# High-Resolution Modeling of Strip Source Infiltration: Three-Dimensional Synthetic Experiment Analogous to Las Cruces Trench Experiment

by

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## ABSTRACT

A high-resolution, three-dimensional finite difference model based on a mixed variable formulation of partially saturated or unsaturated flow is used to model strip source infiltration and natural drainage in a randomly heterogeneous and imperfectly stratified soil. The flow regime, soil properties, and boundary conditions are analogous to those of the first Las Cruces strip source experiment, albeit with some differences. The nonlinear behavior and statistical properties of the unsaturated soil are inferred, in part, from preliminary hydrodynamic data collected at the trench site. A 15 m x 15 m x 5 m computational domain is discretized into 300,000 finite difference cells or grid points. The parameters of the unsaturated conductivity curve are assumed to be single realizations of spatially correlated random fields. Each finite difference cell possesses its own, distinct conductivity function. The detailed simulation captures the complex three-dimensional heterogeneity of the transient moisture plume, and provides direct evidence of horizontal spreading and moisture-dependent anisotropy due to imperfect, spatially variable stratification.

## 1.0 INTRODUCTION

### 1.1 Modeling Group Identification

The numerical model and simulation results described here were previously generated and partially analyzed by the M.I.T. group [Ababou 1988; Ababou and Gelhar 1988]. The Center for Nuclear Waste Regulatory Analyses is currently exploiting these results and developing new simulations toward model validation [Ababou, 1990].

### 1.2 Purpose and Overview

The simulations to be described below were developed with two distinct objectives in mind. The first objective was to test the linearized analytical theory of stochastic flow [Mantoglou and Gelhar, 1987 a,b,c], and particularly the moisture-dependent anisotropy of effective flow behavior, under more realistic conditions of nonlinearity, randomness, and flow geometry than allowed for in theory. The second objective was, given the constraints of the first theoretical objective, to mimic as closely as possible the conditions of the first Las Cruces strip-source experiment.

## 2.0 NUMERICAL EXPERIMENT SET-UP

### 2.1 Input Data

The problem set-up, described below, involves a strip-source geometry and discharge rate similar to those of the first Las Cruces strip-source experiment. However, the initial soil moisture ($\theta = 0.15$, or $\Psi = 150$ cm) used in the model was higher than that observed at the field site in order to avoid an excessive conductivity contrast near the wetting front. Note that relatively low rate infiltration in moderately dry soil can produce large conductivity contrasts, owing to the very sharp decrease of conductivity with increasing suction for the exponential conductivity model adopted here.

One of the main reasons for selecting the exponential conductivity model was its convenience for developing analytical solutions of the stochastic flow equations [Mantoglou and Gelhar, a,b,c]. The exponential relationship is not adequate for modeling the very dry range of unsaturated flow. Recognizing this restriction, we studied the discrepancy between exponential and other conductivity models (Mualem-Van Genuchten) for the field site data. The discrepancy was found to be relatively minor in the suction range 50 cm $\le \Psi \le$ 150 cm. This is illustrated in *Figure 1* from Ababou [1988, Chap. 7, Fig. 7.10].

Besides being highly nonlinear, the two-parameter exponential conductivity curve $K(h,\underline{x}) = Ksat(\underline{x}) \exp(\alpha(\underline{x})h)$ was highly variable in space as well. The parameters $Ksat(\underline{x})$ and $\alpha(\underline{x})$ were assumed to be spatially correlated replicates of two log-normally distributed, independent random fields. Furthermore, the three-dimensional correlation structure was taken to be anisotropic, with a vertical-to-horizontal anisotropy ratio of 1/4 in terms of the directional correlation scales.

A summary of input data is given in *Table 1*, from Ababou [1988, Chap. 7, Table 7.2]. Note that the coefficients of variation of Ksat and $\alpha$ are 67% and 22%, respectively. Single-point and two-point statistics were inferred more or less directly from in-situ field observations such as those reported in Wierenga et al.[1989]. During infiltration, the top boundary condition was a fixed flux of 2 cm/day imposed on the 4 m wide strip source, and zero flux elsewhere. The lateral boundary conditions were zero flux. The bottom boundary condition was gravity drainage (zero pressure gradient). The gravity drainage condition was quite successful in allowing moisture plumes to migrate downward, through the bottom boundary, with minimal disturbance. For more details on problem set-up, see Ababou [1988, Section 7.3.1]. For random field generation by the Turning Band method, see also Tompson et al. [1989].

### 2.2 Simulation and Output Data

The numerical code "BIGFLO", previously developed at MIT [Ababou, 1988], was used to generate the results discussed here. The BIGFLO code is a fully three-dimensional finite difference simulator for saturated or partially saturated flow in highly heterogeneous porous media. The algorithms are described in detail in Ababou [1988, Chap. 5]. Summaries of solution algorithms and model problems can be found in Ababou and Gelhar [1988] for the case of unsaturated flow, and Ababou et al. [1989] for the case of saturated flow.

The strip source simulation comprised two phases, an infiltration phase ($q=2$ cm/day) and a natural drainage phase ($q=0$). Given the depth of the computational domain (5 m) and the particular choice of initial conditions discussed earlier, infiltration was turned off after a relatively short time (10 days) and natural drainage was simulated for 10 more days. The simulation outputs were expressed mainly in terms of three-dimensional pressure fields. Output times of interest here are $t=5$ days and $t=10$ days (infiltration phase), and $t=15$ days (drainage phase).

A preliminary visualization of the results was obtained by contouring the pressure fields along selected slices [Ababou, 1988, Chap. 7.3]. More recently, the fully three-dimensional pressure fields have been visualized using 3D color graphics techniques such as perspective views of solid, color-coded iso-surfaces in 3D space [Ababou, 1990]. Each frame represents a snapshot of the moisture plume at a fixed, pre-selected output time.

## 3.0 ANALYSIS OF SIMULATION RESULTS

Some of the heterogeneous suctions obtained for three vertical slices are shown in *Figure 2* ($t=5$days), *Figure 3* ($t=10$ days), and *Figure* 4 ($t=15$ days). We recall from the previous section that the infiltration phase ended at $t=10$ days. Also, note that the heterogeneous moisture content distribution follows the same pattern as pressure, due to the fact that a single one-to-one relation $\theta=\theta(\Psi)$ was assumed, regardless of spatial location.

The detailed moisture patterns at any time differ considerably from section to section, reflecting the three-dimensional nature of the local flow process. If the soil was uniformly layered, rather than randomly stratified as here, the moisture patterns in any vertical cross-section would be nearly the same everywhere except near the free edge of the finite length strip source.

It is interesting to analyze the vertical versus horizontal extent of the moisture movement as seen in these figures. Let us define the moisture plume by $\theta \geq \theta_F$, where $\theta_F$ is a relatively dry moisture content, e.g. close to the initial value. The contours shown in *Figures* 2, 3, 4 reveal significant lateral spread of the moisture plume. A number of localized wet lenses appear to be hanging over drier regions, reflecting the statistical anisotropy, or imperfect stratification, of the synthetic soil. This feature can be observed near the geometric center of the $x_2=9.8$ m cross-section (around depth $x_1=2.5$m and abscissa $x_3=0$). Another, more subtle phenomenon is the relatively larger spread of the relatively dry margins of the moisture plume (light gray tones), compared to the wet core of the plume (dark gray tones). This behavior is consistent with the moisture-dependent anisotropy predicted by Mantoglou and Gelhar [1987 a,b,c].

The above-mentioned features appear more clearly in full three-dimensional representation. The attached black-and-white reproductions of color plates, *Figure 5* and *Figure 6*, show three-dimensional views of the moisture plume after 10 days of infiltration. The amount of detail in this simulation helps capture the heterogeneity of the moisture pattern over a wide range of scale. The horizontal spread due to random stratification is clearly far from uniform. Layers have "holes". Horizontal "fingers" and wet lenses tend to remain suspended over dryer lenses of soil.

These results are encouraging, and suggest the feasibility of similar simulations under conditions more closely related to the Las Cruces Trench experiment. This may involve, for instance, using both probabilistic and site-specific deterministic input data, combined through stochastic conditioning techniques (work in progress).

## 4.0 REFERENCES

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ATTACHMENT: Tables, Figures, and Color Plates

# TABLE 1

**SUMMARY OF INPUT DATA FOR THE SINGLE-REALIZATION SIMULATION OF STRIP-SOURCE INFILTRATION IN A STATISTICALLY ANISOTROPIC SOIL ("TRENCH EXPERIMENT")**

| Type of Data | Description | Value |
|---|---|---|
| Domain Geometry, Boundary Conditions, and Initial Conditions | Vertical domain size | $L_1$ = 5.0 m |
| | Transverse horizontal domain size | $L_2$ =15.0 m |
| | Transverse longitudinal domain size | $L_3$ =15.0 m |
| | Strip source width | $W_s$ = 4.0 m |
| | Strip source length | $L_s$ = 9.9 m |
| | Flux at the surface of the strip | $q_o \equiv$ 2 cm/day |
| | Condition at the bottom boundary | $q_1$ = - K(h) |
| | Initial pressure head | $h_{in}$ = - 150 cm |
| Space-Time Discretization | Time step | Variable |
| | Mesh size $\Delta x_i$ (i=1,2,3) | $\Delta x_i$= 0.10,0.20,0.20 m |
| | Unidirectional number of nodes $n_i$ | $n_i$= 52, 76, 76 |
| | Total number of nodes of 3D grid | N = 300352 |
| Exponential Conductivity Curve (Random) | Geometric mean saturated conductivity | $K_G$ = 100 cm/d |
| | Standard deviation of $\ell n\ K_s$ | $\sigma_f$ = 0.6083 |
| | Geometric mean of the $\ell n$ K-slope | $\alpha_G$ = 0.0494 $cm^{-1}$ |
| | Standard deviation of $\ell n\ \alpha$ | $\sigma_a$ = 0.2202 |
| | Anisotropic correlation scales $\lambda_i$ | $\lambda_i$ = 0.25,1.0,1.0 m |
| Van-Genuchten Retention Curve (Deterministic) | Saturated moisture content | $\theta_s$ = 0.368 |
| | Residual moisture content | $\theta_r$ = 0.102 |
| | Scaling parameter | $\beta$ = 0.0334 $cm^{-1}$ |
| | Shape factor (real number) | n = 1.982 |

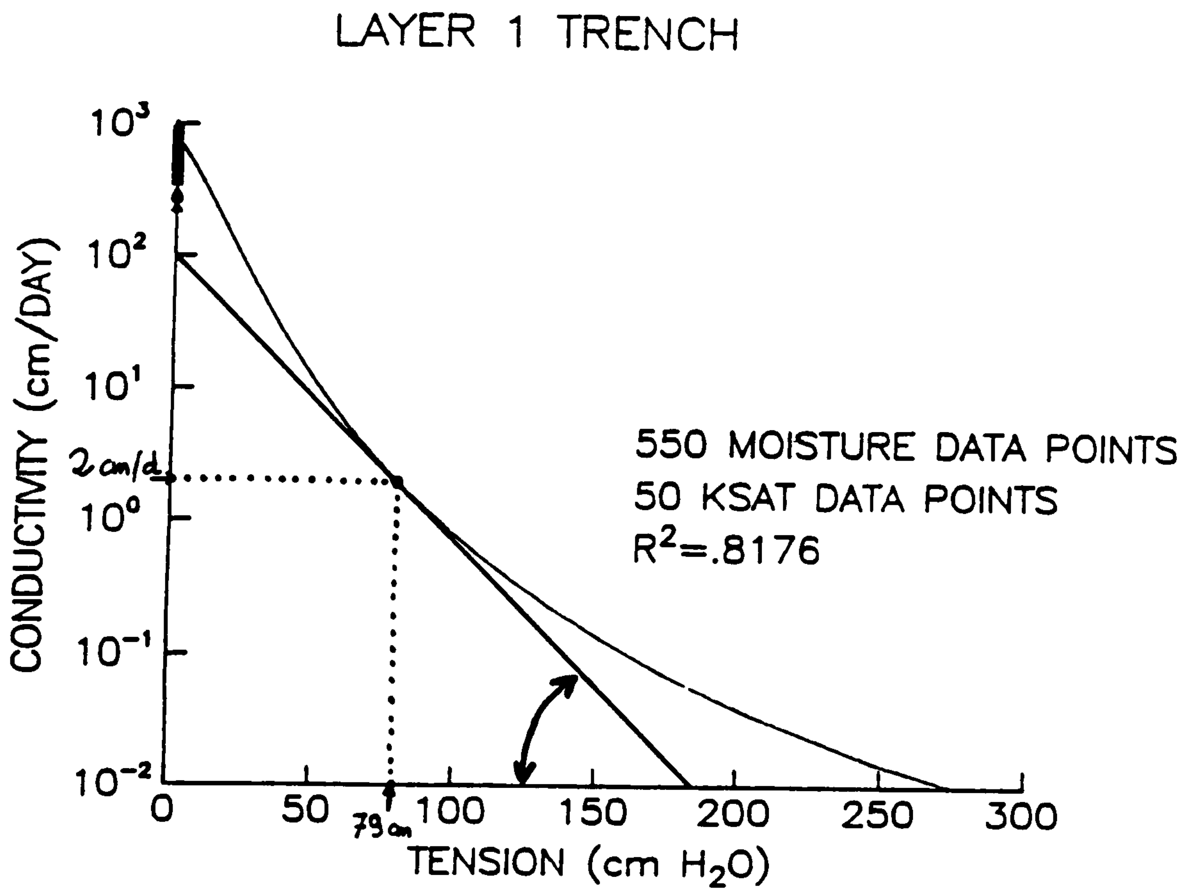


Figure 1. Mean unsaturated conductivity curve K(h) for the soil of the strip-source "trench experiment": the straight line corresponds to the exponential model actually used in the numerical simulation; the other curve is the Mualem-Van Genuchten model indirectly fitted to field data by Wierenga et. al., 1986.

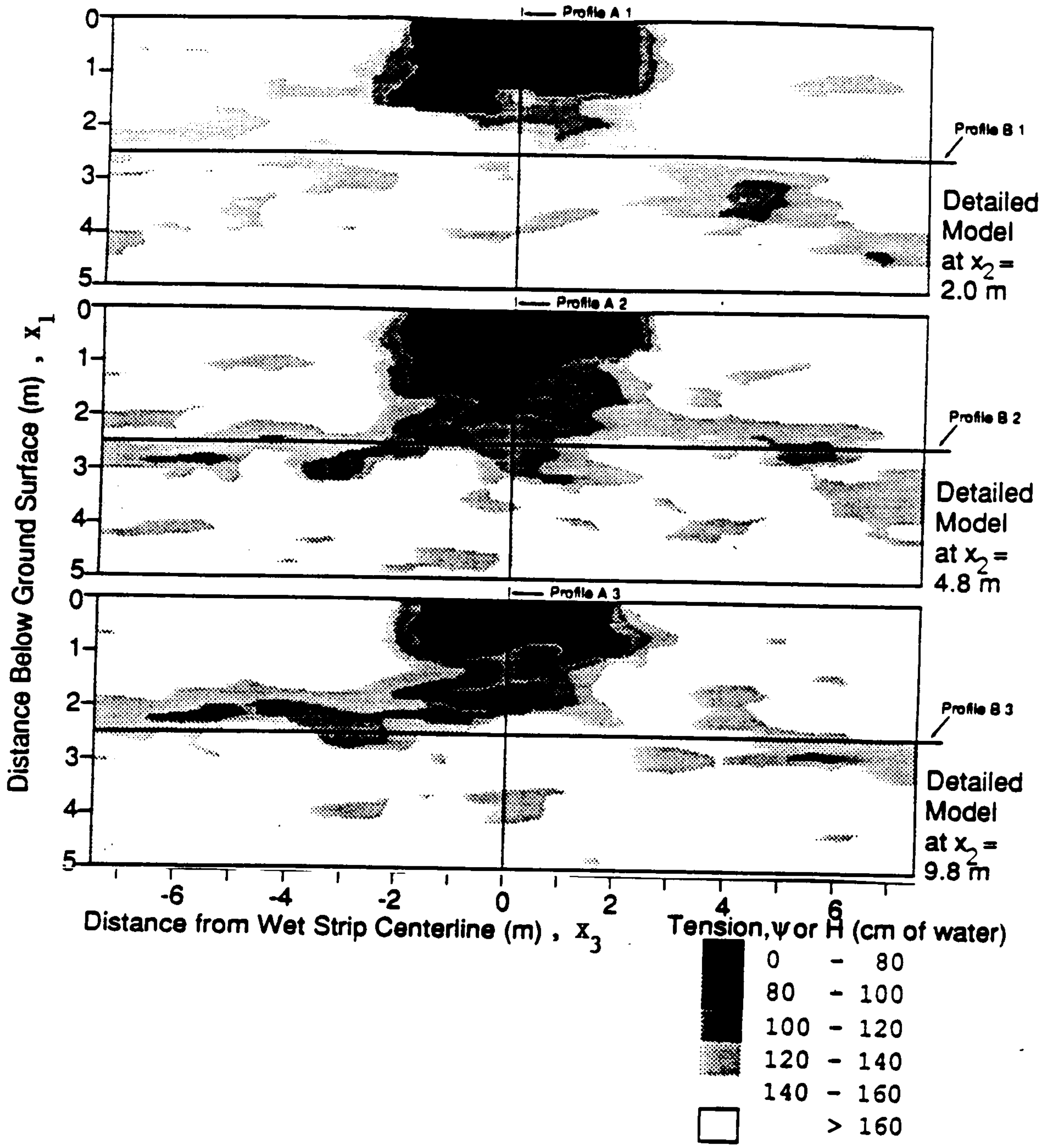


Figure 2. Infiltration (t=5 days)

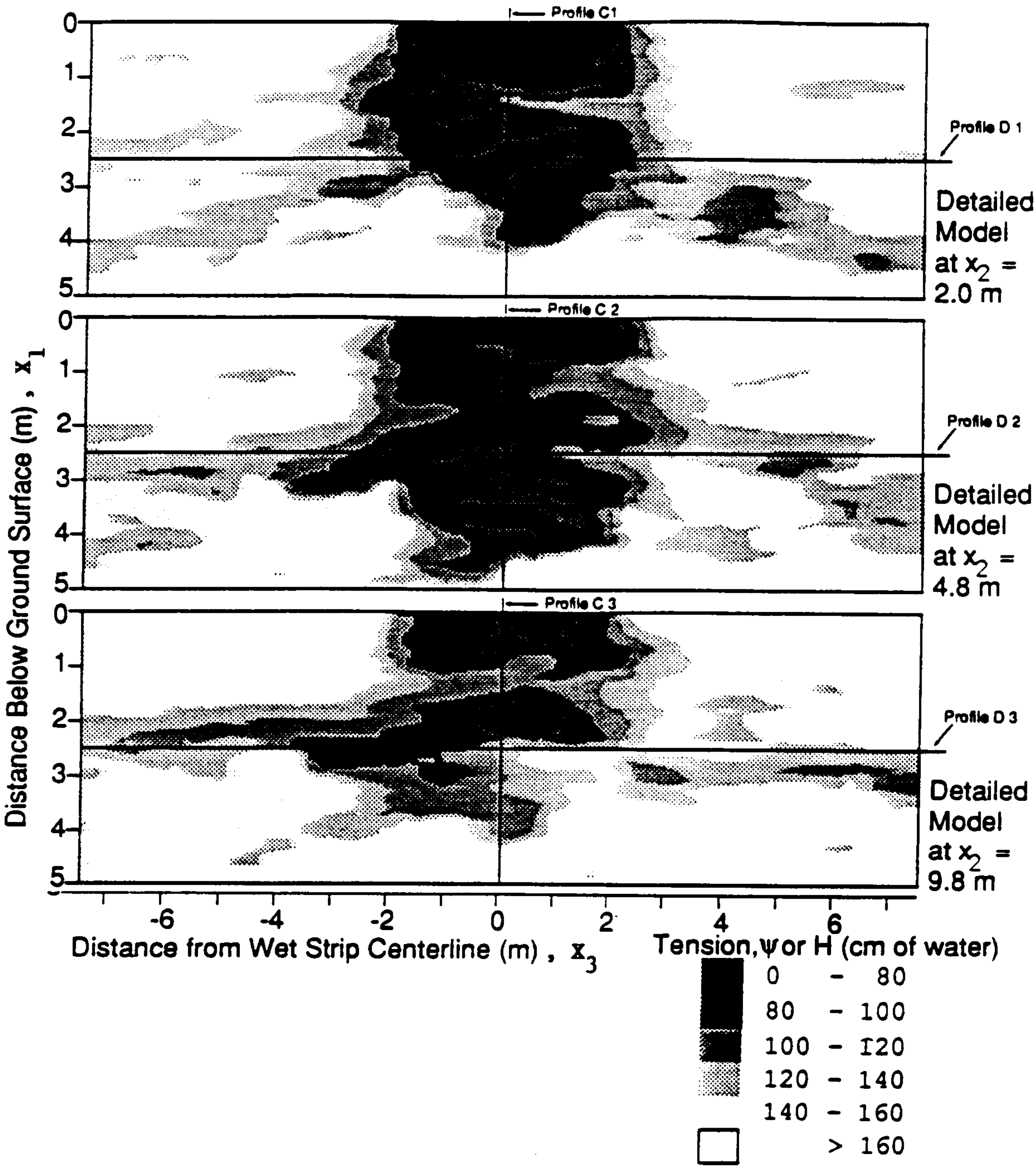


Figure 3. Infiltration (t=10 days)

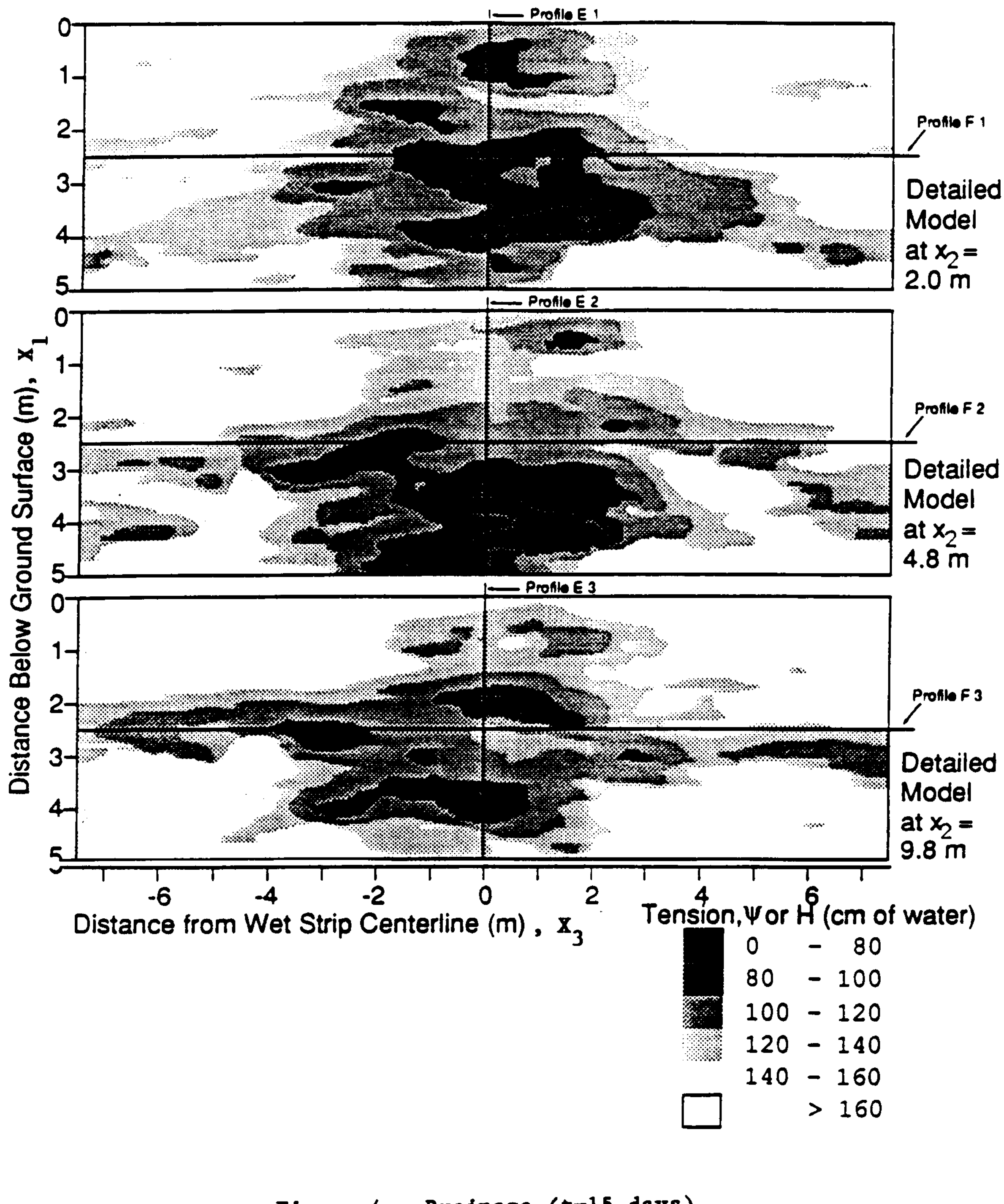


Figure 4. Drainage (t=15 days)

Figure 5. Front View of Three-Dimensional Moisture Plume, from Stochastic Flow Simulations of Ababou (1988).

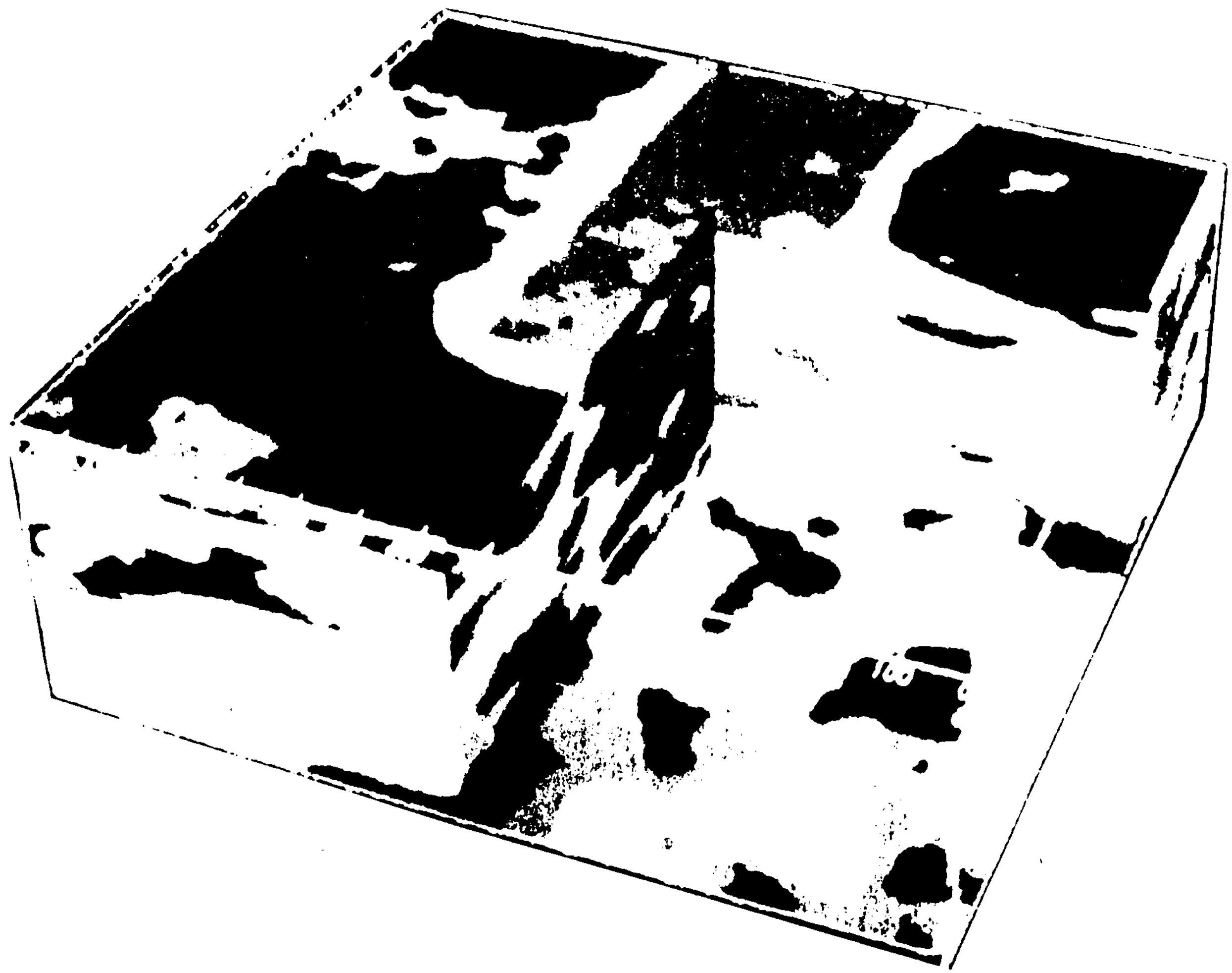

Figure 6. Back View of Three-Dimensional Moisture Pattern, with Moisture Plume Visible in Purple and Blue (Simulations from Ababou, 1988).

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The nonlinear behavior and statistical properties of the unsaturated soil were inferred, in part, from preliminary hydrodynamic data collected at the trench site. A 15 m x 15 m x 5 m computational domain was discretized into 300,000 finite difference cells or grid points. The parameters of the unsaturated conductivity curve are assumed to be single realization of spatially correlated random fields. Each finite is different, all possess its own, distinct conductivity function. The detailed simulation captures the complex three-dimensional heterogeneity of the transient moisture plume, and provides direct evidence of moisture-dependent anisotropy and horizontal spreading due to imperfect, spatially variable stratification.

## 1.0 INTRODUCTION

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# 2.0 NUMERICAL EXPERIMENT SET-UP

## 2.1 Input Data

The final problem set-up, described below, involves a strip-source geometry and discharge rate similar to those of the first Las Cruces strip-source experiment. However, the initial soil moisture ($\theta \approx 0.15$, or $\Psi \approx 150$ cm) used in the model was ~~taken~~ higher than that observed at the field site in order to avoid an excessive conductivity contrast near the wetting front. Even low rate infiltration in moderately dry soil yields large conductivity contrasts, owing to the very sharp decrease of conductivity with increasing suction for the exponential conductivity model adopted here.

One of the main reasons for selecting the exponential conductivity model was its convenience for analytical solutions of the stochastic flow equations [Mantoglou and Gelhar, a,b,c]. That model is not adequate for modeling the very dry range of unsaturated flow. This restriction was taken into account by studying the discrepancy between exponential and other conductivity models (Mualem-Van Genuchten) for the field site data. That discrepancy was found to be relatively minor in the suction range 50 cm $\le \Psi \le$ 150 cm. This is illustrated by *Figure 1* from Ababou [1988, Chap. 7, Fig. 7.10].

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A summary of input data is given in *Table 1*, from Ababou [1988, Chap. 7, Table 7.2]. Spatial statistics were inferred more or less directly from in-situ field observations such as those reported in Wierenga et al.[1989]. During infiltration, the top boundary condition was a fixed flux of 2 cm/day on the 4 m wide strip source, and zero flux elsewhere. The lateral boundary conditions were zero flux, and the bottom boundary condition was a gravity drainage (zero pressure gradient) condition. The latter assumption was quite successful in allowing moisture plumes to migrate downward, through the bottom boundary, with minimal disturbance. For more details on problem set-up, see Ababou [1988, Section 7.3.1]. For random field generation, see Tompson et al. [1989].

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The simulation comprised two phases, an infiltration phase (q=2 cm/day) and a natural drainage phase (q=0). Given the depth of the computational domain (Z=5 m) and the particular choice of initial condition discussed earlier, infiltration was turned off after a relatively short time (10 days) in order to observe natural drainage as well (10 more days). The simulation results were examined mainly in terms of three-dimensional pressure fields. Output times of interest here are t=5 and 10 days (infiltration phase).

Preliminary visualization of the results was done by containing the pressure fields along selected slices [Ababou, 1988, Chap. 7.3]. More recently, the fully three-dimensional pressure field on moisture plume have been visualized using 3D color graphics techniques such as color-coded solid iso-surfaces in 3D space [Ababou, 1990]. In both cases, each frame represents a snapshot at a fixed, pre-selected output time.

## 3.0 SIMULATION RESULTS

Some of the heterogeneous suctions (or moisture contents) obtained for three vertical slices are shown in Figure 2 (t=5days), Figure 3 (t=10 days), and Figure 4 (t=15 days). We recall from the previous section that the infiltration phase stopped at t=10 days.

The detailed moisture patterns at any time differs considerably from section to section, reflecting the three-dimensional nature of the local flow process. If the soil were uniformly layered, rather than randomly stratified as here, the moisture patterns in any vertical cross-section would be nearly the same (except near the edges of the finite length strip source).

It is interesting to analyze the vertical versus horizontal extent of the moisture movement as seen in these Figures. Define the moisture plume by $\theta \geq \theta_F$, where $\theta_F$ is a relatively dry moisture content close to the initial value. The contours shown in Figures 2, 3, 4 reveal significant lateral spread of the moisture plume. A number of localized wet lenses appear to be hanging over drier regions, reflecting the statistical anisotropy, or imperfect stratification, of the synthetic soil. This feature can be observed near the geometric center ($x_2$=0, $x_3$=2.5 m) of the $x_3$=9.8 m cross-section. Another, more subtle phenomenon is the relatively larger spread of the marginally wet parts of the moisture plume (light gray tones), compared to the wet core of the plume (dark gray tones). This behavior is consistent with the moisture-dependent anisotropy predicted by Mantoglan and Gelhar [1987 a,b,c,].

The above-mentioned features appear more clearly in full three-dimensional representation. The attached color plates, *Figure* 5 and *Figure* 6, show three-dimensional views of the moisture plume after 10 days of infiltration. The amount of detail in this simulation helps capture the heterogeneity of the moisture pattern over a wide range of scale. The horizontal spread due to random stratification is far from uniform. Layers have "holes" horizontal wet lenses and "tongues" tend to remain suspended over dryer lenses of soil.

These results are encouraging, and suggest the feasibility of developing similar simulations under conditions more closely related to that of the Las Cruces Trench experiment, including for instance both stochastic and deterministic input data via conditioning techniques.

## 4.0 REFERENCES


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| | Transverse longitudinal domain size | $L_3$ = 15.0 m |
| | Strip source width | $W_s$ = 4.0 m |
| | Strip source length | $L_s$ = 9.9 m |
| | Flux at the surface of the strip | $q_0$ = 2 cm/day |
| | Condition at the bottom boundary | $q_1 = -K(h)$ |
| | Initial pressure head | $h_{in}$ = − 150 cm |
| Space-Time Discretization | Time step | Variable |
| | Mesh size $\Delta x_i$ (i=1,2,3) | $\Delta x_i$ = 0.10,0.20,0.20 m |
| | Unidirectional number of nodes $n_i$ | $n_i$ = 52, 76, 76 |
| | Total number of nodes of 3D grid | N = 300352 |
| Exponential Conductivity Curve (Random) | Geometric mean saturated conductivity | $K_G$ = 100 cm/d |
| | Standard deviation of $\ell n\ K_s$ | $\sigma_f$ = 0.6083 |
| | Geometric mean of the $\ell n$ K-slope | $\alpha_G$ = 0.0494 $cm^{-1}$ |
| | Standard deviation of $\ell n\ \alpha$ | $\sigma_a$ = 0.2202 |
| | Anisotropic correlation scales $\lambda_i$ | $\lambda_i$ = 0.25,1.0,1.0 m |
| Van-Genuchten Retention Curve (Deterministic) | Saturated moisture content | $\theta_s$ = 0.368 |
| | Residual moisture content | $\theta_r$ = 0.102 |
| | Scaling parameter | $\beta$ = 0.0334 $cm^{-1}$ |
| | Shape factor (real number) | n = 1.982 |

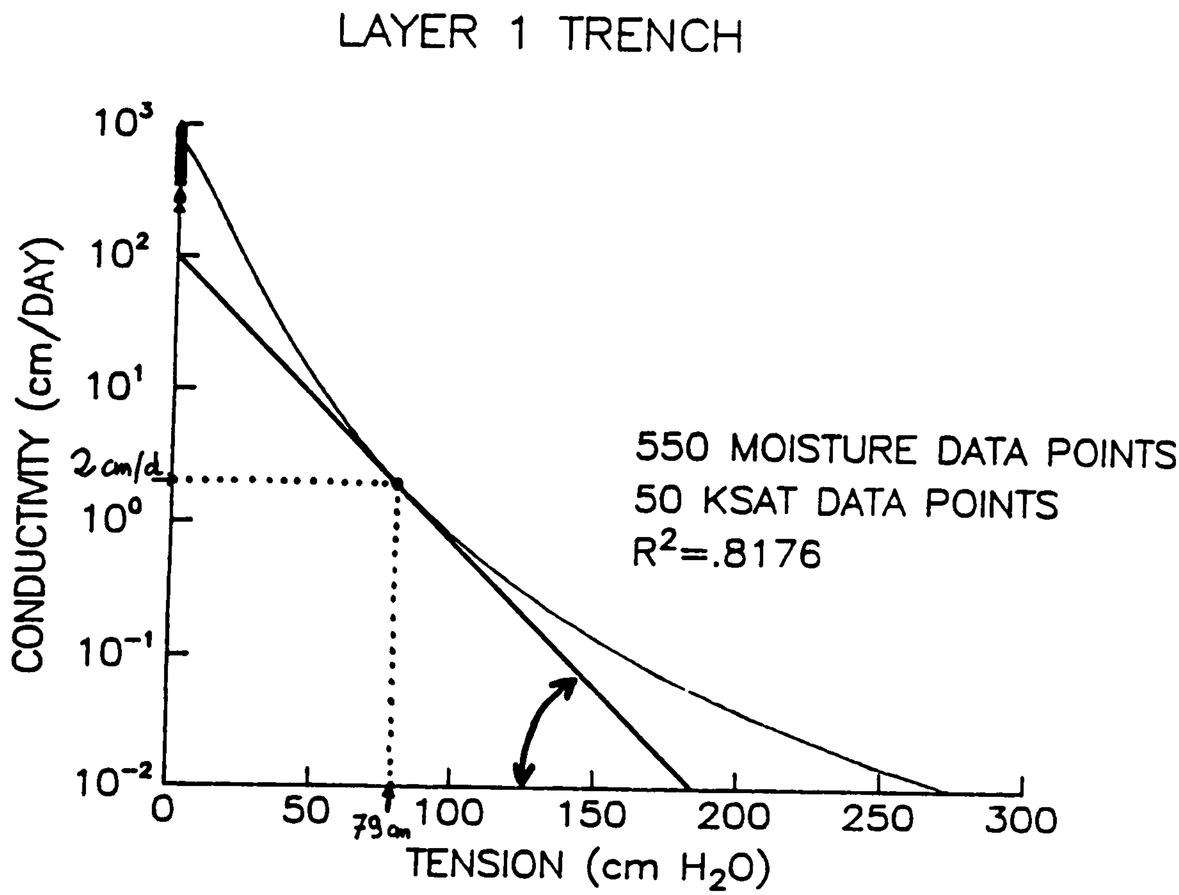


Figure 1. Mean unsaturated conductivity curve K(h) for the soil of the strip-source "trench experiment": the straight line corresponds to the exponential model actually used in the numerical simulation; the other curve is the Mualem-Van Genuchten model indirectly fitted to field data by Wierenga et. al., 1986.

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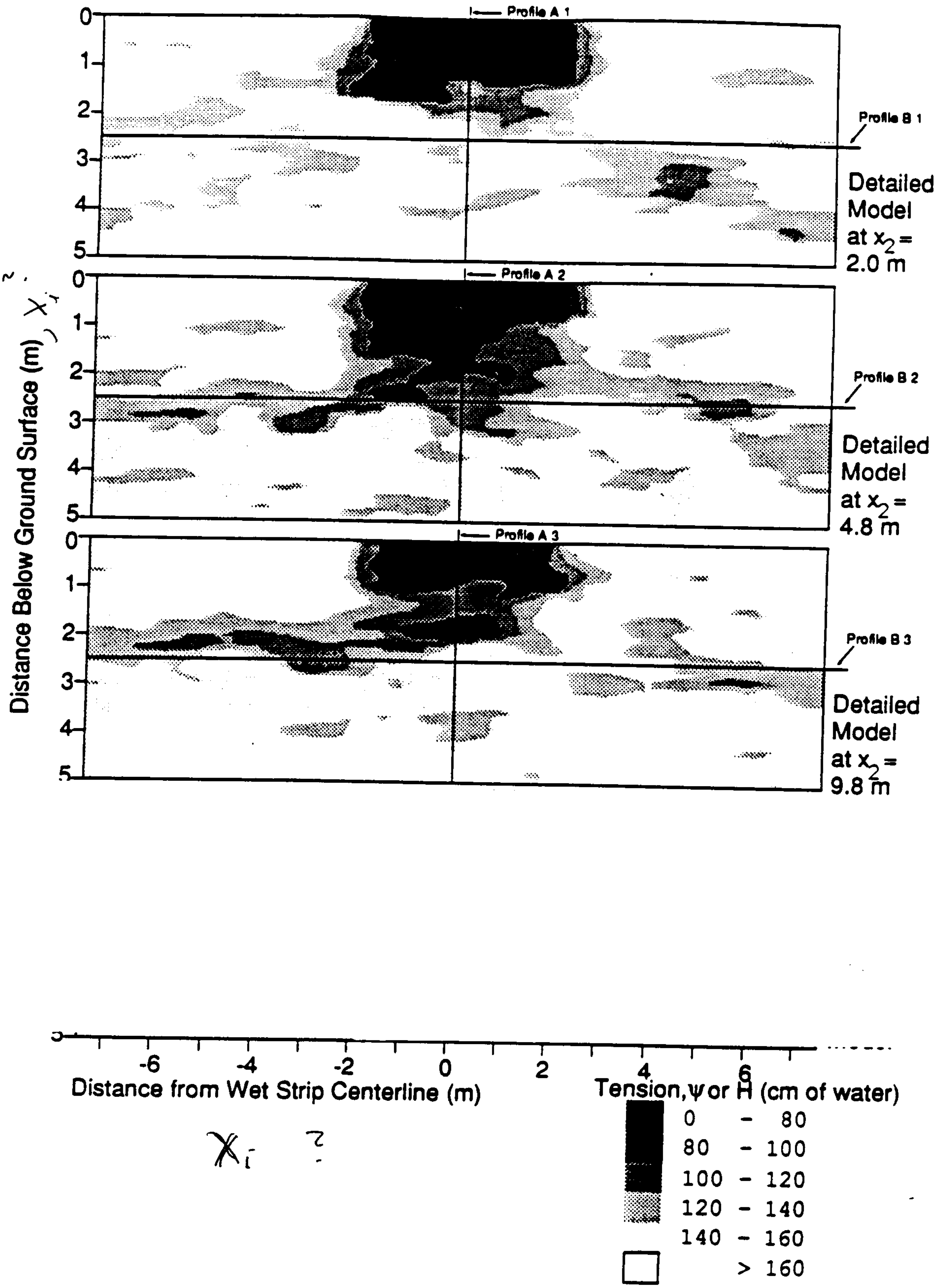
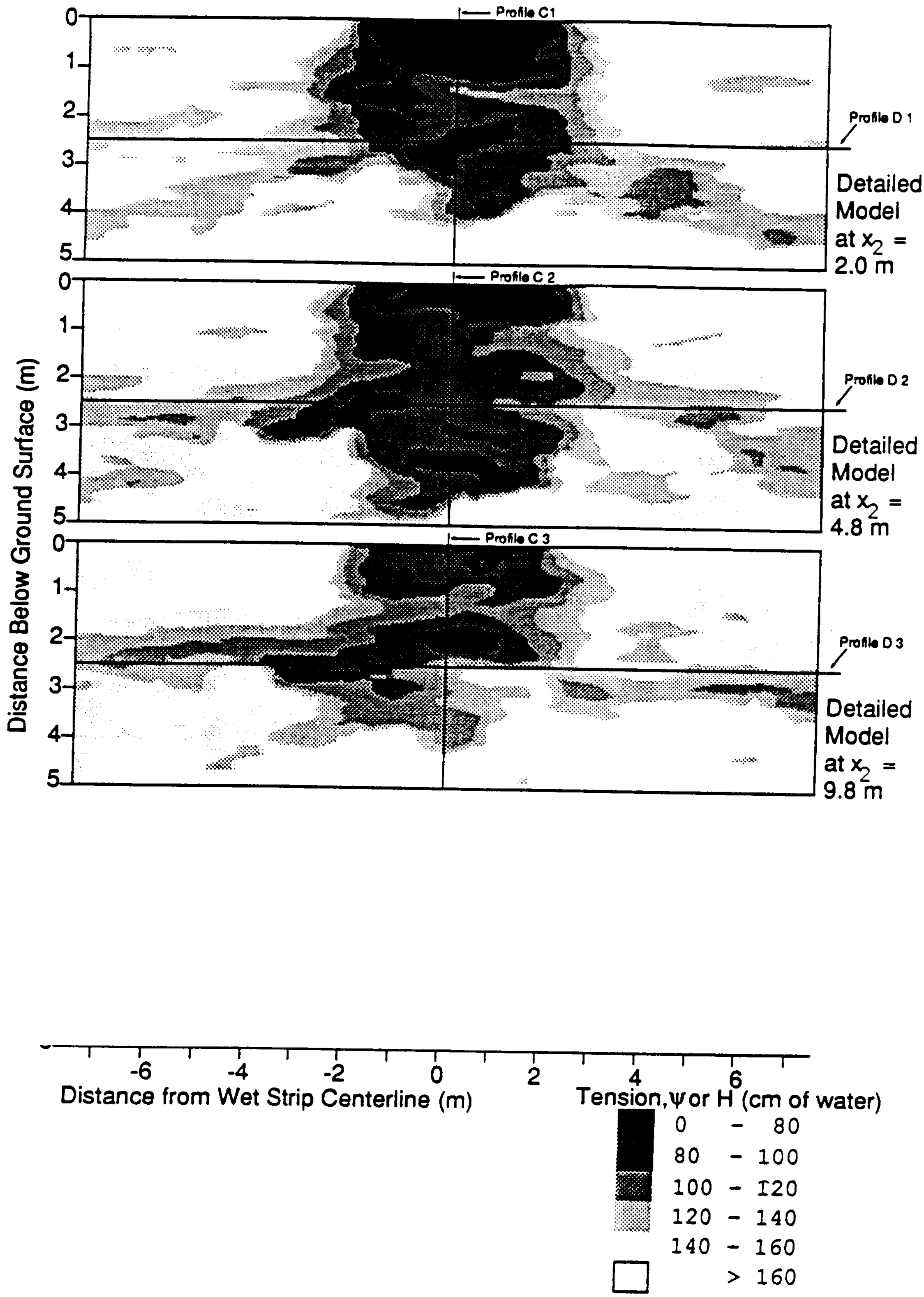


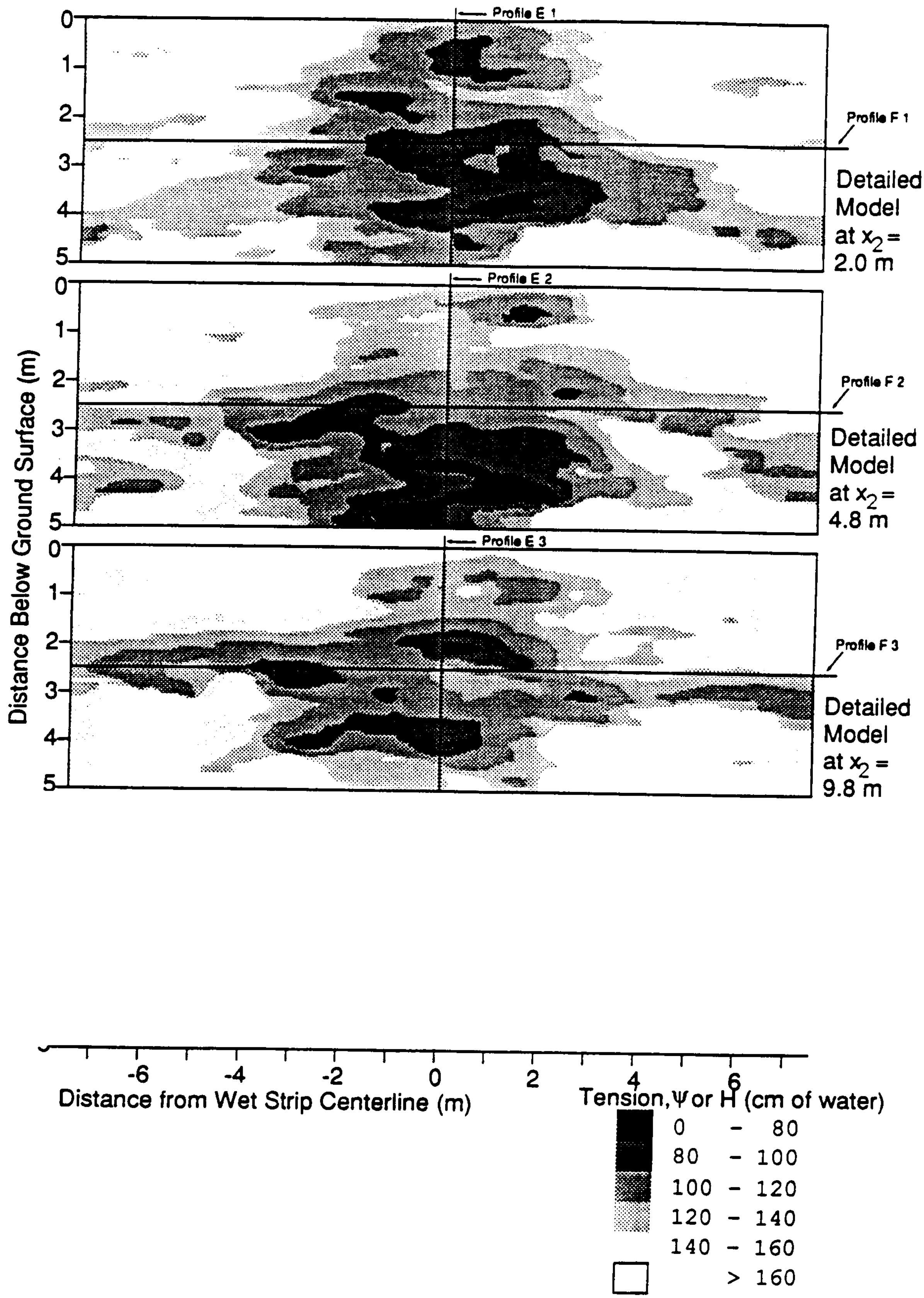

Figure 2.



Profile C1
Profile D 1
Detailed Model at $x_2$ = 2.0 m
Profile C 2
Profile D 2
Detailed Model at $x_2$ = 4.8 m
Profile C 3
Profile D 3
Detailed Model at $x_2$ = 9.8 m
Distance Below Ground Surface (m)
Distance from Wet Strip Centerline (m)
Tension, ψ or H (cm of water)
0 - 80
80 - 100
100 - 120
120 - 140
140 - 160
> 160


Figure 3.

5


Profile E 1
Profile F 1
Detailed Model at $x_2$ = 2.0 m
Profile E 2
Profile F 2
Detailed Model at $x_2$ = 4.8 m
Profile E 3
Profile F 3
Detailed Model at $x_2$ = 9.8 m
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Distance from Wet Strip Centerline (m)
Tension, Ψ or H (cm of water)
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80 - 100
100 - 120
120 - 140
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> 160

Figure 4.

6

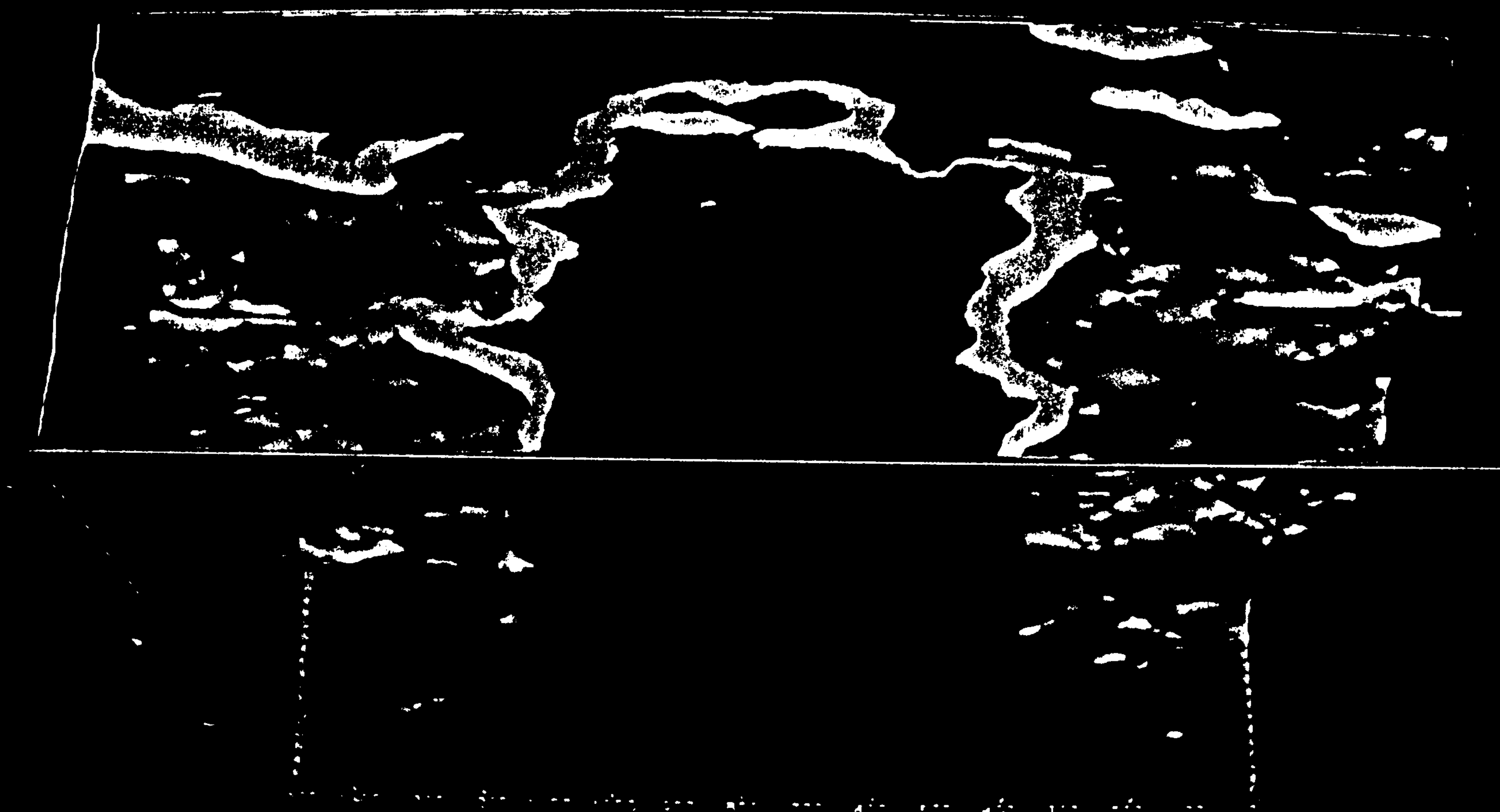

Figure 5. Front View of Three-Dimensional Moisture Plume, from Stochastic Flow Simulations of Ababou (1988).

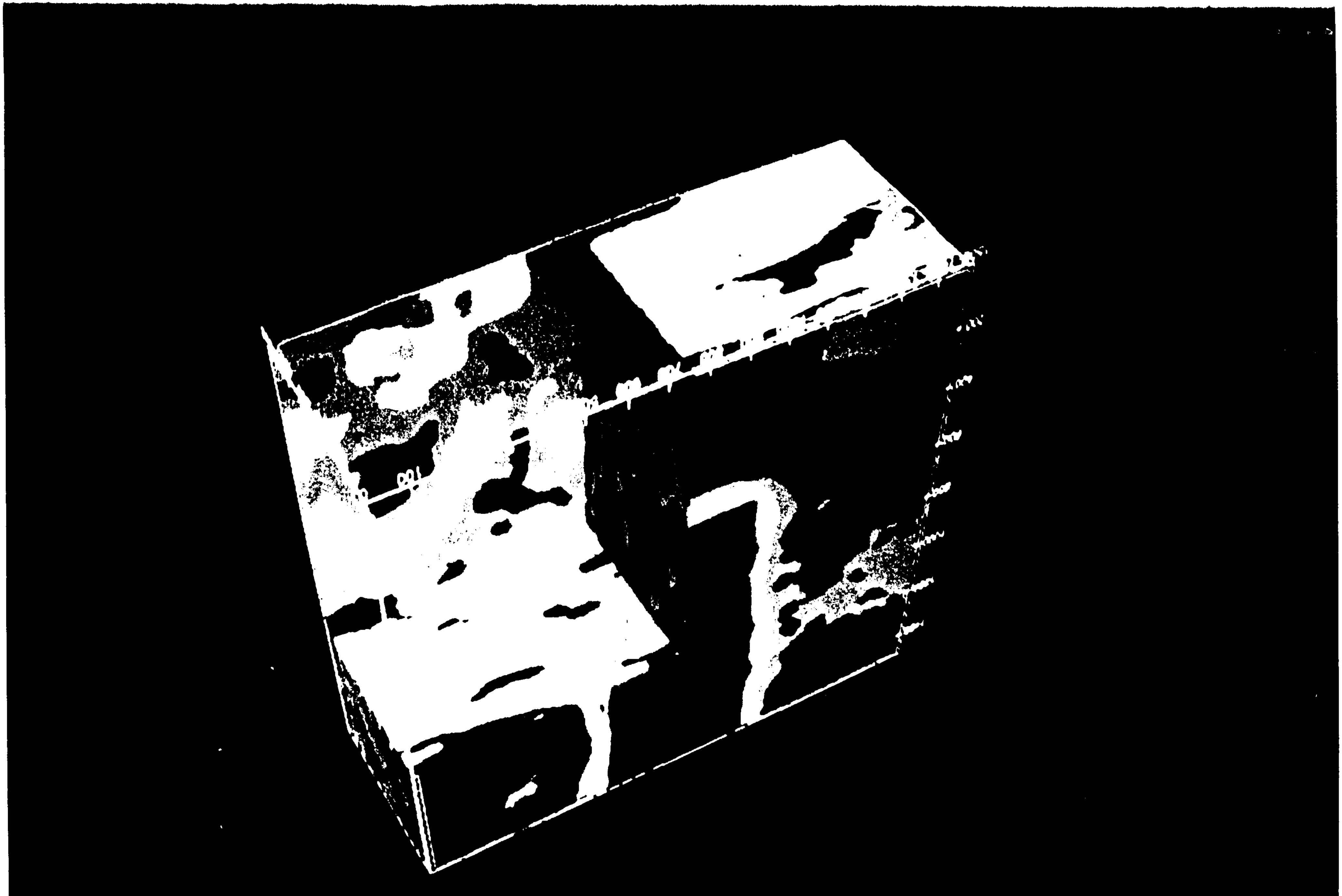

Figure 6. Back View of Three-Dimensional Moisture Pattern, with Moisture Plume Visible in Purple and Blue (Simulations from Ababou, 1988).