Kansas Geological Survey

Preliminary Evaluation of Unsaturated-Saturated Flow and Mass Transport Models: First NSF-EPSCoR Progress Report

by

M. Sophocleous and M. Bagheri

March 1994
Open-File Report 94-12
GEOHYDROLOGY

The University of Kansas, Lawrence, KS 66047 Tel. (913) 864-3965

Preliminary Evaluation of Unsaturated-Saturated Flow and Mass Transport Models: First NSF-EPSCoR Progress Report

M. Sophocleous and M. Bagheri
March 1994
KGS Open-File Report 94-12

Introduction

Nitrate is the most common contaminant of the subsurface, and nitrate contamination of ground water plagues many rural areas of the United States. The transition between the unsaturated and saturated soil zones may be a biologically active zone through which natural and anthropogenic chemicals must pass before entering the ground water. Factors that control nitrogen and carbon dynamics in such transitional systems are poorly understood. The objectives of this three-year project are to: (1) describe temporal and spatial variation in the physical, chemical, and biological aspects of pristine and agriculturally impacted subsurface ecosystems with special emphasis on the transitional zone between groundwater and soil; (2) observe the functional responses of microbes in this transitional zone to nitrogen and carbon availability and the relative flux rates of different forms of nitrogen; (3) delineate the biotic and abiotic controls of the microbial community in the transition zone.

The study will involved (1) characterization of the physical, chemical, and biological properties of the profile to the water table at two sites (one pristine, the other agricultural) on the Konza Prairie of Kansas; (2) microcosms to evaluate flux rates and microbial activity due to perturbations; (3) field manipulations to determine transport of N, C, and microorganisms from the surface; and (4) modeling of transport and transformations. The proposed research will foster development of a multi-disciplinary team to tackle a complex but extremely important problem to Kansas and the U.S. The basic understanding will generate expertise and resources for future research.

One of the objectives of this study is to compare and evaluate a number of well-known soil-water and solute transport models of varying complexity using the field and laboratory data collected from this study. Also, a sensitivity analysis of the various parameters involved in these models will be performed and their relative effect in NO_3^- breakthrough curves will be assessed. Other objectives of the modeling aspect are to better understand the transport mechanisms involved, to test the adequacy of existing theories, to establish a framework for the collection of data, and to provide a means for predicting, and thus controlling, the fate of agrichemicals in soils and aquifers.

Although we examined a number of available models, we evaluated and tested the following models, which we considered as most suitable for our project: SWMS_2D, UNSAT2, LEACHM, and HYDRUS. We also employed the RETC code for quantifying the hydraulic functions of unsaturated soils. A general overview of each one of these models follows.

SWMS_2D model

SWMS_2D is an acronym for Simulating Water Flow and Mass Transport in Two-Dimensional Variably Saturated Media, developed by Simunek, Vogel and van Genuchten (1992). The SWMS_2D computer program simulates water and solute movement in two-dimensional variably saturated media. The program numerically solves the Richards' equation for saturated-unsaturated water flow and the advection-dispersion equation for solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The transport equation includes provisions for linear equilibrium adsorption, zero-order production, and first-order degradation. ~~The program may be used by plant roots~~. The transport equation includes provisions for linear equilibrium adsorption, zero-order production, and first-order degradation. The program may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. SWMS_2D can handle flow regions delineated by irregular boundaries. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the vertical plane, the horizontal plane, or in a three-dimensional region exhibiting radial symmetry about the vertical axis. The water flow part of the model can deal with prescribed head and flux boundaries, as well as boundaries controlled by atmospheric conditions.

The governing flow and transport equations are solved numerically using Galerkin-type linear finite element schemes.

The input data for SWMS_2D are given in four separate input files. These input files consist of one or more input blocks identified by the letters from A through J. The input files and blocks are arranged as follows:

SELECTOR.IN

A. Basic Information
B. Material Information
C. Time Information
D. Seepage Information
E. Solute Transport Information

GRID.IN

F. Nodal Information
G. Element Information
H. Boundary Geometry Information

ATMOSPH.IN

I. Atmospheric Information

SINK.IN

J. Root Water Uptake Information

The program output consists of 15 output files which are organized into 3 groups:

T-level information—This group of output files contains information which is printed at the end of each time step.

H_MEAN.OUT—Mean pressure heads

V_MEAN.OUT—Mean and total water fluxes

CUM_Q.OUT—Total cumulative water fluxes

RUN_INF.OUT—Time and iteration information

SOLUTE.OUT—Actual and cumulative concentration fluxes

P-level information - P-level information is printed only at prescribed print times. The following output files are printed at the P-level:

H.OUT	Nodal values of the pressure head
TH.OUT	Nodal values of the water content
CONC.OUT	Nodal values of the concentration
Q.OUT	Discharge/recharge rates assigned to boundary or internal sin/source nodes
VX.OUT	Nodal values of the x-components of the Darcian flux vector
VZ.OUT	Nodal values of the z-components of the Darcian flux vector
BOUNDARY.OUT	This file contains information about each boundary node, n, for which $Kode(n) \neq 0$, including the discharge/recharge rate, $Q(n)$, the boundary flux, $q(n)$, the pressure head $h(n)$, the water content $\theta(n)$, and the concentration $Conc(n)$.
BALANCE.OUT	This file gives the total amount of water and solute inside each specified subregion, the inflow/outflow rates to/from that subregion, together with the mean pressure head (*hMean*) and the mean concentration (*cMean*) over each subregion (see Table 9.6). Absolute and relative errors in the water and solute mass balances are also printed to this file.

A-level information—A-level information is printed each time a time-dependent boundary condition is specified.

A_LEVEL.OUT—Mean pressure heads and total cumulative fluxes

In addition, some of the input data are printed to file CHECK.OUT. The file CHECK.OUT contains a complete description of the finite element mesh, the boundary code of each node, and the hydraulic and transport properties of each soil material.

UNSAT2 - Variably saturated flow model

The UNSAT2 computer program was developed by S. P. Neuman and documented in Davis and Neuman (1983). The theory is fully described in a series of papers by Neuman (1973, 1975) and Neuman et al. (1975). A variety of applications have been reported by Feddes et al. (1974), Kroszynski and Dagan (1975), Zaslavsky and Sinai (1981), as well as others.

The program is intended for the analysis of flow in unsaturated, partially saturated, or saturated porous media. UNSAT2 can handle flow regions delineated by irregular boundaries and composed of nonuniform soils having arbitrary degrees of local anisotropy. Flow can occur in the vertical plane, in the horizontal plane, or in a three dimensional region exhibiting radial symmetry about a vertical axis. In addition to conventional prescribed head and flux boundaries, the program can also deal with boundaries controlled by atmospheric conditions such as seepage faces and evaporation or infiltration surfaces. The type of boundary condition, as well as the value of the boundary data, can be conveniently varied with time by means of a unique restart feature that does not require tabulating such data. Water uptake by plants is computed in a manner that accounts for both soil and atmospheric conditions and allows for plant growth. A special provision is made for the analysis of flow to a partially or fully penetrating well of finite radius that pumps at an arbitrary rate. The analysis takes full account of wellbore storage. The method of solution is based on a lumped-mass Galerkin finite element scheme utilizing quadrilateral and triangular elements.

The necessary input to program UNSAT2 has been divided into 19 groups identified by letters from A to S. These groups are arranged as follows:

A - Problem Title
B - General Control Data
C - Special Control Data

D - Material Control Data
E - Seepage Face Data
F - Atmospheric Control Data
G - Soil Surface Geometric Data
H - Root Zone Grid Data
I - Plant Species Data
J - Root Zone Data
K - Well Descriptive Data
L - Well Control Data
M - Time Step Data
N - Unit Conversion Factors
O - Material Constant Properties
P - Unsaturated Material Properties
Q - Nodal Point Data
R - Element Data
S - Execution Terminator

The program output, which is assigned to a standard output unit, consists of a listing of all user supplied and computer generated input information including a complete description of the finite element mesh, the boundary code of each node, and the properties of each material

At the end of each time step, the cumulative inflow into the system is printed together with the values of total head, pressure head, and discharge into or out of the system (not flow through the system) at each node. Moisture content at unsaturated nodes is printed for each material. If the well option is being used, the well discharge and water level are also printed. If the surface flux option is being used, the potential surface flux and minimum surface pressure head are printed. If water uptake by plants is taking place, the potential transpiration rate and the pressure head in the roots are printed for each plant species.

LEACHM Model

LEACHM is a general acronym (Leaching Estimation And CHemistry Model) that refers to five versions of a simulation model which describes the water regime and the chemistry and transport of solutes in unsaturated or partially saturated soils to a depth of about two meters. The LEACHM suite of models was developed by Hutson and Wagenet (version 3, 1992). These versions utilize similar numerical solution schemes to simulate water and chemical movement. They differ in that LEACHN describes nitrogen transport and transformation, LEACHP simulates pesticide displacement and degradation, LEACHC describes transient movement of inorganic ions (Ca, Mg, Na, K, SO_4, Cl, CO_3, HCO_3), LEACHB describes microbial population dynamics in the presence of a single growth-supporting substrate and LEACHW describes the water regime only. These models are intended to be applied to laboratory and field situations. Estimates of plant growth and absorption of water and solutes by plant roots are included in all five models, together with a flexible means of describing precipitation and surface evaporation of water. A heat flow simulation, producing soil temperature profiles, is included in LEACHN and LEACHP, which provides the opportunity to adjust rate constants according to both temperature and water content.

The numerical differencing procedures were developed from several earlier models (Hanks and Bowers, 1962; Bresler, 1973; Nimah and Hanks, 1973; Tillotson et al., 1980). The chemical equilibrium and cation exchange subroutines evolved from those of Robbins et al. (1980a, b). Improvements to these models include applicability to a wider range of field conditions, flexibility of simulating layered or non-homogeneous profiles, improved mass balancing and orderly and self-explanatory input and output tables. Experience with earlier versions of LEACHM has led to continual improvements in these procedures.

The models are organized on a modular basis. In each of the five versions, a main program initializes variables, calls subroutines and performs mass balancing. Subroutines deal with data input and output, time step calculation, evapotranspiration, water flow, solute movement, sources and sinks (degradation, transformation, volatilization, microbial growth), chemistry, leaf and root growth, temperature, and solute absorption by plants. Segregation of each of these processes into subroutines called by the main program enables any subroutine to be replaced by an improved or different formulation if desired.

Simulations begin at 00h00 on the first day, for which a set of initial conditions are required. The soil need not be homogeneous in the vertical direction. Plants can be present or absent. If present, crop cover and root expansion can be simulated, or a static, established root system and crop cover can be defined. All versions of LEACHM require the following inputs, which are read from data files constructed appropriately for each version.

•Soil properties and initial conditions for each soil segment:
  - water content or water potential
  - hydrological constants for calculating retentivity and hydraulic conductivity or particle size distribution
  - appropriate chemical contents and soil chemical properties for each version

•Soil surface boundary conditions of:
  - irrigation and rainfall amounts and rates of application
  - mean temperatures and diurnal amplitudes (weekly means), if a temperature simulation is required,
  - potential evaporation (weekly totals)

•Crop details (if it is assumed that no crops are present, a control variable allows bypass of the plant-related subroutines):
  - time of planting
  - root and crop maturity and harvest
  - root and cover growth parameters
  - soil and plant water potential limits for water extraction by plants

Other constants used in determining lower boundary conditions, time steps, dispersion and diffusion coefficients, chemical reactions and transformations and output details.

Each version of LEACHM is organized into a series of subroutines, each of which calculates a different aspect of the fate of the water and solute.

•Output of the model consists of three files

1. - A detailed output file (extension .OUT) at specified times containing:

   - Hydraulic conductivities and water contents for each layer of the soil at soil water matric potential values of 0, -3, 10, -30, -100, and -1500 kPa.

   - Cumulative totals and mass balances of water and all solutes considered in the model being used. This includes the amount of material initially in the soil profile, currently in the profile, the simulated change, additions, losses, and a composite mass error.

- A summary by depth of water content, matric potential, water flux between layers, soil temperature, evapotranspiration, and mass and concentration of individual chemical species.

- A summary by depth of root density, water uptake, and solute uptake. This table presents the information both as a change since the last print, and as a cumulative total from time zero.

2. - A summary file (with the extension .SUM) to which pertinent content and flux data is written at shorter time intervals. This file, in which each record represents one time, is convenient for preparing time series plots.
3. - A breakthrough curve (extension .BTC) which lists cumulative time, pore volumes and leachate concentration at selected drainage increments.

HYDRUS Model

HYDRUS (Kool and van Genuchten, 1991) simulates one-dimensional variably saturated water flow and solute transport in porous media. The solution of the flow problem considers the effects of root water uptake and hysteresis in the unsaturated soil hydraulic properties. The solute transport equation incorporates the effects of ionic or molecular diffusion, hydrodynamic dispersion, linear or nonlinear equilibrium adsorption and first-order decay. The boundary conditions for the flow and transport equations may be constant or time-varying. Soil hydraulic properties in HYDRUS can be described by the parametric functions of van Genuchten (van Genuchten and Nielsen, 1985). Uptake of water by plant roots includes evapotranspiration, a normalized root uptake distribution function, and a pressure-salinity stress response function. The code is written in FORTRAN-77 and employs fully implicit, Galerkin type linear finite element solutions of the governing flow and transport equations.

HYDRUS is a modification of the program WORM previously developed at the U.S. Salinity Laboratory.

Data input for HYDRUS is specified in 12 groups, arranged as follows:

Group 1. Problem Description
Group 2. Simulation Parameters
Group 3. Control Parameters
Group 4. Time Stepping Parameters
Group 5. Problem Geometry
Group 6. Soil Hydraulic Properties
Group 7. Solute Transport Properties
Group 8. Root Water Uptake Parameters
Group 9. Initial Conditions
Group 10. Boundary Conditions
Group 11. Output Times
Group 12. Observation Point Locations

HYDRUS uses three output files. The main output file is used to echo most of the input data and also contains simulation results at the requested output time values. The second output file is used to write nodal values of the pressure head, water content, and concentration at the requested output times for use in plotting simulation results. The third output file contains a time record of computed dependent variables at the user-specified observation points.

RETC Computer program

The RETC (RETension Curve) computer code (van Genuchten, Leij, and Yates, 1991) is designed to analyze the soil -water retention and hydraulic conductivity functions of unsaturated soils. These hydraulic properties are key parameters in any quantitative description of water flow into and through the unsaturated zone of soils. The program uses the parametric models of Brooks-Corey and van Genuchten to represent the soil water retention curve, and the theoretical pore-size distribution models of Mualem and Burdine to predict the unsaturated hydraulic conductivity function from observed soil water retention data. This model employs the nonlinear least-squares parameter optimization method to estimate the unknown coefficients in the different soil hydraulic expressions.

Initial Results

Because the required data to run these models are still being collected and thus are not available at the project start, we used our time evaluating and purchasing the proper computer equipment (Sparc 10 UNIX workstation), learning how to operate under the UNIX environment, installing and executing various numerical models and graphics/spreadsheet programs, modifying and adjusting the selected models to better suit our requirements, and running numerous hypothetical test cases and comparing results and analyzing model differences.

For example, the LEACHM model uses the simplified Campbell's equation (Campbell, 1974) for predicting the hydraulic conductivity function. We modified the program and programmed the more versatile van Genuchten functions (van Genuchten and Nielsen, 1985) into the LEACHM model. In order to easily compare outputs from different models, we modified the output routines of some of the models to display soil water content and hydraulic conductivities at commonly specified pressures. We also developed a post processor for displaying the results of UNSAT2, among other changes.

In order to demonstrate some of the capabilities of such models, we ran a one-dimensional test case with boundary conditions similar to the one encountered at the Konza Prairie site. The test case layout and boundary conditions are shown in fig. 1. The hydraulic conductivity and characteristic functions employed are shown in figs. 2 and 3, respectively. (The initial conditions of soil-water content or capillary pressure distributions are shown in the next set of figures.) Using these input data and initial and boundary conditions, we simulated the soil-water content and capillary pressure profiles in the soil profile at different times, as well as the cumulative water fluxes (figs. 4, 5, and 6, respectively). We also simulated nitrogen transport and transformations by applying 50 kg/ha urea fertilizer in the first soil segment (25 mm) of the test soil column. The resulting NO_3-N solution profile with depth and time is shown in fig. 7 (fig. 7b is an expanded view of fig. 7a).

In order to partially verify our results, we run another soil-water flow test case using all four previously-mentioned numerical simulators (LEACHM, UNSAT2, SWMS_2D, and

HYDRUS). The test case is similar to the one shown in fig. 1 except that the total column length was 60 cm, and the bottom boundary condition was a fixed water table. The same soil hydraulic characteristics shown in figs. 2 and 3 are also employed in this case. The soil-water content (part a) and capillary pressure (part b) profiles from each one of the four simulation models are shown in figs. 8, 9, 10, and 11. The results of the model intercomparison are indeed very similar, as expected, given minor inconsistencies in output times and in grid design [block-centered (LEACHM) versus finite element node-centered (all other models)].

References

Bresler, E., 1973. Simultaneous transport of solutes and water under transient unsaturated flow conditions. Water Resour. Res. 9:975–986.

Campbell, G., 1974. A simple method for determining unsaturated conductivity from moisture retention data. Soil Sci. 117:311–314.

Davis, L.A., and Neuman, S.P., 1983. Documentation and User's Guide: UNSAT2 Variably Saturated Flow Model (Including 4 Example Problems). Final Report. WWL/TM-1791-1. Water, Waste and Land, Inc., Ft. Collins, Colorado.

Feddes, R.A., Bresler, E., and Neuman, S.P., 1974. Field test of a modified numerical model for water uptake by root systems, Water Resour. Res., 10(6), 1199–1206.

Hanks, R.J., and Bowers, S.A., 1962. Numerical solution of the moisture flow equation for infiltration into layered soils. Soil Sci. Soc. Amer. Proc. 26:530–534.

Hutson, J.L., and Wagenet, R.J., 1992. LEACHM: Leaching Estimation and Chemistry Model, Version 3. Research Series No. 92-3, Dept. of Soil, Crop and Atmospheric Sciences, Cornell University, Ithaca, New York.

Kool, J.B., and van Genuchten, M.Th., 1991. HYDRUS, one-dimensional variably saturated flow and transport model including hysteresis and root water uptake. Research Report No. 124, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.

Kroszynski, U.I., and Dagan, G., 1975. Well pumping in unconfined aquifers: the influence of the unsaturated zone, Water Resour. Res., 11(3), 479–490.

Neuman, S.P., 1973. Saturated-unsaturated seepage by finite elements. Proc. ASCE, J. Hydraul. Div. 99 (HY12):2233–2250.

Neuman, S.P., 1975. Galerkin approach to saturated-unsaturated flow in porous media, Ch. 10 in Finite Elements in Fluids, in: R.H. Gallagher, J.T. Oden, C. Taylor, and O.C. Zienkiewicz, eds, Vol. I: Viscous Flow and Hydrodynamics. John Wiley and Sons, London, p. 201–217.

Nimah, M.N., and Hanks, R.J., 1973. Model for estimation of soil water, plant, and atmospheric interrelations: I. Description and sensitivity. Soil Sci. Amer. Proc. 37:522–527.

Robbins, C.W., Jurinak, J.J., and Wagenet, R.J., 1980a. Calculating cation exchange in a salt transport model. Soil Sci. Amer. J. 44:1195–1199.

Robbins, C.W., Wagenet, R.J., and Jurinak, J.J., 1980b. A combined salt transport-chemical equilibrium model for calcareous and gypsiferous soils. Soil Sci. Soc. Amer. J. 44:1191–1194.

Simunek, J., Vogel, T., and van Genuchten, M.Th., 1992. The SWMS_2D code for simulating water flow and solute transport in two-dimensional variably saturated media. Research Report No. 126, U.S. Salinity Laboratory Agricultural Research Service, U.S. Dept. of Agriculture, Riverside, California.

Tillotson, W.R., Robbins, C.W., Wagenet, R.J., Hanks, R.J., 1980. Soil water, solute, and plant growth simulation. Bulletin 502. Utah State Agr. Exp. Stn., Logan, Utah, 53 pp.

van Genuchten, M.Th., and Nielsen, D.R., 1985. On describing and predicting the hydraulic properties of unsaturated soils. Ann. Geophys. 3:615–628.

van Genuchten, M.Th., Leij, F.J., and Yates, S.R., 1991. The RETC code for quantifying the hydraulic functions of unsaturated soils, EPA/600/2-91/065, Robert S. Kerr Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Ada, Oklahoma.

Zaslavsky, D., and Sinai, G., 1981. Surface hydrology: V. In-surface transient flow, Jour. Hydr. Div. ASCE, 107 (HYI), p. 65–93.

List of Figures

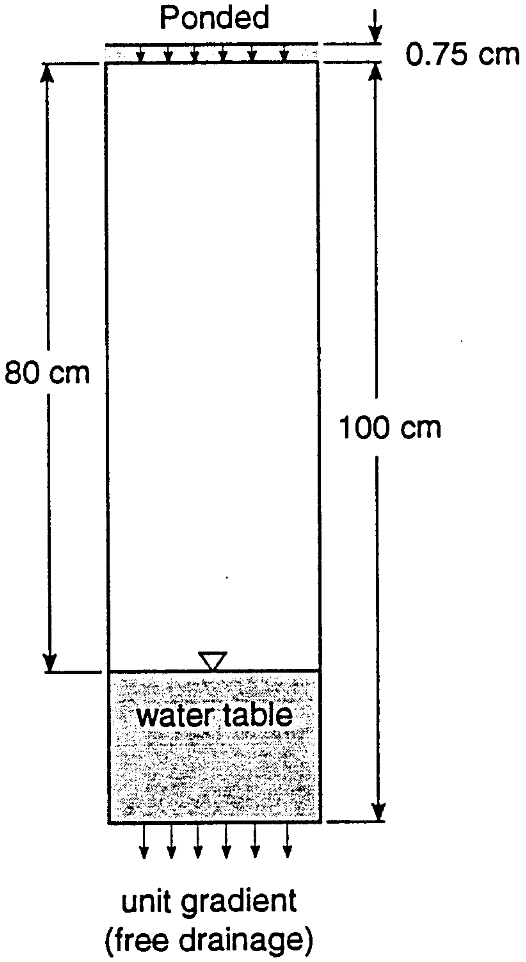

Figure 1. Test case layout and boundary conditions for computer modeling.

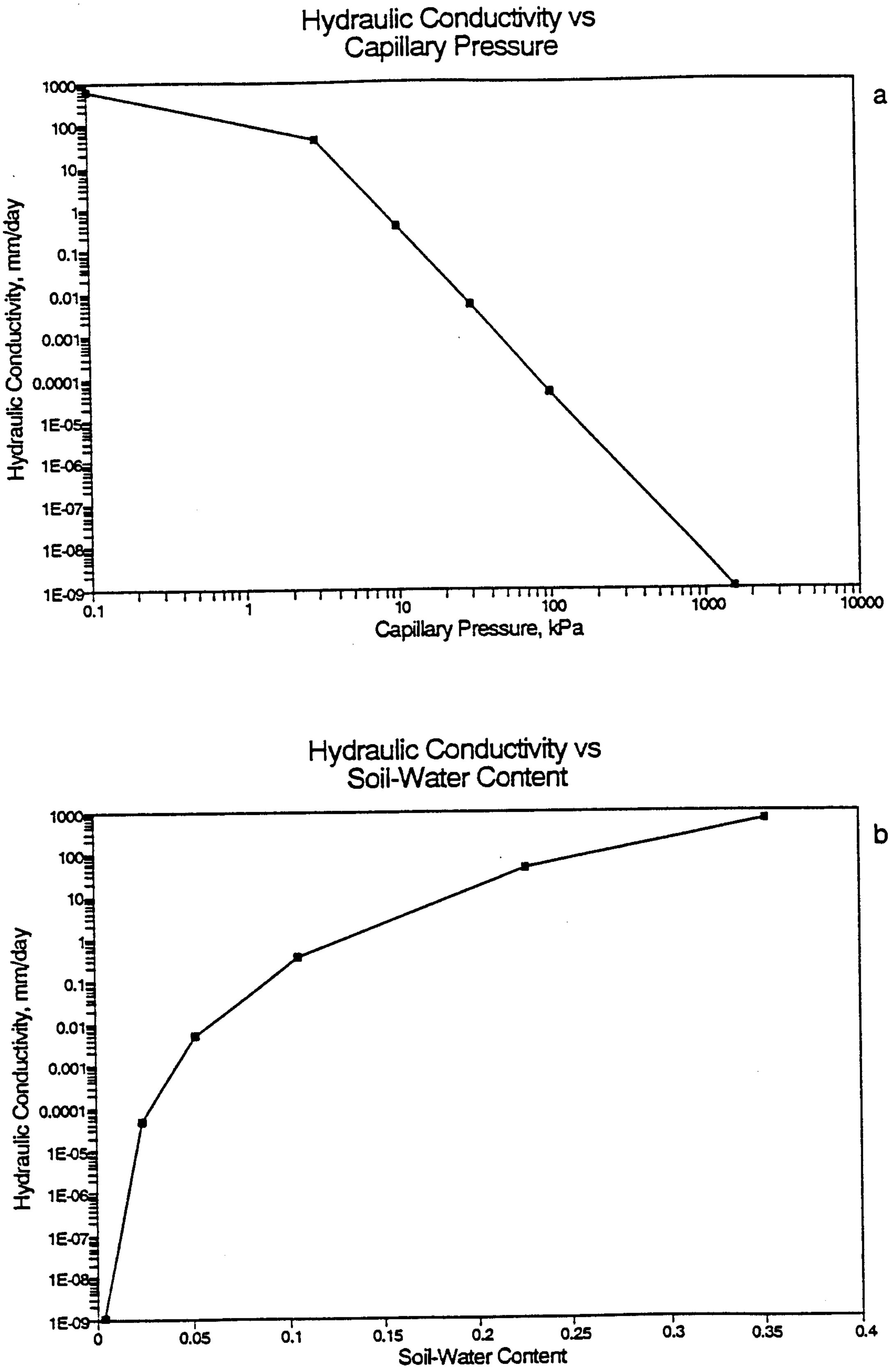

Figure 2. Hydraulic conductivity as a function of capillary pressure and soil water content for the hypothetical soils used in the computer simulations.

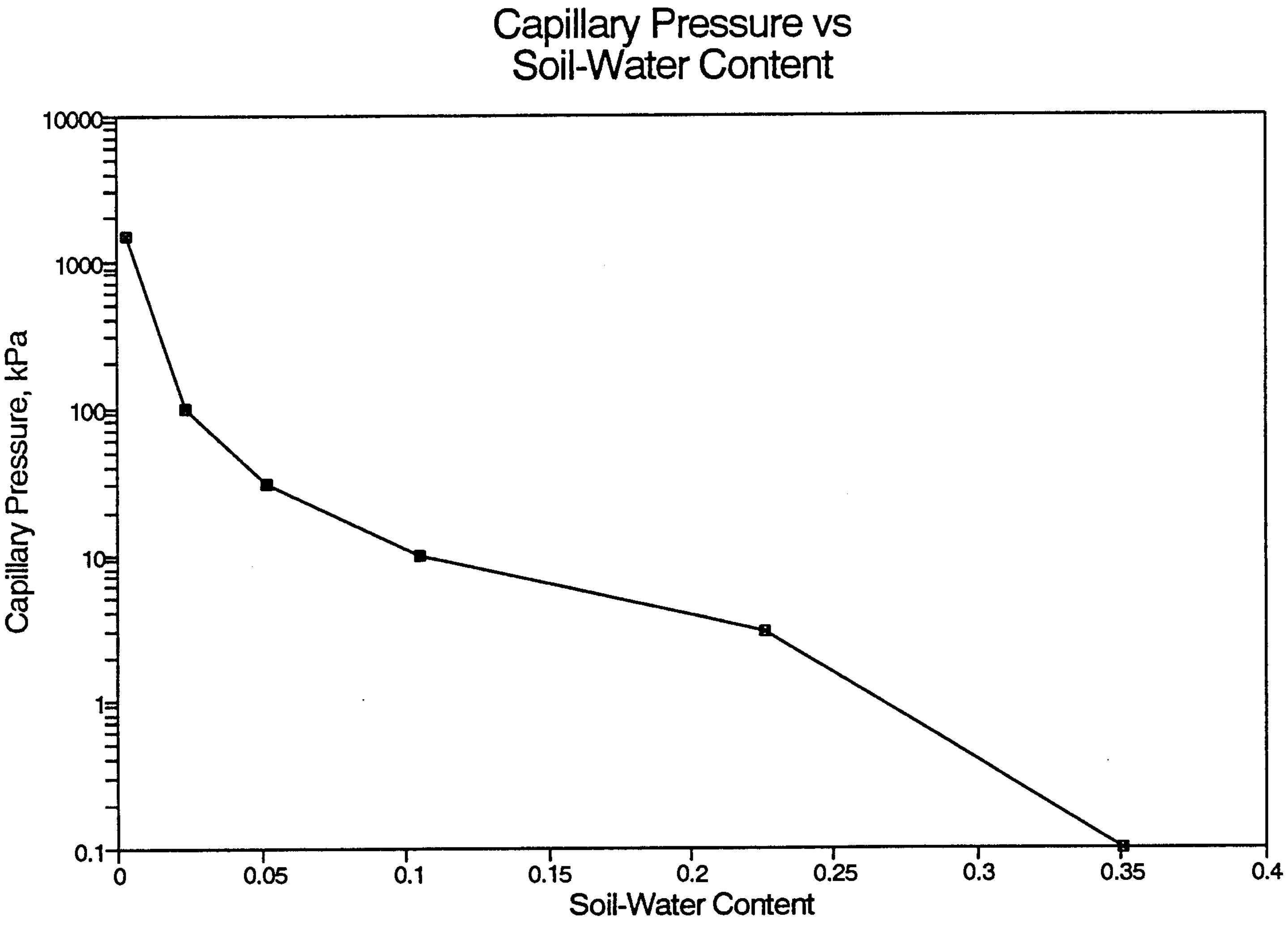

Figure 3. Moisture release curve for the hypothetical soils used in the computer simulations.

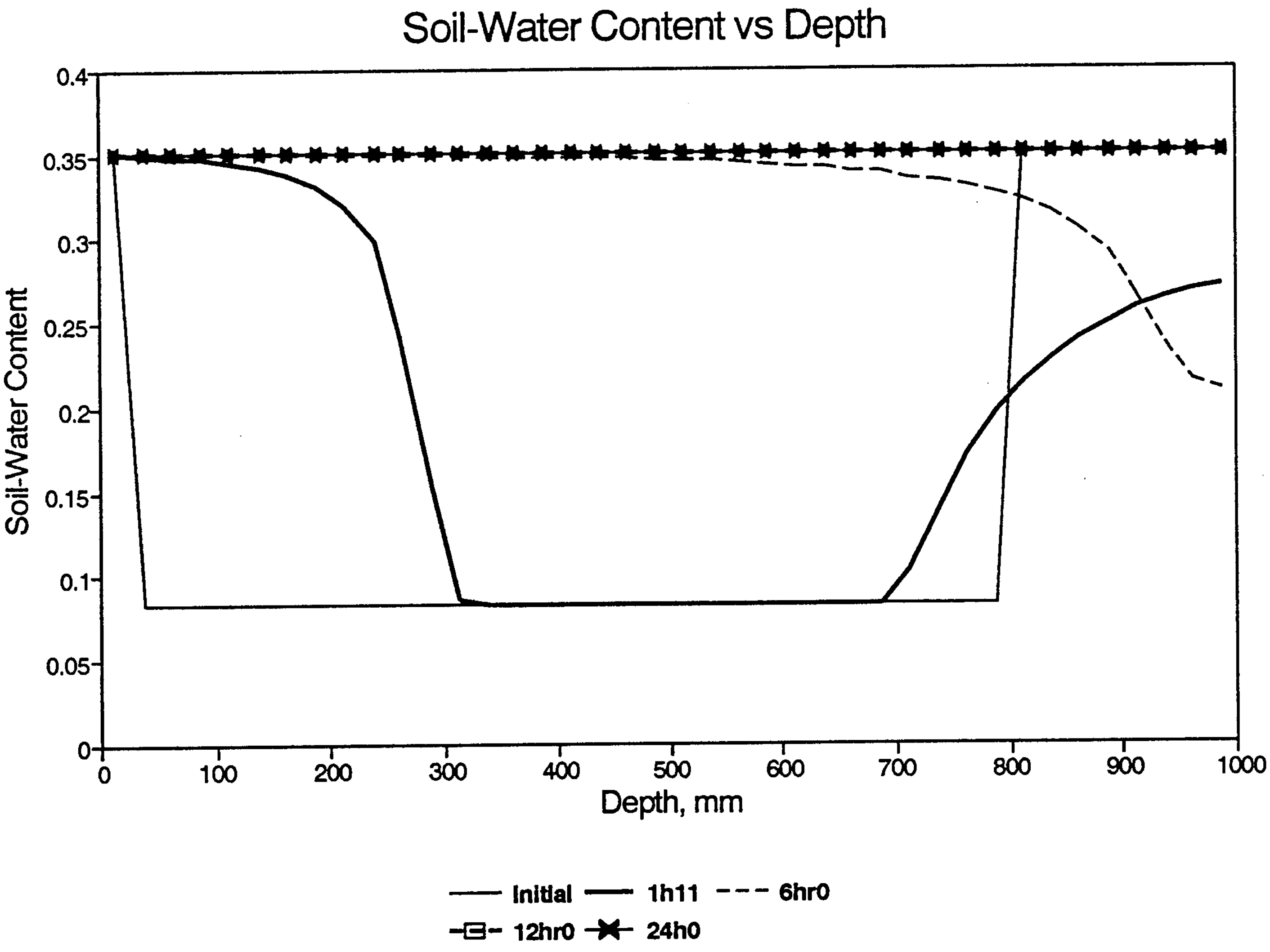

Figure 4. Simulated soil water content versus depth.

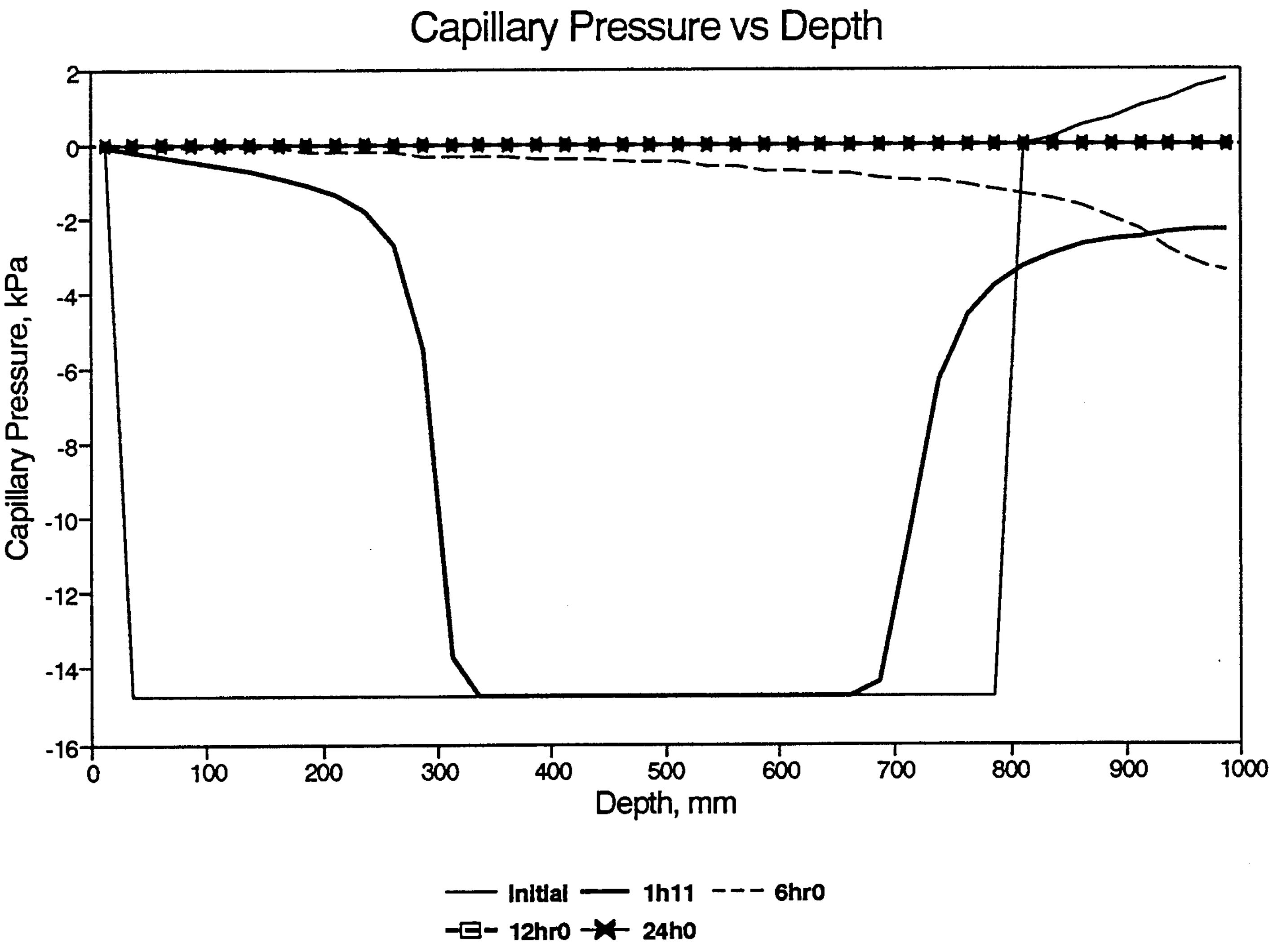

Figure 5. Simulated capillary pressure versus depth.

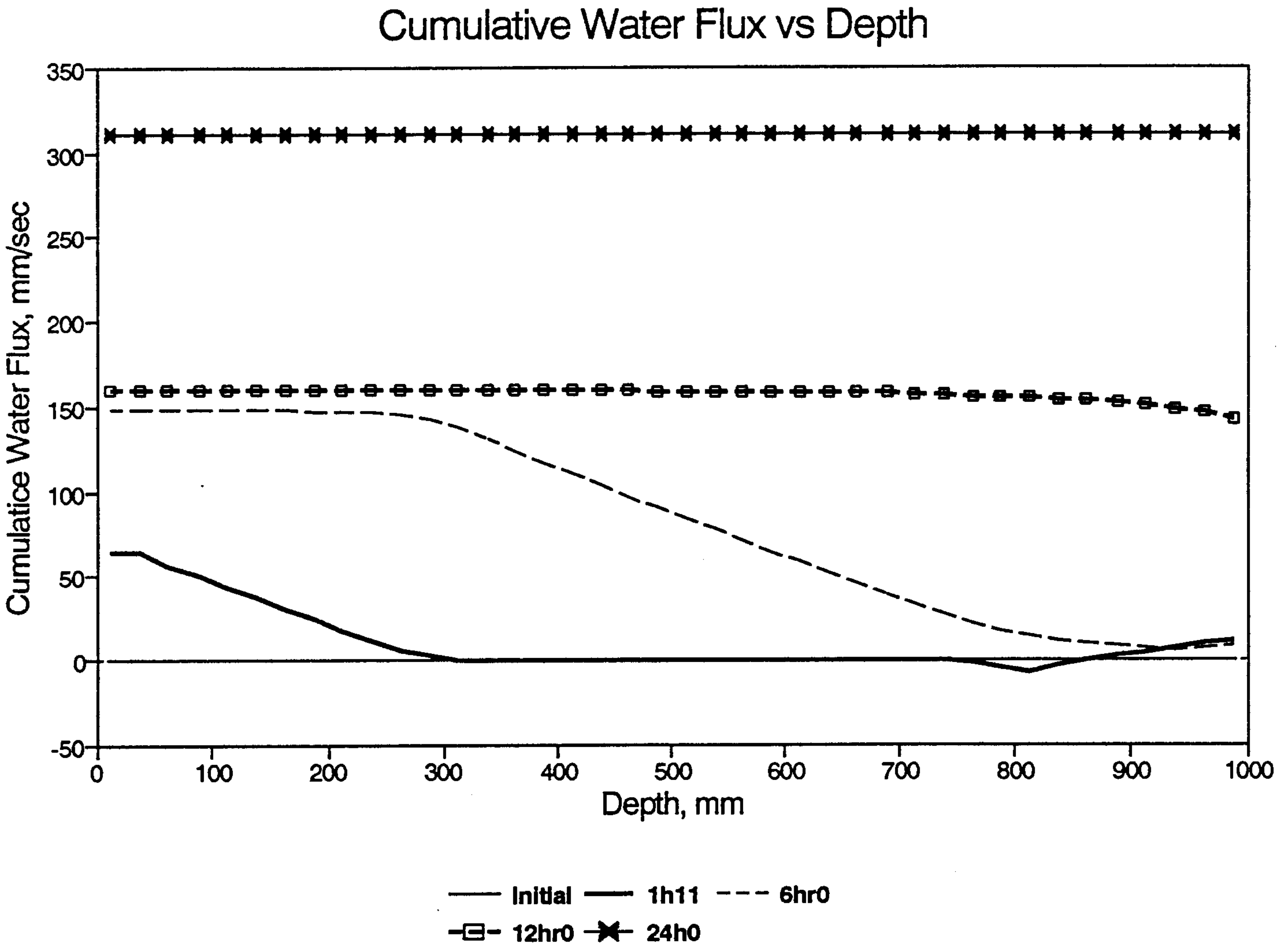

Figure 6. Simulated cumulative water flux versus depth for the hypothetical soils.

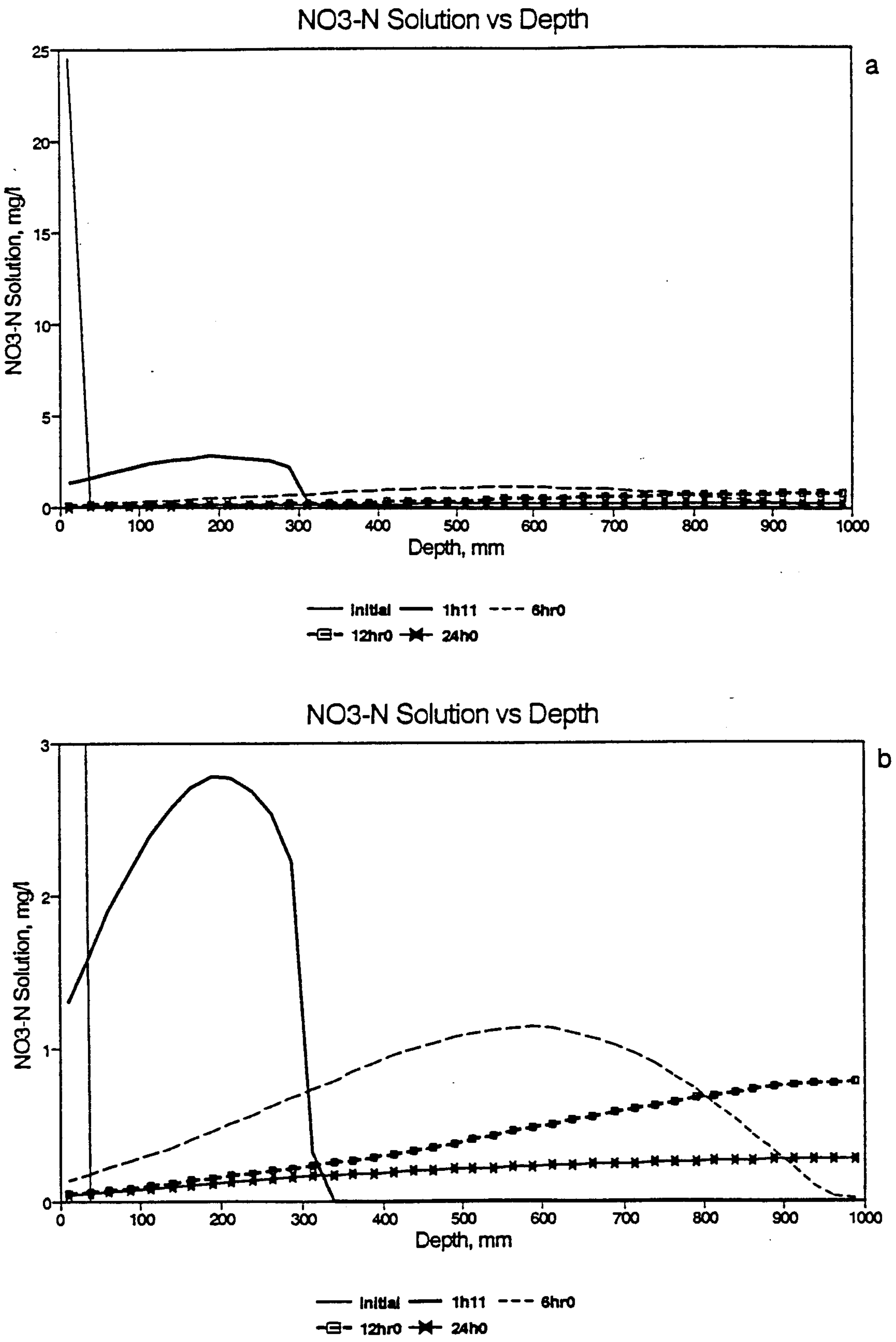

Figure 7. Simulated nitrate transport as a function of depth in soil.

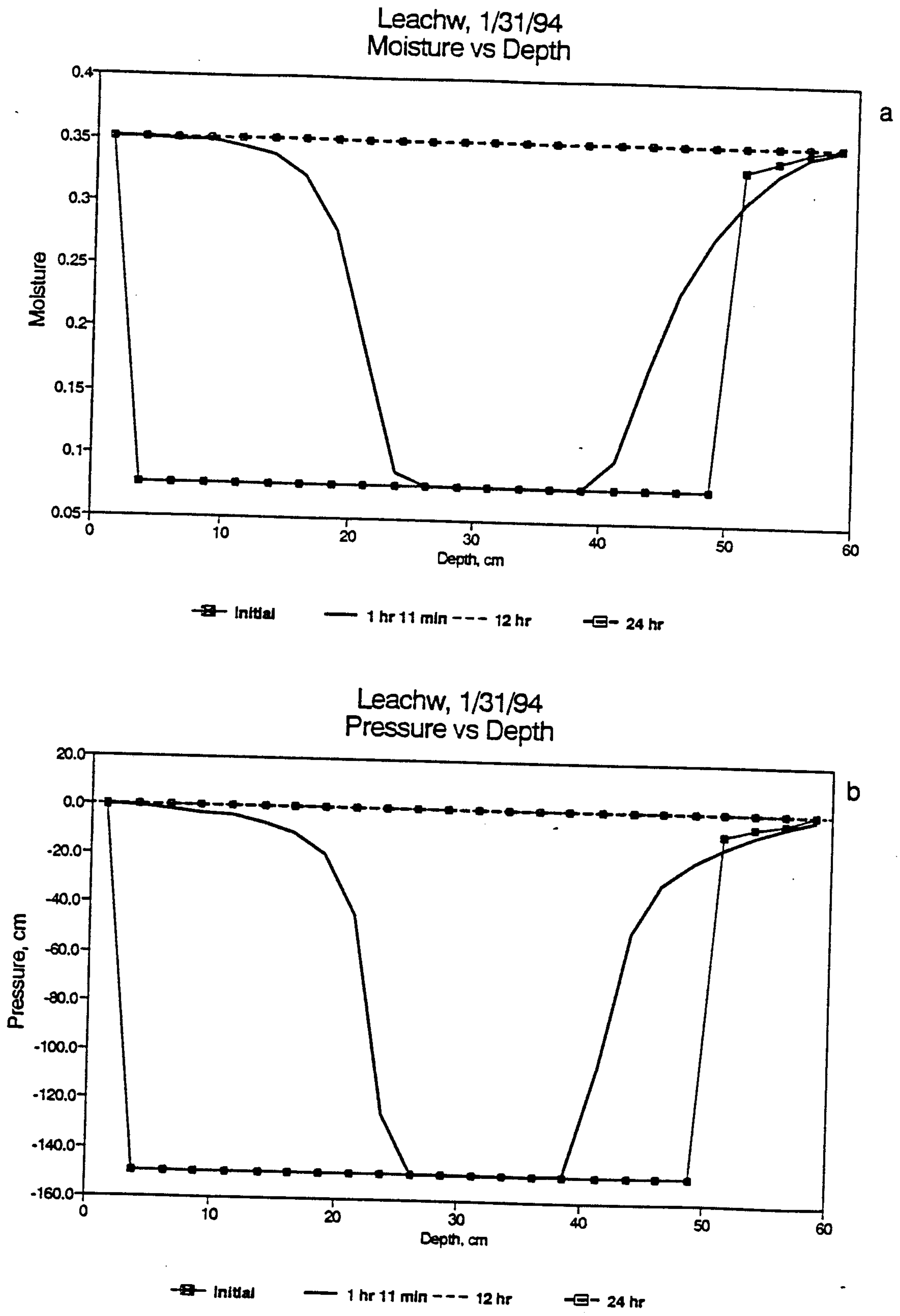

Figure 8. Moisture and pressure versus depth as predicted by LEACHM.

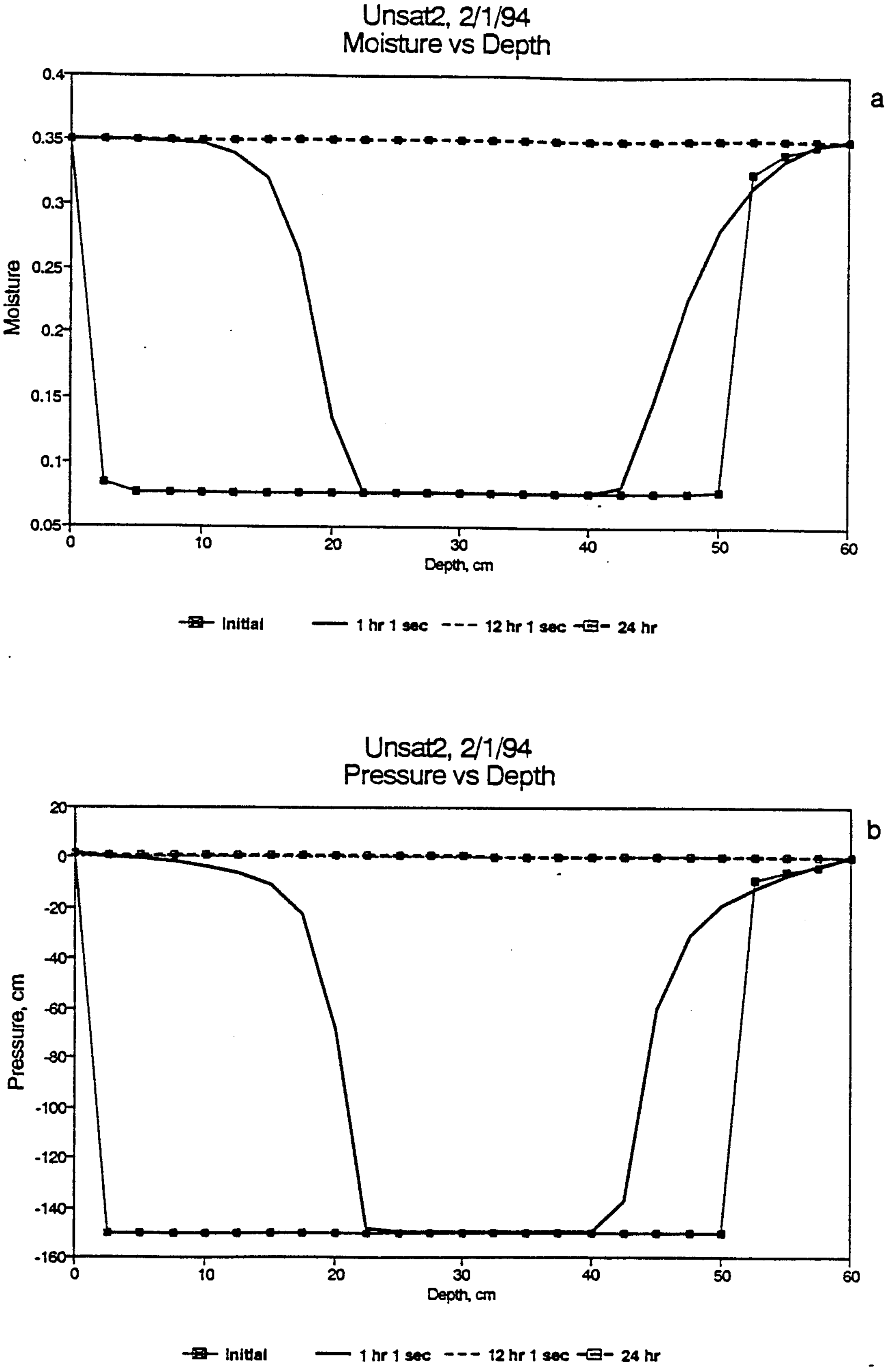

Figure 9. Moisture and pressure versus depth as predicted by UNSAT2.

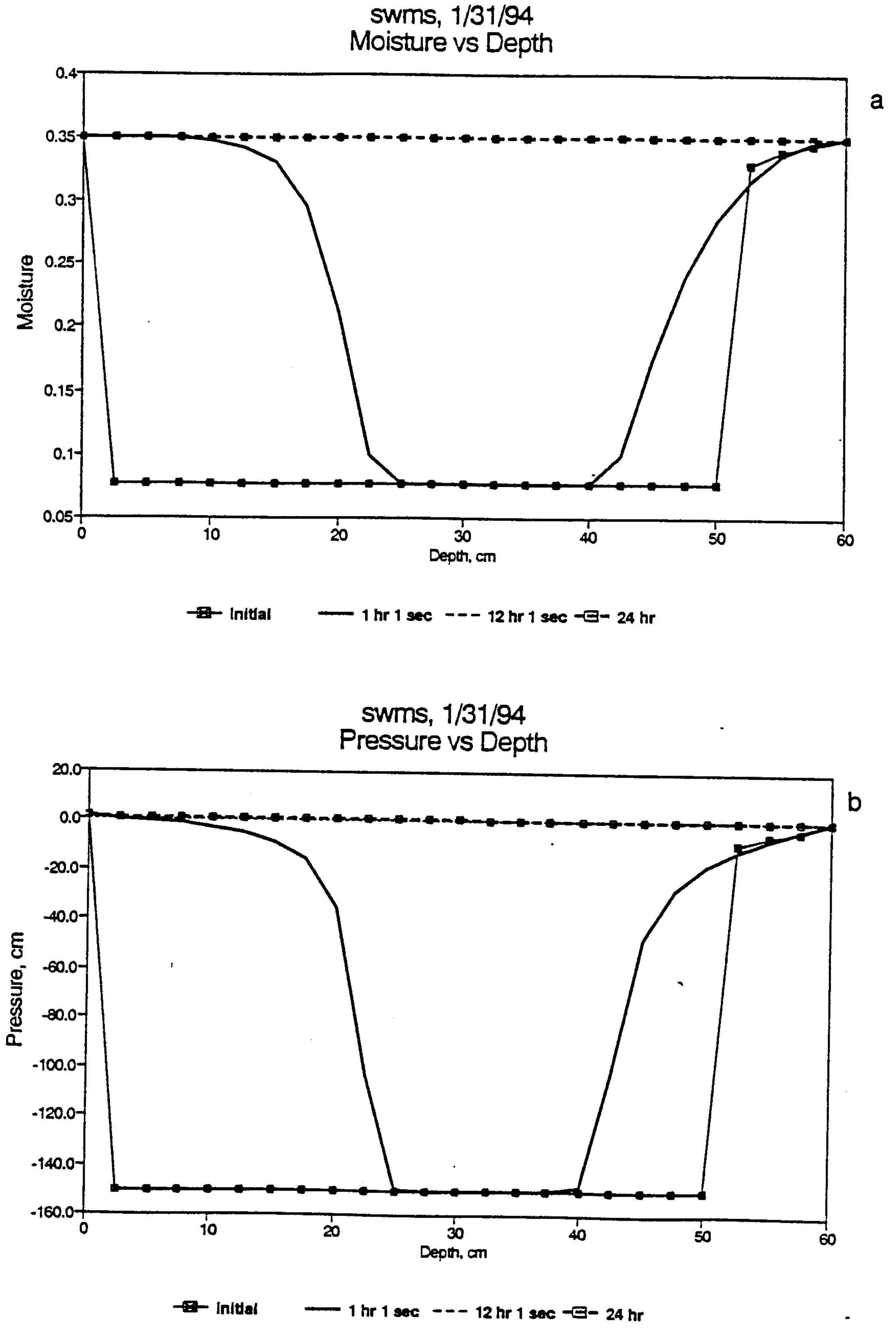

Figure 10. Moisture and pressure versus depth as predicted by SWMS_2D.

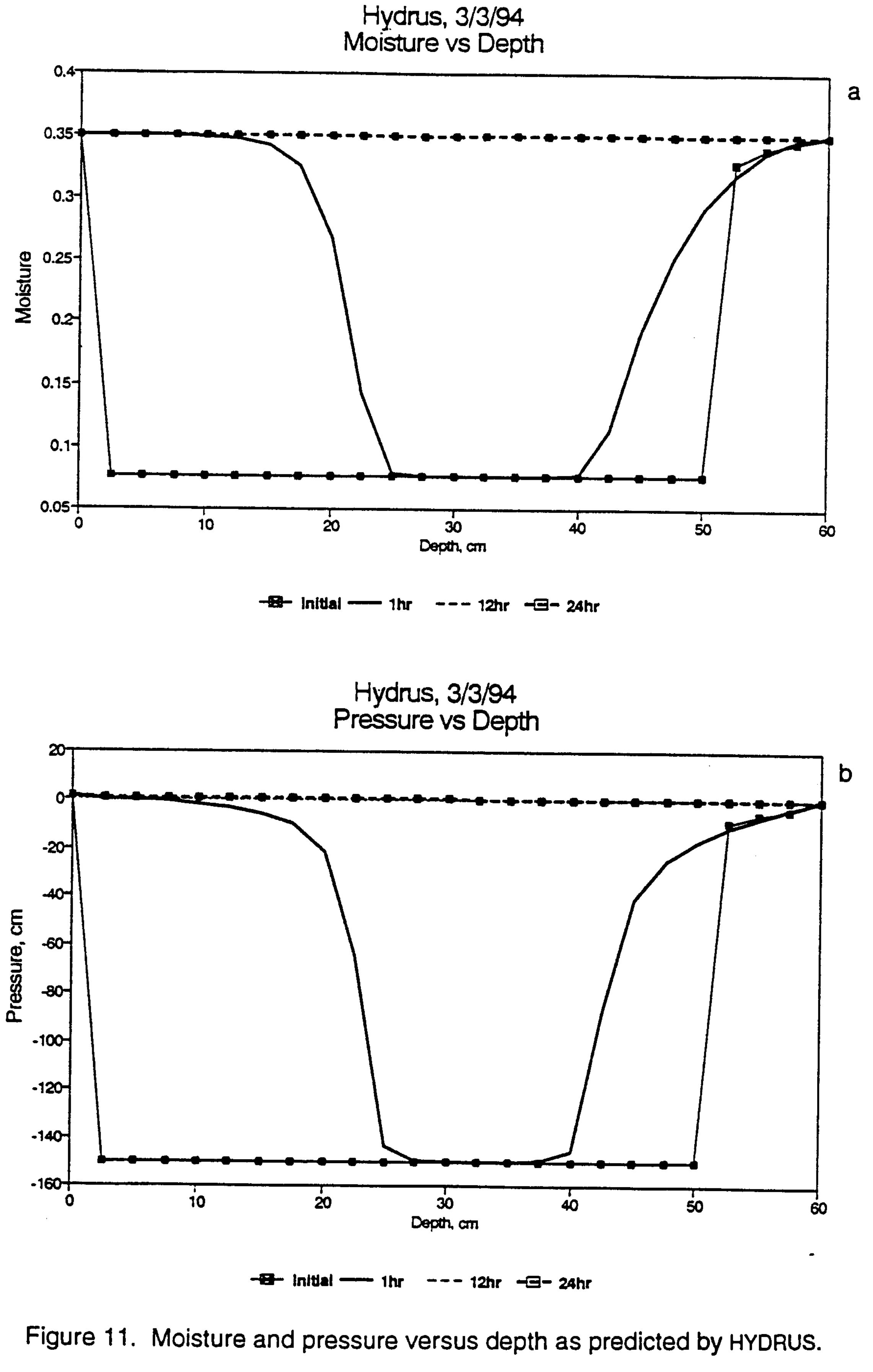

Figure 11. Moisture and pressure versus depth as predicted by HYDRUS.