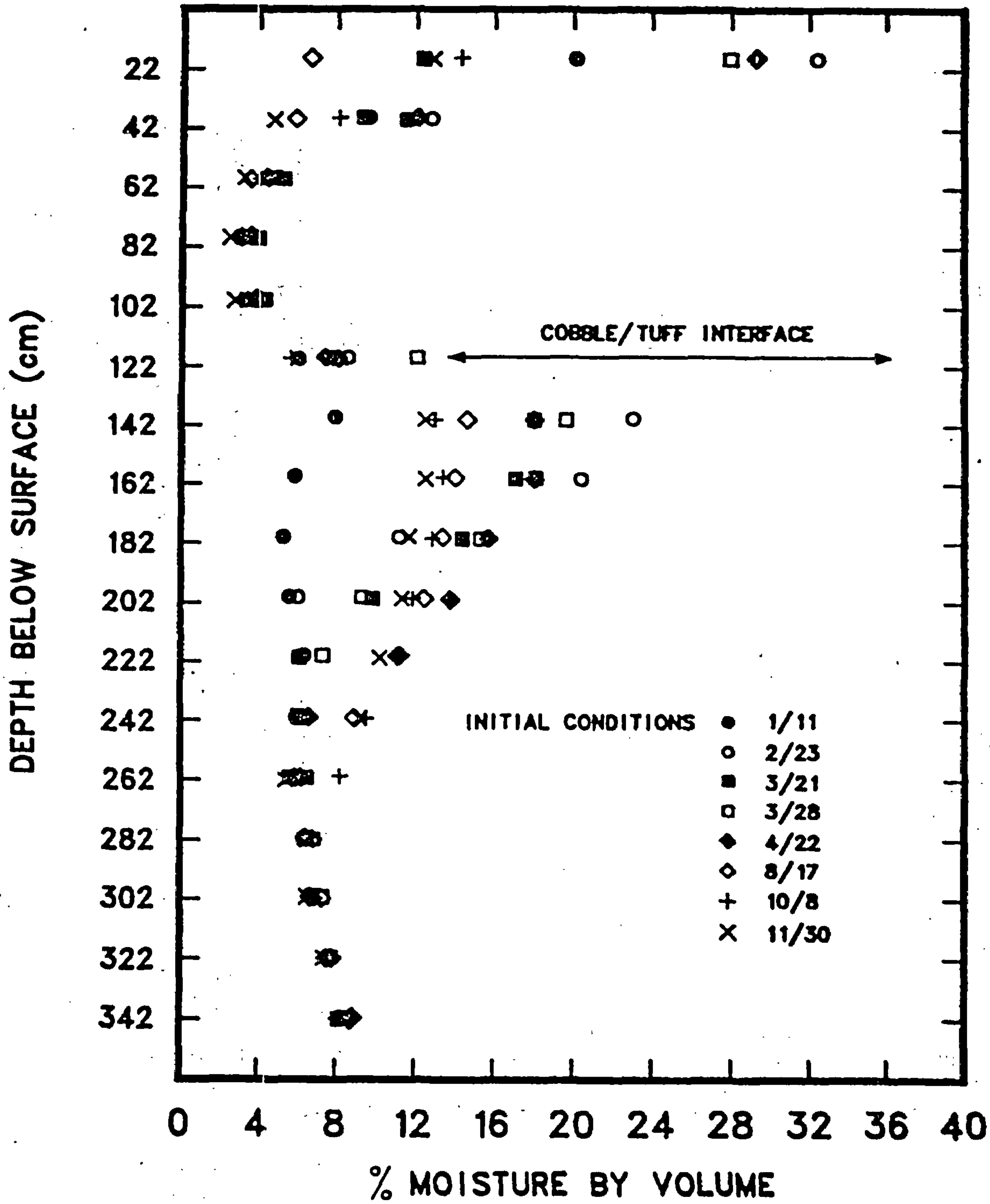

Fig. 21. "Damping" of moisture pulses under field conditions.

TABLE VIII

CONDITIONS FOR TRACR3D SIMULATION OF FIELD EXPERIMENT

Starting Conditions

cm Below Interface	Volumetric Moisture (%)	Per Cent of Total Saturation
20	8.9	0.22
40	6.7	0.17
60	6.0	0.15
80	6.3	0.16
100	7.1	0.18
120	7.0	0.18
140	7.0	0.18
160	7.1	0.18
180	7.4	0.18
200	8.5	0.21
220	9.4	0.24

Moisture Additions

1. Add 8 cm water.
2. Run
3. After 30 days, add 2 cm of water.
4. Run with no additional inputs for 9 months.

Material Properties

Boundary conditions—Use infinitely deep, crushed, tuff fill, no evaporation.
Porosity = 40%.
All other material properties as used in Caisson A simulations.

D. Factors Affecting the Results

1. Experimental

a. Detector. All the experimental results depended on the neutron moisture gauge for volumetric water content measurements. This instrument determines water content by detecting neutrons (produced by a radioactive source located in the instrument probe) that have been moderated and back-scattered by the hydrogen atoms in the soil water. It has been found experimentally that the maximum radius beyond which changes in soil moisture do not affect the results is about 30 cm at 5% volumetric soil water content and 20 cm at 32.4% (Nyhan et al. 1984). The moisture gauge integrates the soil moisture over a region that decreases in size with increase in moisture. Because the gauge is an integrating instrument, sharp changes in soil moisture (such as at interfaces of tuff/gravel or gravel/cobble or where other types of moisture discontinuities exist) cannot be accurately defined.

The probes were calibrated before shipment for use in sand with aluminum access tubes of 5.08 cm diam. The factory calibration of the probe used in the first experiment was checked at one point (12%) by collecting the tuff removed during construction of one of the neutron probe access holes and by comparing the moisture in the collected tuff with the moisture measured with the gauge directly after the access tube had been inserted. The factory calibration agreed with the moisture content of the collected tuff. Other calibration checks were also made (Nyhan et al. 1984).

In the other two experiments, another type of neutron probe with a different source-detector geometry was used. In addition, the diameter of each access tube was 6.35 cm. To convert the original calibration made in a tube diameter of 5.08 cm to a diameter of 6.35 cm, the readings obtained in the vertical 6.35-cm-diam tube were compared with readings taken at the same horizon in 5.08-cm-diam tubes located in caisson B.

Considering problems in intercalibrations of probes, differences in access tube diameters, counting statistics, and associated problems, it is felt that in uniformly crushed tuff, moisture measurements are accurate to approximately 2% of the absolute value (i.e., if 20% were measured, the moisture could range between 18 and 22%).

The error bars shown for the experimental results plotted on the simulation graphs represent the errors in moisture measured by the detectors. They do not represent errors from other factors.

b. Equipment Influencing Neutron Behavior. Because aluminum has a very low neutron cross section, aluminum access tubes were used in all the experiments. In addition, tubes were located at distances greater than 30 cm so that the space in one tube would not influence the neutron detector in an adjacent tube. All vertical tubes were sealed when not in use.

Tensiometers and their associated equipment contain water and other hydrogen-containing materials. This equipment was emplaced at greater than 30 cm from the neutron probe access tubes.

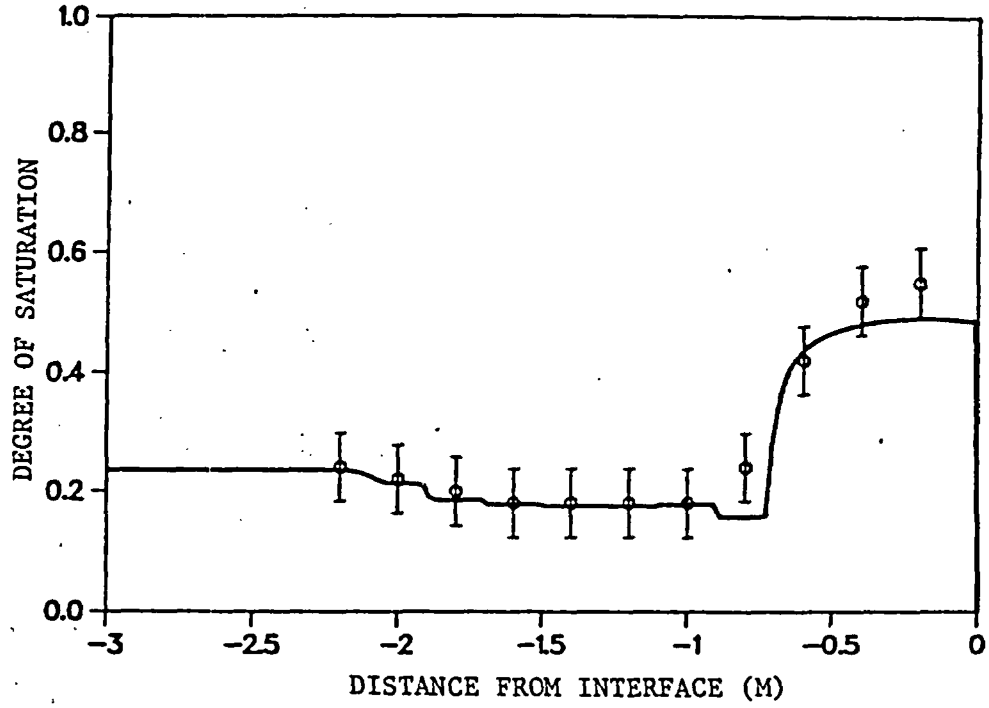

Fig. 22. Field test, 8 cm + 2 cm (10.3 days).

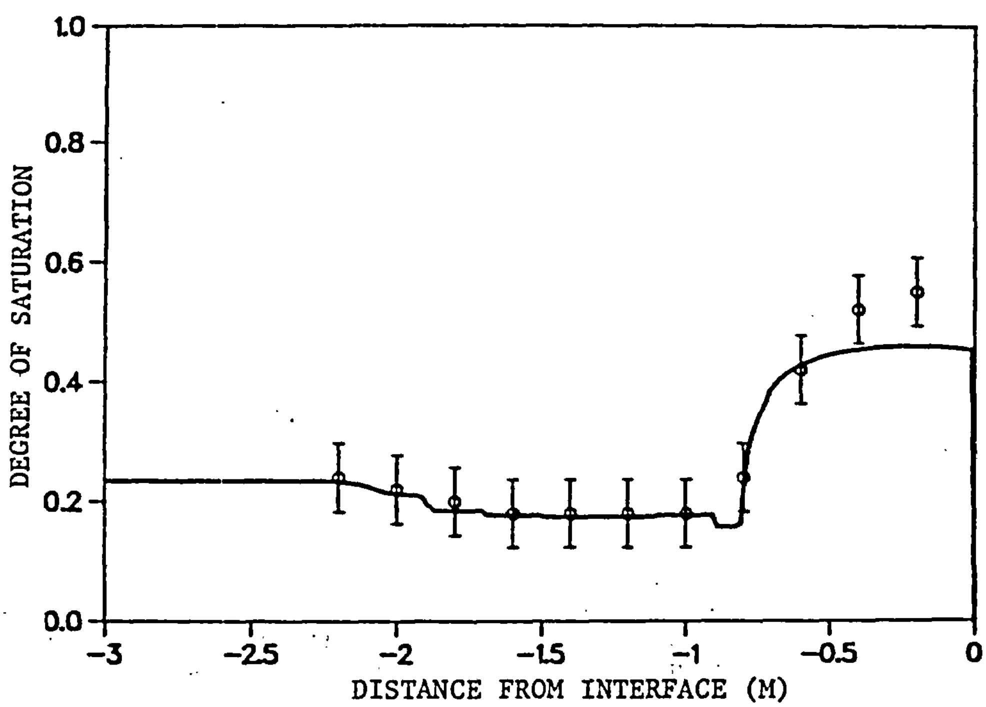

Fig. 23. Field test, 8 cm + 2 cm (20.2 days).

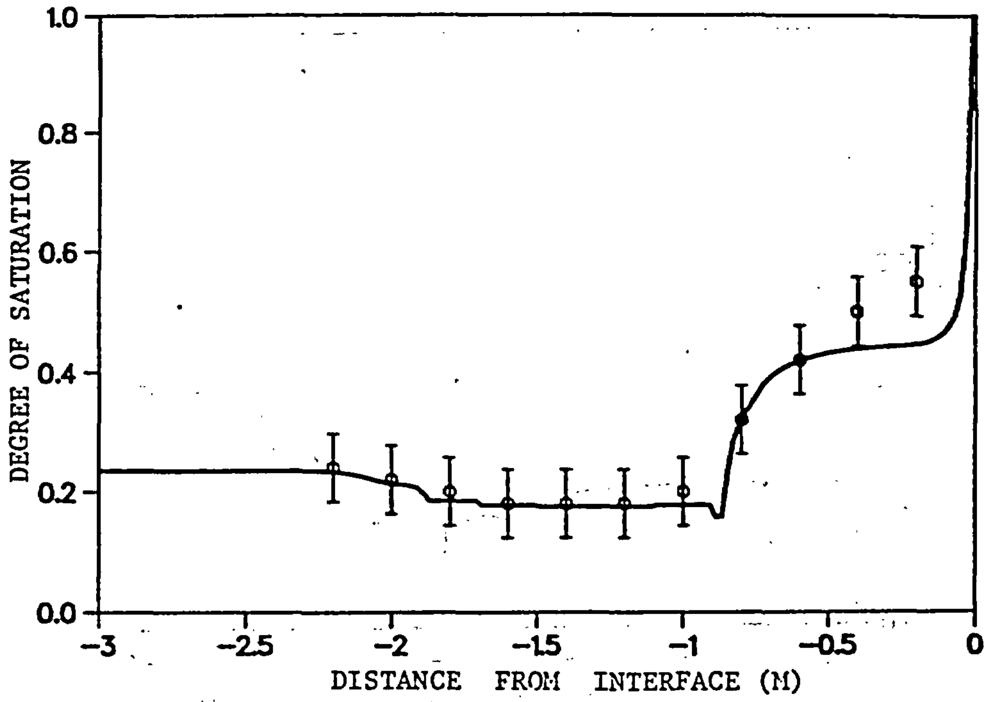

Fig. 24. Field test, 8 cm + 2 cm (1.0 month).

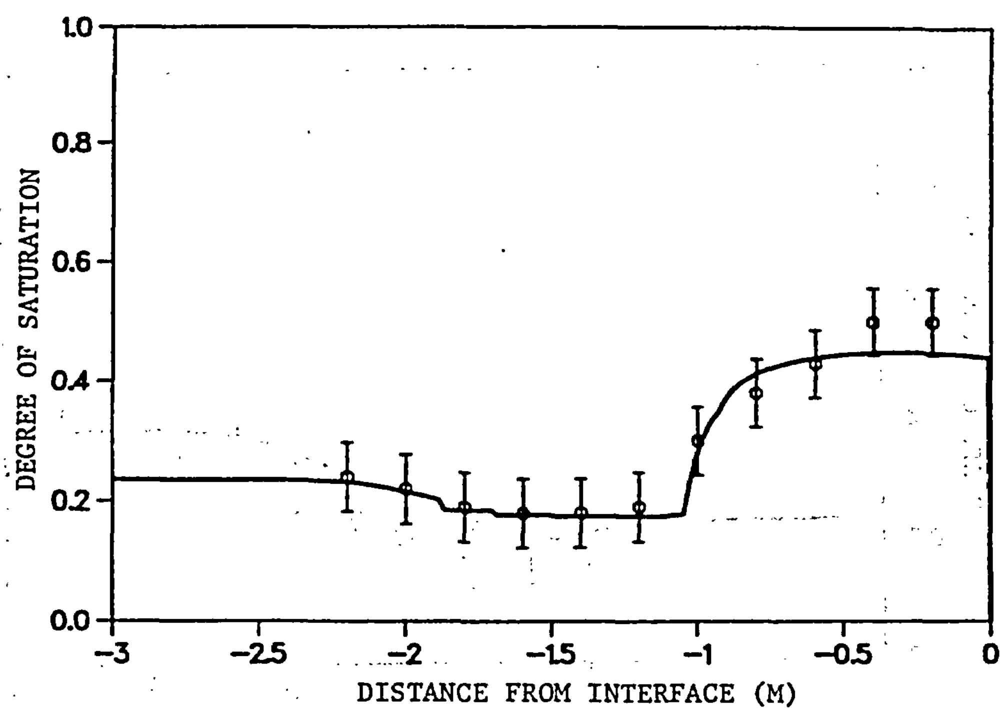

Fig. 25. Field test, 8 cm + 2 cm (2.0 months).

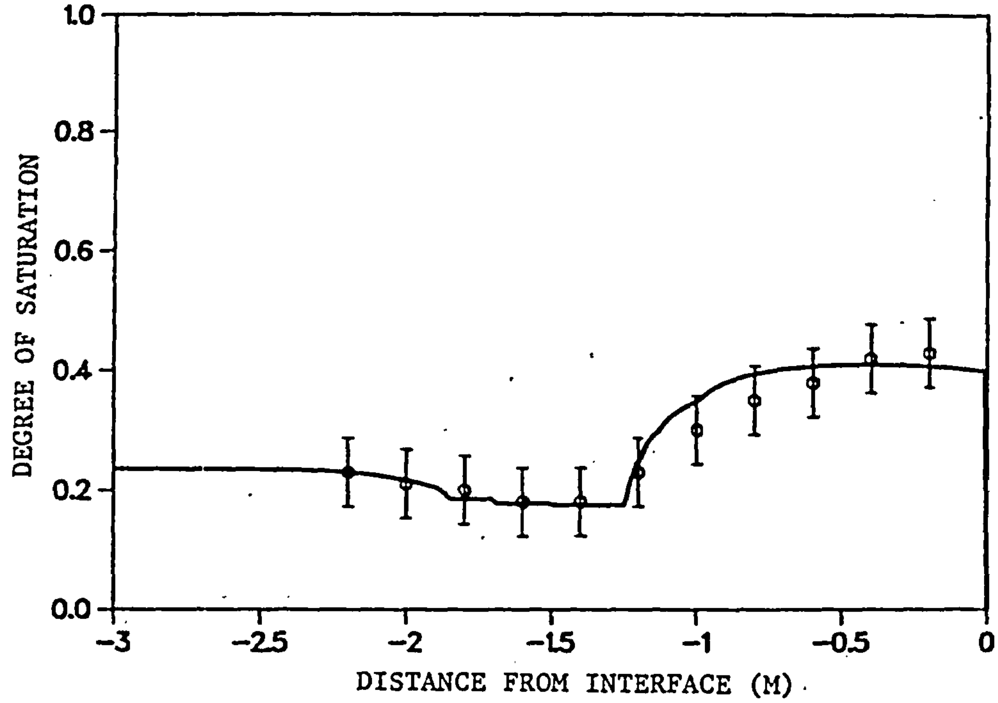

Fig. 26. Field test, 8 cm + 2 cm (4.0 months).

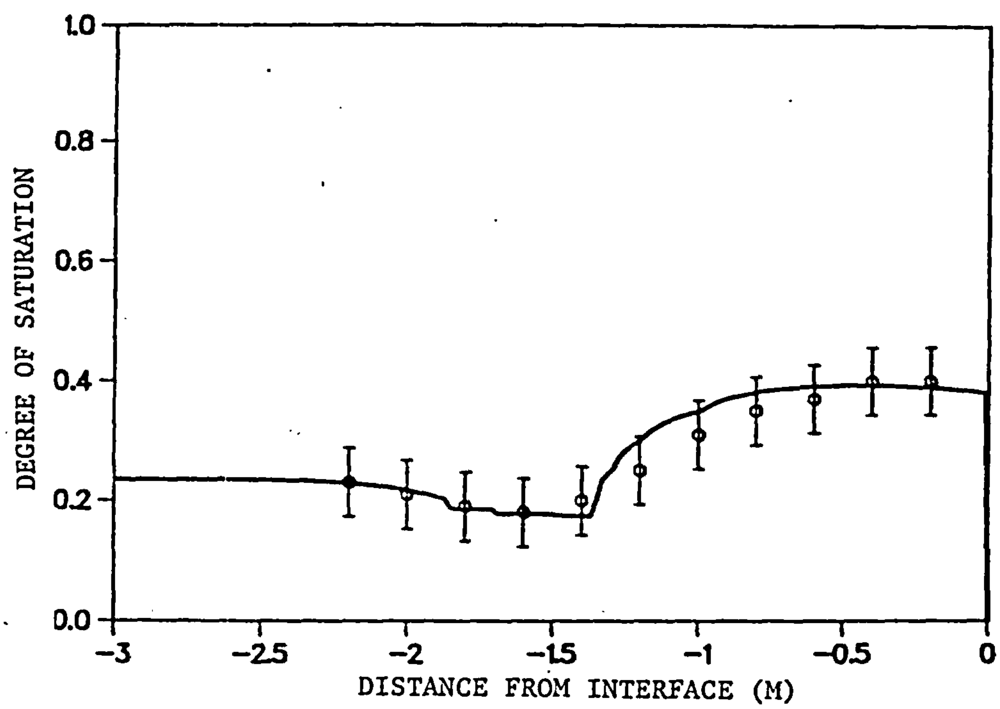

Fig. 27. Field test, 8 cm + 2 cm (6.0 months).

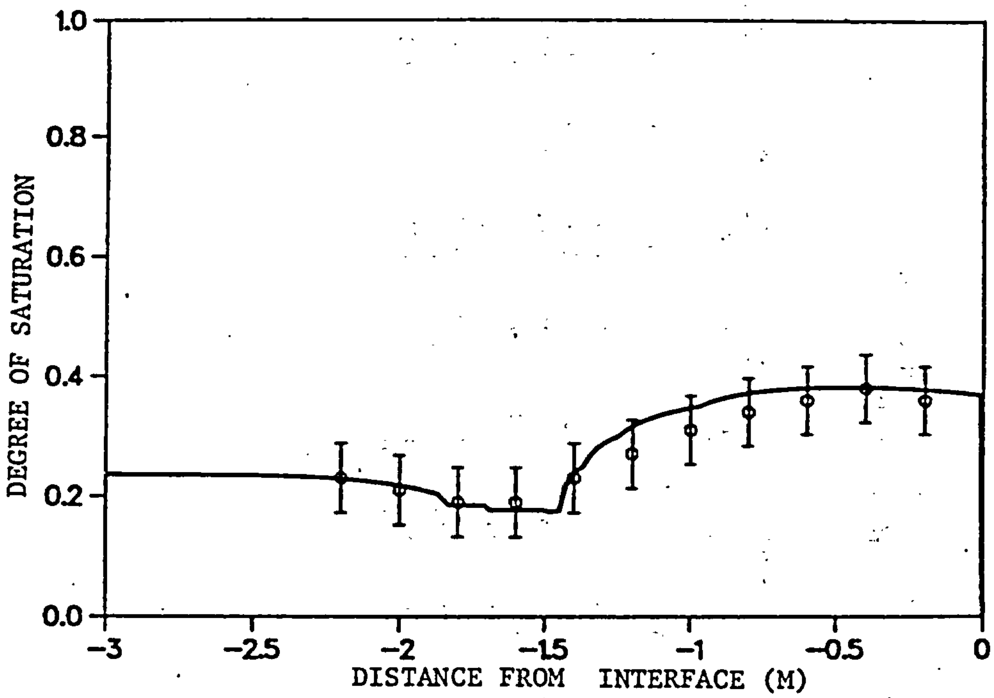

Fig. 28. Field test, 8 cm + 2 cm (8.0 months).

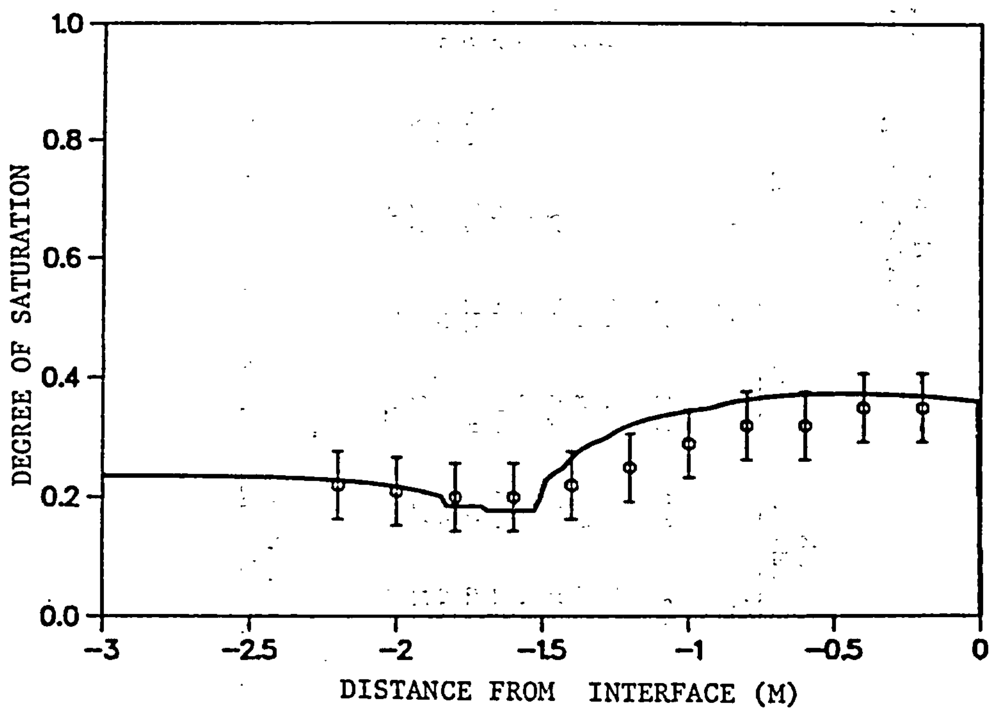

Fig. 29. Field test, 8 cm + 2 cm (10 months).

TABLE IX

FIELD MOISTURE 8 cm + 2 cm PULSE — DEGREE OF SATURATION AS A FUNCTION OF DEPTH AND TIME: EXPERIMENTAL AND SIMULATION RESULTS

Distance Below Interface (cm)	Initial Conditions		10 days		20 days		1 month		2 months		4 months		6 months		8 months		10 months	
	E	S	E	S	E	S	E	S	E	S	E	S	E	S	E	S	E	S
20	0.22	0.21	0.55	0.49	0.51	0.46	0.55	0.45	0.50	0.45	0.43	0.41	0.40	0.39	0.36	0.38	0.35	0.37
40	0.17	0.17	0.52	0.48	0.48	0.45	0.50	0.44	0.50	0.45	0.42	0.41	0.40	0.39	0.38	0.38	0.35	0.37
60	0.15	0.15	0.42	0.43	0.40	0.42	0.42	0.42	0.43	0.44	0.38	0.41	0.37	0.39	0.36	0.38	0.32	0.37
80	0.16	0.16	0.24	0.16	0.33	0.27	0.32	0.32	0.38	0.41	0.35	0.39	0.35	0.38	0.34	0.37	0.32	0.36
100	0.18	0.18	0.18	0.18	0.22	0.18	0.20	0.18	0.30	0.30	0.30	0.35	0.31	0.35	0.31	0.35	0.29	0.34
120	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.19	0.18	0.23	0.24	0.25	0.30	0.27	0.31	0.25	0.32
140	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.20	0.18	0.23	0.23	0.22	0.26
160	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.19	0.18	0.20	0.18
180	0.18	0.18	0.20	0.18	0.19	0.19	0.20	0.19	0.19	0.19	0.20	0.19	0.19	0.19	0.19	0.19	0.20	0.19
200	0.21	0.21	0.22	0.21	0.22	0.21	0.22	0.21	0.22	0.22	0.21	0.22	0.21	0.22	0.21	0.22	0.21	0.22
220	0.24	0.24	0.24	0.23	0.24	0.23	0.24	0.23	0.24	0.23	0.23	0.23	0.23	0.23	0.23	0.23	0.22	0.23

E — Experimental.
S — Code simulation.
Total saturation — 40% by volume.
Degree of saturation — volumetric moisture/total volumetric moisture at saturation.

c. Soil Matrix. Inhomogeneities in the soil matrix will result in inhomogeneities in the soil material properties. Inhomogeneities in the soil material properties influence soil water content. Therefore, measurements of soil water content can indicate possible inhomogeneities in the soil matrix.

The horizontal access tubes in caisson A were used to determine at regular intervals water content as a function of distance from the center of the caisson at a given depth. These series of measurements indicated that moisture varied across the caisson from the center outward. Figures 30 and 31 indicate the results of traverses at 350 and 426 cm below the surface. The surface was ponded, so moisture input should have been uniform. However, even if it were not, at the depths of 350 and 426 cm if the soil matrix were uniform, dispersion should have resulted in nearly uniform moisture levels. Thus, data from the traverses suggest that the crushed-tuff matrix was not uniform.

The data from the vertical traverse of B indicate a region of low moisture 178-258 cm from the bottom of the caisson (Fig. 19). Inhomogeneities in moisture levels were also found in all the horizontal traverses at levels 44, 120, 195, 274, 350, and 426 cm below the surface. Figure 32 indicates data from a traverse at 350 cm.

If moisture data from the carefully emplaced caisson tuff indicated possible inhomogeneities in the soil matrix, greater differences may have also existed in the field experiment, which was not so carefully implaced.

The inhomogeneities in the soil matrix will influence the movement of water and, therefore, will contribute to differences in the computer simulation and experimental results.

2. Code

a. Moisture Input. To see how a change in moisture input into the code simulation might influence the results, the TRACR3D code simulation was run with a pulse input of 11 cm and compared with the input of 13 cm for the Caisson A experiment.

As would be expected with 13 cm, the pulse amplitude is slightly larger and the early effects at the sand/tuff interface are more pronounced.

b. Boundary and Initial Conditions. Except for a steady-state condition (such as was modeled for caisson B), initial conditions must be known and used as input into the code. Thus, for the code simulation to be possible, experimental data for both boundary conditions and initial moisture levels must be available. Errors in these inputs will affect the simulator results.

c. Material Properties. To determine what influence an error in the relevant material properties might have on the computer code simulation, two different cases were run. In both cases, lack of precise experimental data made the chosen changes in material properties reasonable numbers to use.

In the caisson A experiment, the saturated permeability of the tuff was changed from 0.25 to 0.17×10^{-5} m/sec; other parameters remained the same in the simulation. The lower saturated permeability results in a pulse that moves slightly slower, with the differences between the two cases decreasing with time.

In the field experiment, the porosity (defined as the total saturation) was changed from 40% to 34.6% water content by volume, with other parameters remaining the same. After 20.2 days (Fig. 33), the simulation indicates that the pulse will have traveled farther for the lower porosity. At 10 months (Fig.34), in the case of 40% porosity, no change in soil moisture is noted below depths of 150 cm, whereas with 34.6% porosity, damping is not complete until 200 cm. Thus, the porosity has a large influence on pulse shape and on the depth at which the pulse is "damped".

Although no test cases were run on the computer, the formulation of the computer code would indicate that the matric potential used in the input also has a large influence on the results of the simulation.

The properties of the sand and gravel used in the experiments have not been measured. These properties, therefore, had to be estimated. Changes in the properties would make the behavior at the interfaces change. Because these interface regions could not be measured accurately for volumetric moisture, it is difficult to know how well the code simulation agreed with actual conditions at the interfaces.

III. CONCLUSIONS

A. Validation of TRACR3D Code

The close agreement between the code simulations and the experimental data indicates that the code is valid under the conditions tested. However, in using the code, several factors influencing the reliability of the simulations must be understood.

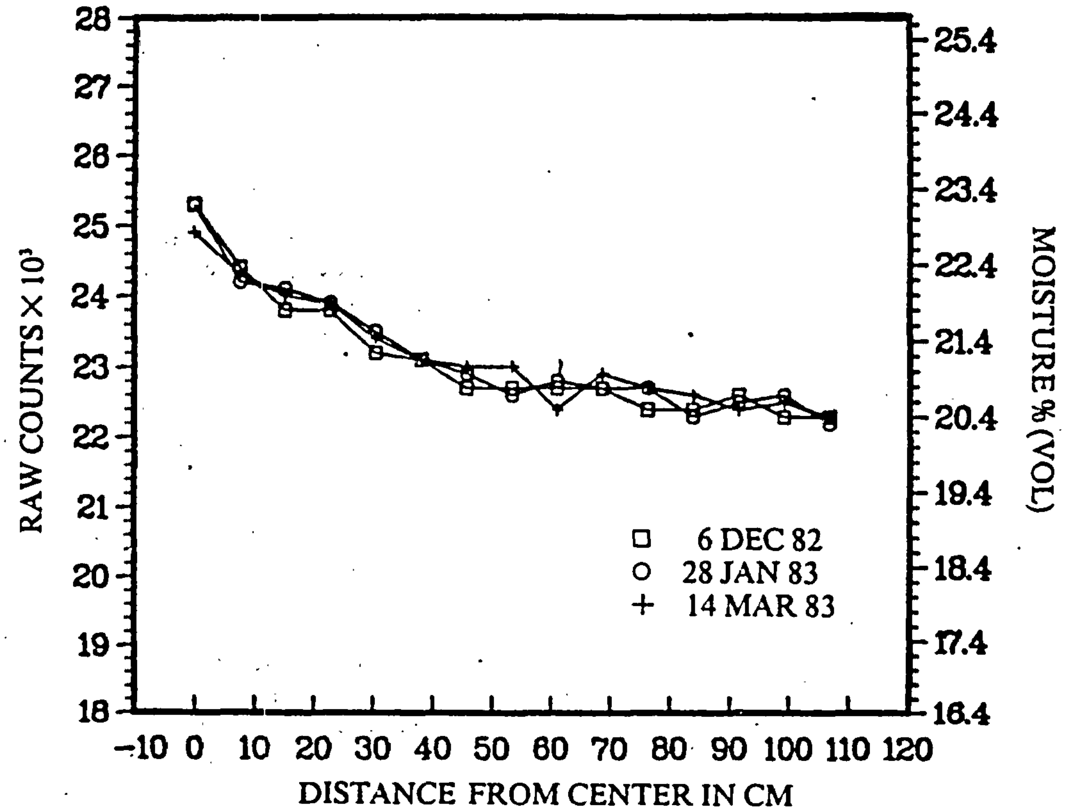

Fig. 30. Distribution of soil moisture in a horizontal traverse 350 cm below soil surface.

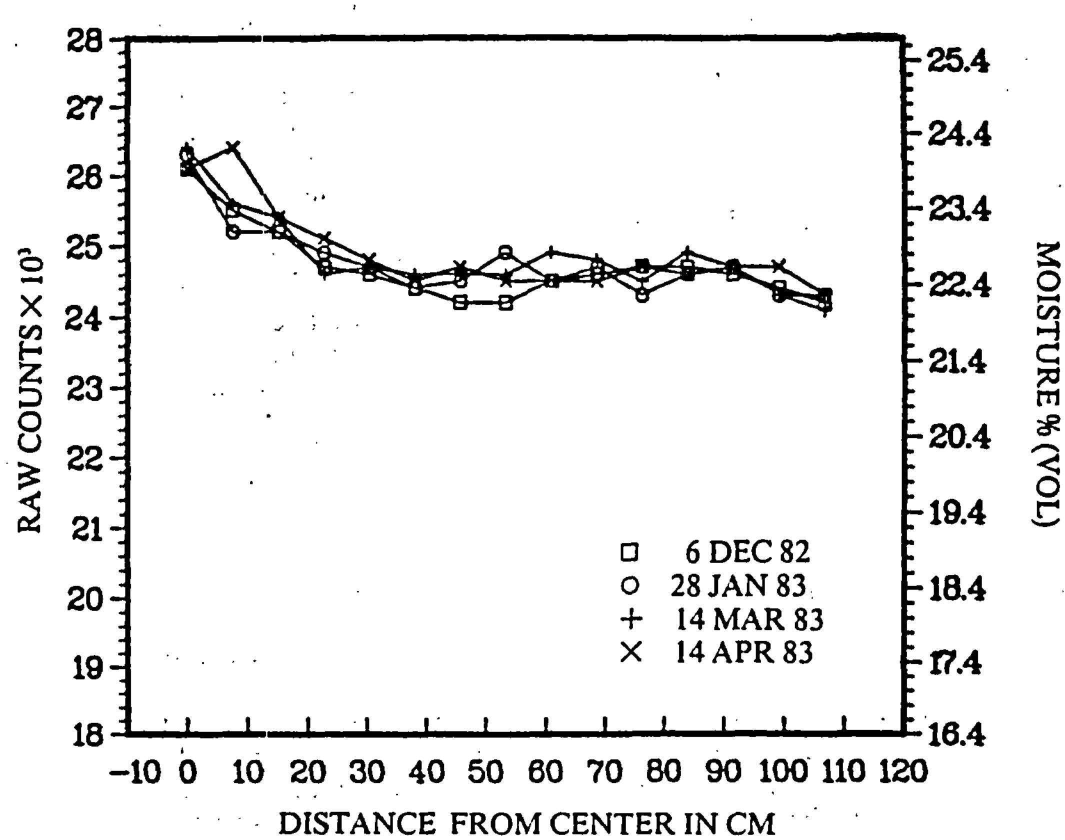

Fig. 31. Distribution of soil moisture in a horizontal traverse 426 cm below soil surface.

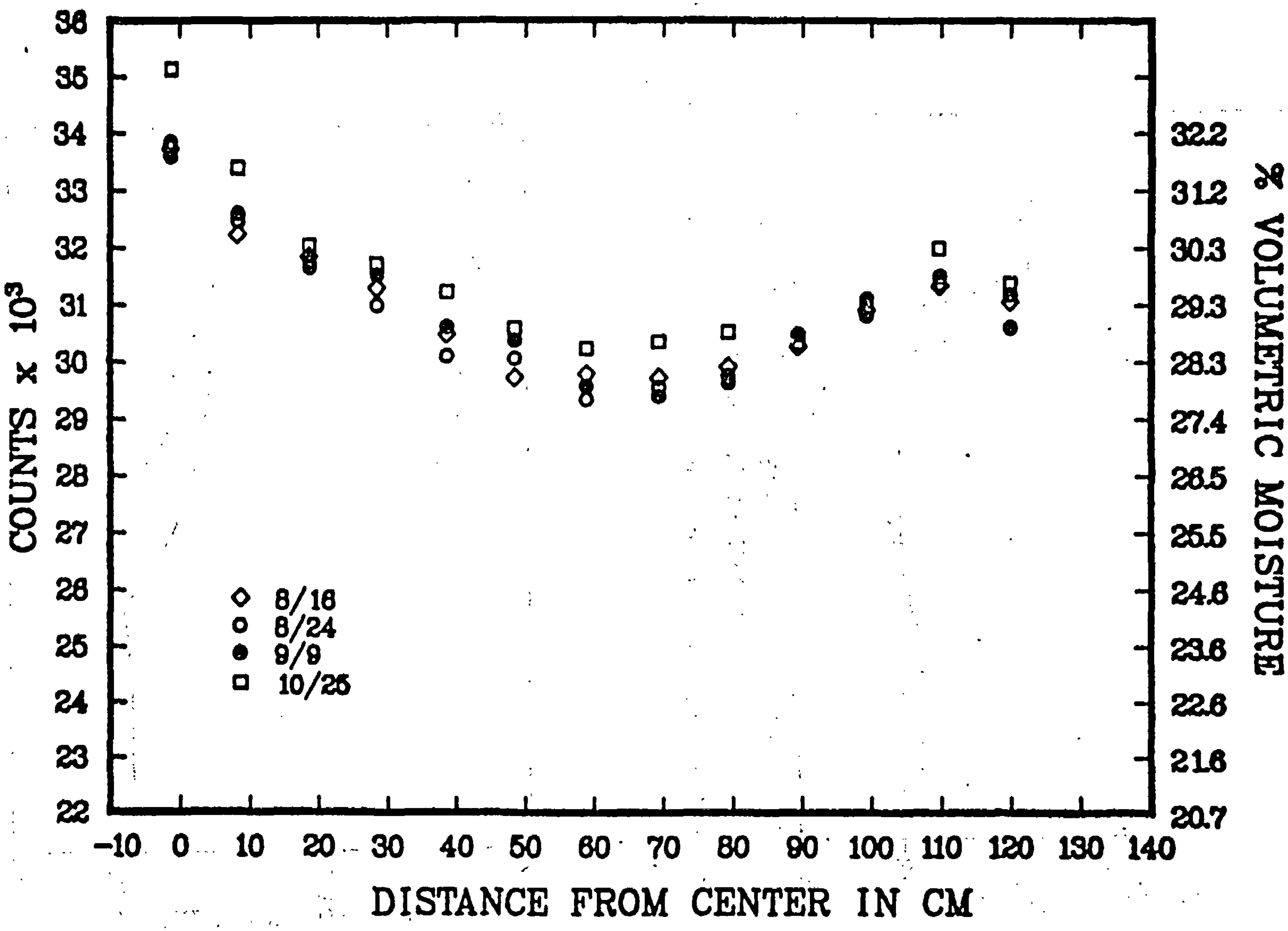

Fig. 32. Distribution of moisture, Caisson B, in a horizontal traverse 350 cm below surface.

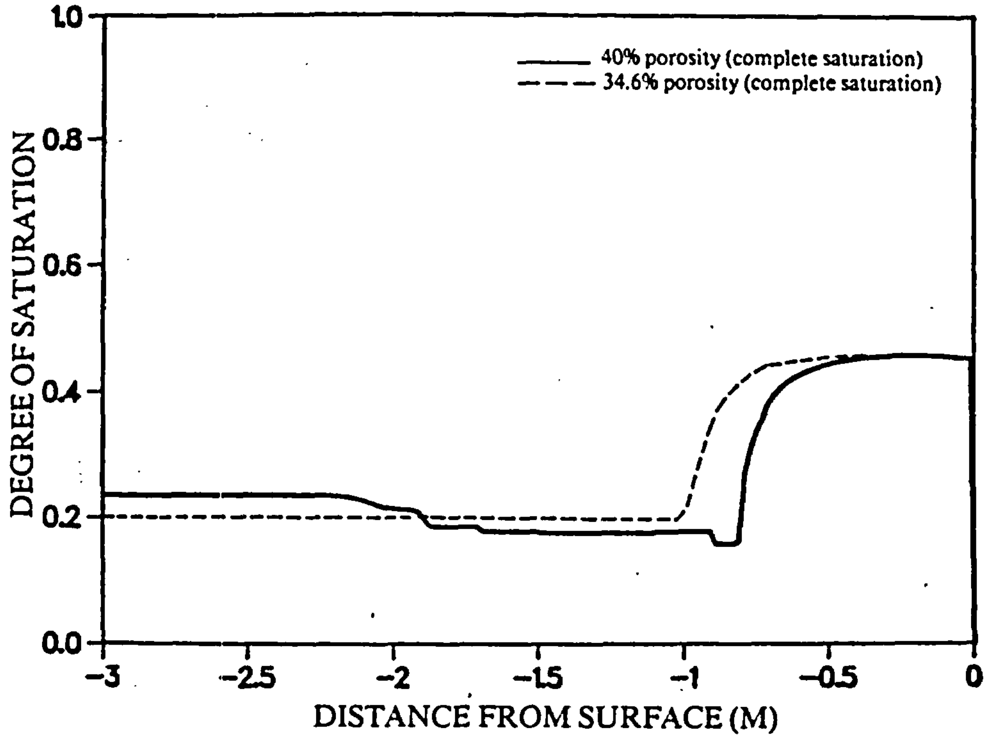

Fig. 33. Simulated degree of saturation at 20.2 days using two different input porosities.

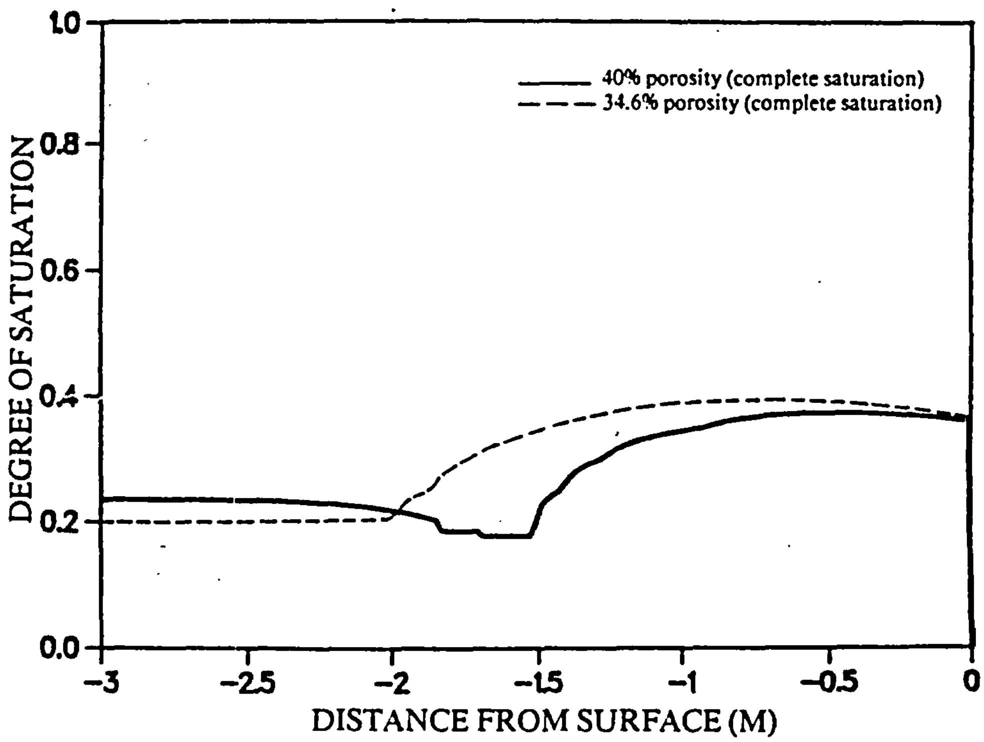

Fig. 34. Simulated degree of saturation at 10 months using two different input porosities.

1. Experimental Data Input

A simulation requires that boundary conditions, initial soil moisture, amount and duration of moisture input, and all relevant material properties throughout the system be supplied as data input. It would appear that porosity and matric potential are especially important.

2. Soil Inhomogeneities

Porous media are generally nonuniform in their properties on almost any scale. A soil's permeability and porosity usually are spatially distributed in a quasi random or stochastic manner. Most flow and transport models use only average property values for a soil region. If the standard deviation in the distribution of a material property is large, simulations using only average values could be seriously in error in some parts of the region. Monte Carlo calculations can be performed to give more accurate results, but this requires data on how soil properties are distributed.

B. Field Monitoring

1. Detecting Water Movement

In monitoring waste burial sites located in unsaturated zones, one of the parameters monitored can be the change in volumetric soil water content with time. If changes are detected, mass flow of soil water is occurring.

The pulse experiments, both in caisson A and in the field, indicated that there is a region below which changes in soil water content are "damped" and no changes in water content can be detected. Flux into the region is equal to flux out. The minimum depth below which there is little change is dependent on initial conditions, size of water pulse, and material properties of the soil.

As the caisson A experimental data indicate, water movement out of the bottom of the caisson occurred quickly after introduction of the pulse at the surface.

2. Nonuniform Mass Flow

The horizontal moisture measurements in caisson A and the vertical and hoizontal moisture measurements under constant inflow in caisson B indicate that inhomogeneities exist in the caisson crushed tuff or water inflow was not uniform or both.

Because waste burial pits must, by their very nature, be inhomogeneous at these sites, the differences in moisture changes from one region to another might be expected to be larger than in the caissons. Water content measurement in a burial site at one location may not represent conditions in a nearby location.

In addition, if neutron moisture probes are used, since these are integrating instruments, changes within small volumes in the region of influence of the neutron probe may also occur without being experimentally detectable as changes in soil water content.

Thus, under unsaturated flow, movement of soil water in an inhomogeneous matrix may be diffucult to detect. Unless the inhomogeneous material properties of the matrix are known, they are also difficult to simulate in computer codes.

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