Saturated-Unsaturated 3D Groundwater Model. II: Verification and Application

Ahmet Dogan[1] and Louis H. Motz, M.ASCE[2]

Abstract: Verification and application results are presented for a new saturated-unsaturated 3D groundwater flow model (SU3D) developing in Dogan and Motz, which can be used to calculate the pressure distribution over the entire groundwater flow domain in response to rainfall and evapotranspiration. SU3D solves the nonlinear 3D, modified mixed form of the Richards equation continuously throughout the groundwater flow domain, including both the unsaturated and saturated zones. The block-centered finite-difference method, a modified Picard iteration scheme, and the preconditioned conjugate gradient method are used to solve the governing partial differential equations in the new model. SU3D can simulate evaporation from land surface and transpiration from the root zone. Potential evapotranspiration is partitioned into potential evaporation and potential transpiration as a function of the leaf area index; actual evaporation and actual transpiration are then calculated individually. As shown in this paper, SU3D has been verified by reproducing the results of five analytical and numerical studies and a 3D unconfined-aquifer pumping test from the published literature.

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Introduction

A new saturated-unsaturated 3D rainfall-driven groundwater flow model (SU3D) has been developed to simulate most of the important elements of the hydrological cycle (Dogan and Motz 2005) (Fig. 1). The uniqueness of SU3D is its 3D hydrological completeness, such that recharge, evapotranspiration, unsaturated flow, and saturated flow are all simulated continuously. The model utilizes precipitation data as input, calculates recharge, evaporation, and transpiration, and simulates both unsaturated and saturated flow in a basin using a robust, fast, and stable numerical solution and iteration methods. As described in this paper, SU3D has been verified by reproducing the results of problems involving 1D infiltration and redistribution, 1D transient infiltration in layered soils, transient 2D variably saturated water table recharge, a 2D response to rainfall and evapotranspiration, and a 3D response to pumping. Also, SU3D has been verified by reproducing the results of a field-scale unconfined-aquifer pumping test.

[1]Assistant Professor, Dept. of Civil Engineering, Suleyman Demirel Univ., 32001 Isparta, Turkey. E-mail: dogan@mmf.sdu.edu.tr

[2]Associate Professor, Water Resources Research Center, Dept. of Civil and Coastal Engineering, Univ. of Florida, P.O. Box 116580, Gainesville, FL 32611-6580. E-mail: lmotz@ce.ufl.edu

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Model Description and Input Parameters

Governing Finite-Difference Equation of Model

The mathematical equation governing the groundwater flow system in SU3D is the modified 3D Richards equation. The Darcy-Buckingham equation is substituted into the continuity equation, in which the storage term is modified to represent saturated-unsaturated flow conditions, to obtain the following form of the 3D Richards equation in partial differential form in terms of the pressure head h (Dogan and Motz 2005):

$$\left[\frac{\partial}{\partial x}\left(K_x(h)\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y(h)\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z(h)\left(\frac{\partial h}{\partial z}+1\right)\right)\right]\pm Q_{\text{ext}}$$
$$=\frac{\partial\theta}{\partial t}+S_w S_s\frac{\partial h}{\partial t} \tag{1}$$

where $K_x(h)$, $K_y(h)$, and $K_z(h)$ are hydraulic conductivities that are functions of pressure head (h) in the x-, y-, and z-directions, respectively (LT^{-1}); z is the elevation head; Q_{ext} is a volumetric source or sink term $(L^3L^{-3}T^{-1})$; θ is the moisture content; η is the porosity; S_w is the saturation ratio$=\theta/\eta$; and S_s is the specific storage (L^{-1}). Eq. (1) is the general 3D saturated-unsaturated flow equation that is called the mixed form of the modified Richards equation due to the inclusion of the saturated zone (Celia et al. 1990) and the occurrence of the moisture content θ and pressure head h in the same equation (Clement et al. 1994).

Description of Model

SU3D can be used to simulate the hydrogeologic system by solving the nonlinear, 3D mixed form of the modified Richards equation continuously throughout the flow domain from the land surface to the impervious bottom of the lowest layer (Dogan 1999; Dogan and Motz 2005). The finite-difference method with a variable grid is used to solve the governing equation. The upper

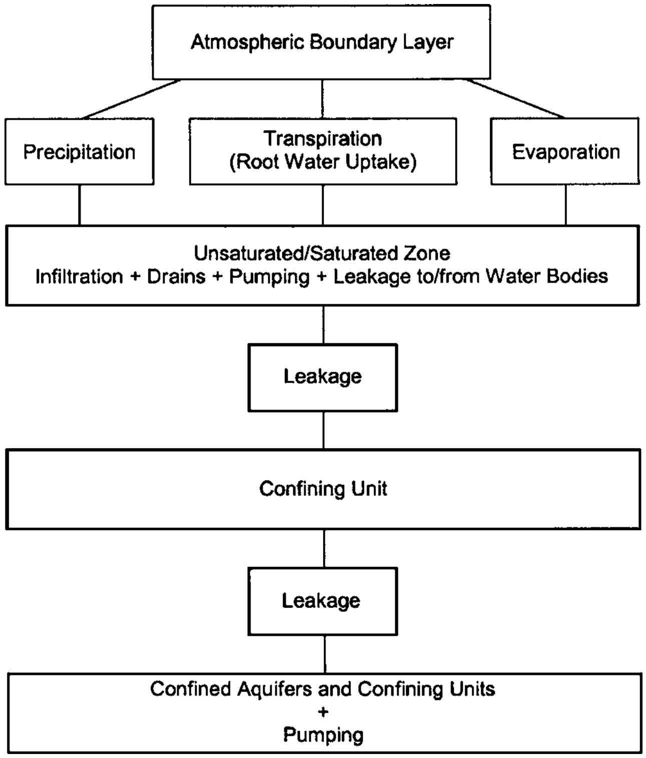

Fig. 1. Schematic representation of physical components of SU3D and interaction among components

boundary in the model is at land surface where values for the boundary conditions are determined using soil characteristics and meteorological data. The model treats the complete subsurface regime as a unified whole, and the flow in the unsaturated zone is integrated with saturated flow in the underlying unconfined and confined aquifers. SU3D allows modeling of heterogeneous and anisotropic geologic formations.

In SU3D, evapotranspiration is considered a combination of evaporation and transpiration, which are calculated separately. Accordingly, potential evapotranspiration (*PET*) is divided into its components—potential evaporation (E_p) and potential transpiration (T_p)—based on the leaf area index (*LAI*), which is the ratio of the leaf area to the total area of land surface. *PET* can be calculated in SU3D based on the pan evaporation method or the energy conservation method using the Priestly-Taylor (1972) equation (Dogan 1999). The actual evaporation (E_a) from the soil surface and actual transpiration (T_a) from the root zone are calculated from E_p and T_p, respectively. A plant root water uptake (transpiration) model and an evaporation model are included as a sink term and an upper boundary condition, respectively, in the governing flow equation in the model.

In SU3D, infiltration is conceptualized as a two-stage procedure. In the first stage, all rainfall enters the system at the applied rate as long as the conductivity and sorptive capacities of the medium are not exceeded. When these capacities are exceeded, in the second stage, water starts ponding on the land surface, and infiltration decreases asymptotically to a value equal to the saturated hydraulic conductivity of the medium, based on Lappala et al. (1987). The rainfall-runoff process is treated by assigning a maximum ponding depth value ($h_{p\,\max}$) to each cell on the land surface in the flow domain.

After the infiltration rate becomes equal to the hydraulic conductivity of the top soil and the maximum ponding depth is exceeded, then the remaining rainfall on the land surface is assumed to be runoff that is removed from the flow domain. At land surface, during a rainfall event, a flux boundary condition is set if the maximum ponding depth is not reached, and a fixed head boundary condition is set after the maximum ponding depth is reached (Dogan 1999). Thus the rainfall-runoff and infiltration process is conceptualized at the land surface as an upper boundary condition.

Pumping and injection wells can be simulated in SU3D by assigning a well discharge rate (Q) (L^3T^{-1}) to each cell of the saturated zone containing a well. Pumping from a cell is simulated by distributing the total pumping discharge to the neighboring six cells of the pumped cell as surface fluxes from their appropriate faces, based on Freeze (1971). This method prevents the pumped cells from going dry unrealistically during pumping.

Drains and springs are treated as specified head sink terms in SU3D. For simulation, the drain head (or pool elevation of a spring) and a conductance term need to be specified for each cell of the saturated zone containing a drain or spring. The conductance for a drain or spring is a lumped parameter that represents the resistance to the flow due to such features as the geological structure around a drain or spring, the number of the holes in a drainpipe, and the effect of converging streamlines in the immediate vicinity of a drain or spring.

SU3D has a modular structure similar to MODFLOW (McDonald and Harbaugh 1988), which makes it possible to modify the model components, add new features, and/or update the model without changing its general structure. Each item in the source/sink terms and boundary conditions is modeled as a module of the main body of the model. The physical system considered in SU3D includes the coupled physics of the soil and vegetation and atmospheric events such as precipitation and daily maximum and minimum temperatures.

This system, which is conceptualized to be 3D, consists of a vertically dominant flow system in the unsaturated zone and a horizontally dominant flow system in the saturated zone. The simulation of soil moisture flow under moisture extraction by crop roots involves consideration of several variables and factors: rainfall, meteorological data for the prediction of evapotranspiration, crop characteristics such as root depth, growth pattern, *LAI*, root water uptake pattern, and soil layering and soil properties for each soil layer. SU3D predicts actual evaporation loss from the soil surface, transpiration loss from the unsaturated zone, soil moisture content in the unsaturated zone, pressure heads in the saturated zone, and consequently the position of the water table for each time interval as output.

Model Limitations

The main limitation of SU3D is that it does not simulate surface-water runoff. Overland surface-water runoff is calculated and taken out of the model domain without interacting again with the groundwater flow system. Therefore the model should not be applied where surface runoff is a major component of the recharge process in the hydrologic cycle. Also, the model is very sensitive to vertical discretization, and thus finer discretization is required near land surface and in the vicinity of the water table, which is especially true if the capillary rise of the soil is significant. Therefore this model is very useful in small-scale applications where finer vertical discretization is mathematically feasible. In regional applications, SU3D can be used to predict the rainfall-recharge relation and delay time in recharge to the groundwater. Special

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care should be given to the selection of time steps because larger time steps may cause instability in simulations during the rainfall and evaporation processes.

Model Verification and Application

SU3D was verified by reproducing the results of five analytical and numerical examples from the literature. The model also was verified by reproducing the results of a field-scale pumping test. The boundary conditions, input variables, soil hydraulic properties, and results for the analytical and numerical examples and the field-scale pumping test are described in the following sections.

1D Infiltration and Redistribution

Paniconi et al. (1991) described two problems (test cases 2 and 3) in which the unmodified Richards equation was used to compare the performance of six different time discretization strategies. In their study, a very dense fine grid, small time increments, and a very accurate Newton iterative solution technique were used as the base-case "exact" solution for these test problems. In the present study, SU3D was run to verify test case 2.

Paniconi et al. (1991) simulated the problem of infiltration and redistribution in a 10-m column with a flux at the surface that increased linearly with time and a constant pressure head at the bottom to allow for drainage. The boundary conditions for this example are

$$q = t/64 \text{ m/h} \quad \text{at } z = 10 \text{ m} \tag{2a}$$

and

$$h = 0 \quad \text{at } z = 0 \tag{2b}$$

The system is initially in hydrostatic equilibrium, that is, $h+z$ is constant over the entire flow domain. The material properties for this problem are derived from van Genuchten and Nielsen's (1985) closed-form equation. For a moisture-content relation, Paniconi et al. (1991) modified van Genuchten and Nielsen's (1985) relation to permit a nonzero value of specific moisture capacity to occur in the saturated zone. The hydraulic conductivity and moisture-content equations are

$$K_r = \frac{K(h)}{K_s} = (1+\beta)^{-5m/2}[(1+\beta)^m - \beta^m]^2 \quad \text{if } h < 0 \tag{3a}$$

and

$$K_r = \frac{K(h)}{K_s} = 1 \quad \text{if } h \geqslant 0 \tag{3b}$$

and

$$\theta(h) = \theta_r + (\theta_s - \theta_r)(1+\beta)^{-m} \quad \text{if } h \leqslant h_0 \tag{4a}$$

and

$$\theta(h) = \theta_r + (\theta_s - \theta_r)(1+\beta_0)^{-m} + S_s(h - h_0) \quad \text{if } h > h_0 \tag{4b}$$

where $\beta=(|h/h_s|)^n$; h_s is the air entry (or bubbling) pressure head (L^{-1}); n is a fitting parameter in the moisture retention curve; and $m=1-1/n$. The residual water content is θ_r, and θ_s is the saturated moisture-content, which generally is equal to the porosity (η) of the formation; $\beta_0=(h_0/h_s)^n$ and S_s is the value of specific storage when the pressure head h is greater than h_0, which is a parameter determined on the basis of continuity requirements imposed on S_s, which implies that

$$S_s = \left.\frac{(n-1)(\theta_s - \theta_r)|h|^{n-1}}{|h_s|^n(1+\beta)^{m+1}}\right|_{h=h_0} \tag{5}$$

For a given S_s, Eq. (5) can be solved for h_0.

The specific moisture capacity $C(h)$ can be calculated from

$$C(h) = \frac{(n-1)(\theta_s - \theta_r)|h|^{n-1}}{|h_s|^n(1+\beta)^{m+1}} \quad \text{when } h \leqslant h_0; \tag{6a}$$

and

$$C(h) = S_s \quad \text{when } h > h_0 \tag{6b}$$

For $S_s=0$ and $h_0=0$, these modified equations revert to their original form in the van Genuchten and Nielsen (1985) equation.

Values for the parameters in Eqs. (3)-(6) and simulation parameters for SU3D are listed in Table 1. The soil column was discretized into 100 layers vertically for the finite-difference formulation. The pressure head values through the depth of the soil column after 1, 2, 4, 10, and 32 h of infiltration are shown in Fig. 2. The results of SU3D and Paniconi et al. (1991) are in very close agreement.

Table 1. Parameters Used in 1D Infiltration and Redistribution Problem of Paniconi et al. (1991)

Parameter	Value or expression
Flow domain	10-m soil column
Relative hydraulic conductivity $[K_r(h)]$	Eqs. (3*a*) and (3*b*)
Moisture content $[\theta(h)]$	Eqs. (4*a*) and (4*b*)
Saturated hydraulic conductivity (K_s)	5 m/h
Saturated moisture content (θ_s)	0.45
Residual moisture content (θ_r)	0.08
Bubbling (or air entry) pressure head (h_s)	−3.0 m
h_0	−0.19105548 m
van Genuchten parameter (n)	3
$m=1-1/n$	0.667
Specific storage ($h>h_0$) (S_s)	0.001 m^{-1}
Top boundary condition	Specified flux ($q=t/64$ m/h)
Bottom boundary condition	Constant head ($h=0$ m)
Initial pressure heads	Hydrostatic equilibrium ($h+z=0$)
Grid characteristics	Uniform grid with 100 elements
Nodal spacing (dz)	0.1 m
Time increment (dt)	Variable from 0.001 to 0.1 h
Maximum simulation time	32 h

1D Transient Infiltration in Layered Soils

Analytical solutions for 1D, transient infiltration toward the water table in layered soils developed by Srivastava and Yeh (1991) were used to test SU3D as a second example. In their solution, the Richards equation governing 1D vertical flow in the unsaturated zone was linearized using exponential hydraulic conductivity and moisture content versus pressure-head relations. Although the exponential relations may be very restricted for practical applications, they do serve as a means of verifying many numerical models for unsaturated flow, especially for infiltration in very dry,

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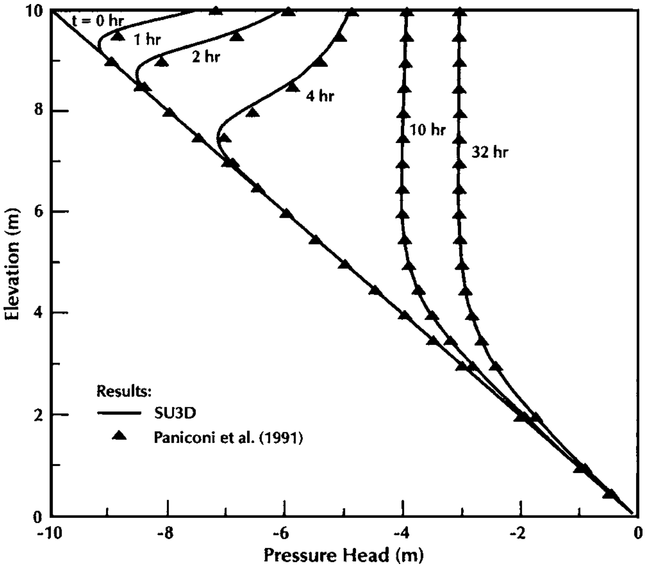

Fig. 2. Comparison of SU3D with Paniconi et al. (1991)

layered soils where numerical models often suffer from convergence and mass balance problems (Srivastava and Yeh 1991).

The following relations were used by Srivastava and Yeh (1991) for hydraulic conductivity and moisture content as a function of the pressure head

$$K = K_s e^{\alpha_h} \tag{7}$$

and

$$\theta = \theta_r + (\theta_s - \theta_r) e^{ah} \tag{8}$$

where K and K_s are unsaturated and saturated hydraulic conductivities (LT^{-1}), respectively; h is pressure head (L); θ_r and θ_s are residual and saturated moisture contents, respectively; and α (L^{-1}) is a soil pore-size distribution parameter representing the rate of reduction in hydraulic conductivity or moisture content as h becomes more negative.

In this problem, Srivastava and Yeh (1991) developed an analytical solution for layered soils by considering a case where the soil profile consists of two distinct soil layers. The datum ($z=0$) is assumed to be at the interface between the two layers, and L is the depth to the water table. The bottom boundary is a prescribed head boundary condition with $h_0=0$. At $t=0$, q_a is the initial flux at the soil surface, which determines the initial pressure distribution in the soil (along with h_0), and q_b is the prescribed flux at the soil surface for times greater than 0. For convenience, the following dimensionless parameters (indicated by *) were defined and used by Srivastava and Yeh (1991) in the rest of the equations, with subscript 1 denoting the lower layer and subscript 2 denoting the top layer:

$$z_* = \alpha_1 z \quad \text{for } -L_1 \leqslant z \leqslant 0.0 \text{ so that } L_{1^*-} = \alpha_1 L_1 \tag{9a}$$

$$z_* = \alpha_2 z \quad \text{for } 0.0 \leqslant z \leqslant L_2 \text{ so that } L_{2^*-} = \alpha_2 L_2 \tag{9b}$$

$$K_{1^*} = K_1/K_{s1}; \quad q_{a1} = q_a/K_{s1}; \quad q_{b1} = q_b/K_{s1} \tag{9c}$$

$$K_{2^*} = K_2/K_{s2}; \quad q_{a2} = q_a/K_{s2}; \quad q_{b2} = q_b/K_{s2} \tag{9d}$$

and

$$t_* = \frac{\alpha_1 K_{s1} t}{\theta_{s1} - \theta_{1r}} \tag{9e}$$

The initial condition in layer 1 (K_{*10}) is

$$K_{*10} = K_{*1}(z_*, 0) = q_{a1} - (q_{a1} - e^{\alpha_1 h_0}) e^{-(L_{1^*} + z_*)} \tag{10a}$$

and the initial condition in layer 2 (K*20) is

Table 2. Parameters Used in Analytical Solution of Srivastava and Yeh (1991) Representing 1D, Transient Infiltration in Layered Soils

	Value or expression		
Parameter	Layer 1		Layer 2
Flow domain	100-cm soil column		100-cm soil column
Hydraulic conductivity		Eq. (7)	
Moisture content		Eq. (8)	
Saturated hydraulic conductivity (K_s)	1.0 cm/h		10.0 cm/h
Saturated moisture content (θ_s)		0.40	
Residual moisture content (θ_r)		0.06	
q_a		0.1 cm/h	
q_b		0.9 cm/h	
α	0.1/cm		0.1/cm
Initial pressure heads	Eq. (10*a*)		Eq. (10*b*)
Bottom boundary condition	$h_0=0.0$ at $z=-L_1$		
Top boundary condition			Prescribed flux q_b
Nodal spacing (dz)	2 cm		2 cm
Time increment (dt)		Varies from 0.001 to 0.1 h	
Maximum simulation time		100 h	

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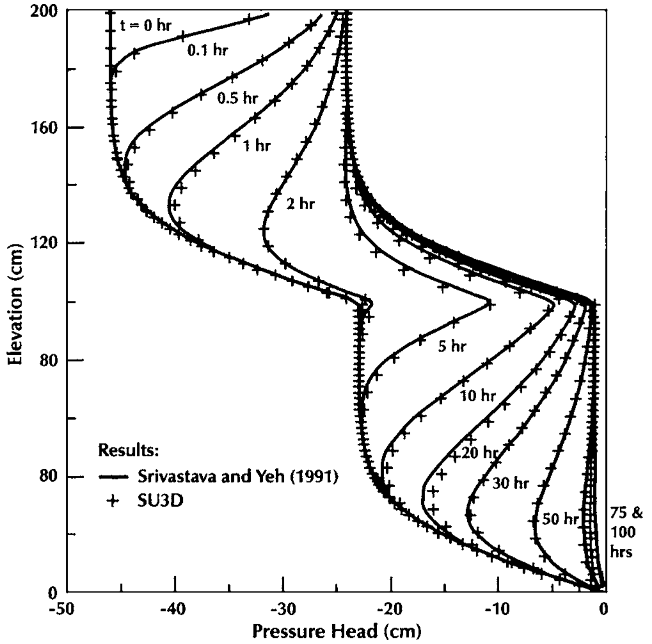

Fig. 3. Comparison of SU3D with analytical solution of Srivastava and Yeh (1991) for layered soils

$$K_{*20}=K_{*2}(z_*,0)=q_{a2}-\{q_{a2}-[q_{a1}-(q_{a1}-e^{\alpha_1 h_0})e^{-L_1{}^*}]^{\alpha_2/\alpha_1}\}e^{-z_*} \qquad (10b)$$

The initial heads are obtained by simultaneous solution of Eqs. (7) and (10). The parameters used in the Eqs. (9) and (10) are listed in Table 2. The results of the analytical solution of Srivastava and Yeh (1991) and SU3D for times of 0, 0.1, 0.5, 1, 2, 5, 10, 15, 20, 30, 50, 75, and 100 h are plotted in Fig. 3. There is an excellent match between SU3D and the analytical model.

Transient, 2D, Variably Saturated Water Table Recharge

A transient, 2D, variably saturated water table recharge problem described by Vauclin et al. (1979) was selected to test SU3D for a 2D case. The same example also was used by Clement et al. (1994) to verify their 2D variably saturated model. The flow domain consists of a rectangular soil slab 6.00 by 2.00 m, with an initial horizontal water table located at a height of 0.65 m. At the soil surface, a constant flux of $q=0.14791$ m/h was applied over a width of 1.00 m in the center. The remaining soil surface was covered to prevent evaporation losses.

Because of the symmetry, only the right side of the flow domain needs to be modeled. The modeled portion of the flow domain is 3.00×2.00 m, with no-flow boundaries on the bottom and on the left side because of the symmetry. At the soil surface, the constant flux of $q=0.14791$ m/h was applied over the left 0.50 m of the top of the modeled domain. The remaining 2.50-m soil surface at the top of the modeled area is a no-flow boundary. The water level at the right side of the model was maintained at 0.65 m as a fixed-head boundary, and a no-flow boundary was specified above the water table at the right side of the model domain.

The soil hydrologic properties from Vauclin et al. (1979) are listed in the Table 3. Clement et al. (1994) fitted the soil properties of Vauclin et al. (1979) to the van Genuchten (1980) model to estimate soil properties α_v and n_v in the van Genuchten model.

Table 3. Parameters Used in Transient, 2D, Variably Saturated Water Table Recharge Problem of Vauclin et al. (1979)

Parameter	Value or expression
Flow domain	3.00×2.00 m
Hydraulic conductivity $[K(h)]$	Eqs. (3*a*) and (3*b*)
Moisture content $[\theta(h)]$	Eqs. (4*a*) and (4*b*)
Saturated hydraulic conductivity (K_s)	0.35 m/h
Saturated moisture content (θ_s)	0.30
Residual moisture content (θ_r)	0.01
Bubbling (or air entry) pressure head ($h_s=1/\alpha$)	1/3.3 m
h_0	0.0 cm/h
van Genuchten parameter (n)	4.1
Specific storage (S_s)	0.0
Bottom boundary condition	Impervious no-flow boundary
Top boundary condition	Prescribed flux (left 0.50 m) and no-flow boundary (right 1.50 m)
Initial pressure heads	Hydrostatic equilibrium with horizontal water table at 0.65 m ($h+z=0.65$ m)
Grid characteristics	$30\times40=1{,}200$ cells with size of $dx=0.1$ m and $dz=0.05$ m
Time increment (dt)	Varies from 0.001 to 0.1 h
Maximum simulation time	8.00 h

The specific storage was neglected in this problem by Clement et al. (1994) because changes in storage are facilitated by the filling of pores, which overshadows the effects of compressibility. Therefore the specific storage coefficient in SU3D was set to zero for this example. The transient position of the water table for times of 0, 2, 3, 4, and 8 h is plotted in Fig. 4. The results obtained using SU3D closely agree with the experimentally observed values reported by Vauclin et al. (1979).

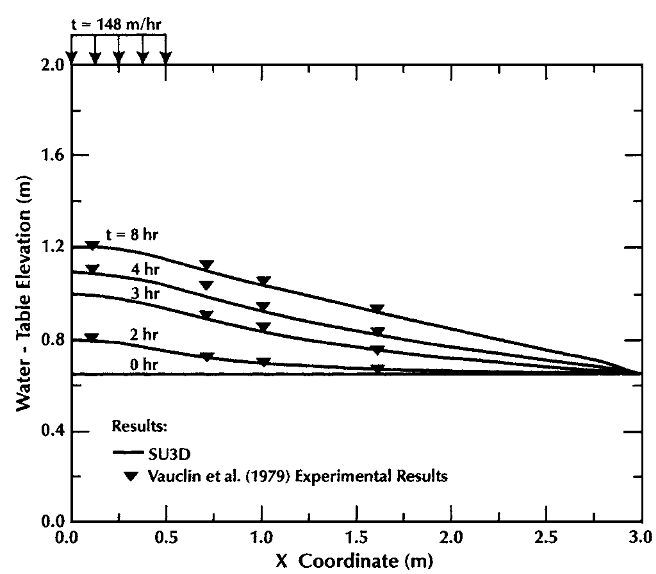

Fig. 4. Comparison of SU3D with experimental results of Vauclin et al. (1979)

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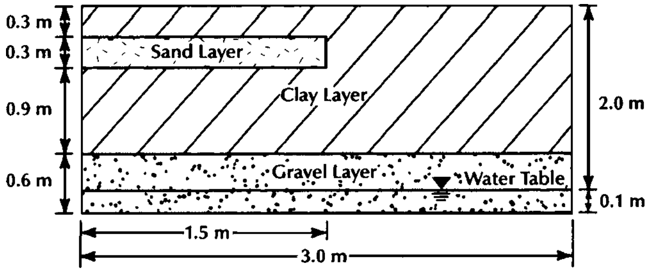

Fig. 5. Description of problem of Lappala et al. (1987)

2D Response to Rainfall and Evapotranspiration

The fourth example used to verify SU3D is a relatively complex 2D problem involving rainfall events, evaporation, and transpiration based on Lappala et al. (1987). The dimensions of the simulated section are shown in Fig. 5. Four recharge periods totaling 77 days were simulated. The first period was a 1-day rainfall event at a rate of 2.5 cm/day, the second period was a 30-day period with bare-soil potential evaporation of 0.2 cm/day, and the third period was a 1-day rainfall event at a rate of 2.5 cm/day. The fourth period was a 45-day period that consists of both evaporation and evapotranspiration.

The user-defined variables that control evaporation and evapotranspiration were assumed to remain constant throughout the simulation, with the exception of the PET, root depth, and root pressure. These parameters were varied linearly between each ET period, which is 30 days. This means that the parameter values are given for time=0, 30, 60, and 90 days, and the intermediate values of those parameters are calculated by linear interpolation between the known values at times 0, 30, 60, and 90 days.

The T_p values are 0, 0, 0.45, and 0.60 cm/day, and root depths are 0, 35, 35, and 35 cm for the four ET periods, respectively. Values of the root activity function $r(z,t)$ were 0.2 and 0.9 cm^{-2} at the top and at bottom of the root zone, respectively; E_p was 0.2 cm/day, surface resistance was 0.6 cm^{-1}, and atmospheric potential was −100,000 cm for all ET periods. The K_s values were 5, 100, and 300 cm/day; θ_s values were 0.45, 0.40, and 0.42; θ_r values were 0.15, 0.08, and 0.05; and the Brooks and Corey (1964) parameters h_b and λ_p were (−50 cm, 0.6), (−15 cm, 1.0), and (−8 cm, 1.2) for the clay, sand, and gravel layers, respectively.

The model domain was discretized into 26 layers and 22 columns that are variably spaced. The initial condition consists of an equilibrium head profile specified above a fixed water table at a depth of 2.0 m. The minimum pressure head was set at −1.00 m. The hydraulic properties of the three different soils were represented by the Brooks and Corey (1964) functions. During the second and fourth periods, when evaporation and transpiration occur, the initial time steps were decreased to 1.0×10^{-5} day to achieve convergence. The input parameters from Lappala et al. (1987) used in SU3D are summarized in Table 4.

The SU3D output file consists of pressure heads and moisture contents at four locations selected to be at the same depth of 0.33 m from land surface but at horizontal distances of 0.11, 1.46, 1.54, and 2.89 m from the left-hand side boundary. The first two locations are in the sand layer and the other two are in the clay layer. The results from SU3D and VS2D match very well for the pressure heads in the sand layer at all simulation times (Fig. 6).

During early time (before transpiration starts), the results in the clay layer are in agreement in both models, but at later times, especially after transpiration becomes more effective, the pressure heads calculated using SU3D are less than the pressure heads calculated using VS2D. This difference may be due to the hydraulic properties of the clay soil. Since SU3D solves the mixed form of the modified Richards equation, which is more mass conservative and more sensitive to the moisture content gradients, a small moisture-content change in the clay layer may require substantial pressure gradients, which may cause the differences in the results between the two models.

3D Pumping Problem Solved Using 3DFEMWATER

A 3D pumping problem was selected from 3DFEMWATER (Yeh and Cheng 1994). This example involves steady-state flow to a pumping well in a model domain bounded on the left and right by hydraulically connected rivers, on the front, back, and bottom by impervious rock formations, and on the top by the soil-air interface (Fig. 7). A pumping well was located at $(x,y)=(540,400\text{ m})$. Initially, the water table was assumed to be horizontal and 60 m above the bottom of the aquifer. The water level at the well was then lowered to an elevation of 30 m. This elevation was held until a steady-state condition was reached. The porous medium in the region was assumed to be anisotropic and to have saturated hydraulic conductivity components K_x=5 m/d, K_y=0.5 m/d, and K_z=2 m/d. The porosity of the medium was 0.25, and the residual moisture capacity was 0.0125. The unsaturated characteristic hydraulic properties of the medium were given by

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{1 + (\alpha|h_a - h|)^{\beta}} \tag{11}$$

and

$$K_r = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r}\right]^2 \tag{12}$$

where h_a, α, and β are parameters used to compute the water content and relative hydraulic conductivity. The values of h_a, α, and β are 0, 2.0, and 0.5, respectively.

The initial condition was set as H=60 m, or $h=60-z$. The boundary conditions are as follows: the pressure head is assumed hydrostatic on the two vertical planes located at $x=0$ and $0<z<60$, and $x=1{,}000$ and $0<z<60$, respectively; and no-flow boundaries are imposed on all the other boundaries of the flow domain.

The model domain was discretized using $27\times17\times100$ =45,900 node-centered cells. The discretization increments in the x-direction change from 20 to 50 m, while the increments in the y-direction are constant at 47 m. The discretization increments in the z-direction change from 0.25 m in the unsaturated zone to 20 m in the saturated zone. The input parameters from Yeh and Cheng (1994) used in SU3D are summarized in Table 5. A cross section in the $x-z$ plane passing through the center of the well shows that the results of SU3D and 3DFEMWATER match very closely (Fig. 8).

3D Field-Scale Unconfined-Aquifer Pumping Test

A pumping test problem described by Nwankwor et al. (1984) was used to test whether SU3D could be used to simulate a field-scale unconfined-aquifer pumping test. The unconfined aquifer in the test results reported by Nwankwor et al. (1984) is 9 m thick and composed primarily of horizontal discontinuous lenses of medium-grained, fine-grained, and silty fine-grained sand (Fig. 9).

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Table 4. Parameters Used in 2D Rainfall and Evapotranspiration Problem of Lappala et al. (1987)

Parameter	Value or expression			
Flow domain	3.0×2.1 m (Fig. 5)			
Hydraulic conductivity $[K(h)]$	Brooks and Corey (1964) (Eq. (22), Dogan and Motz (2005))			
Moisture content $[\theta(h)]$	Brooks and Corey (1964) (Eq. (21), Dogan and Motz (2005)			
Saturated hydraulic conductivity (K_s)	5.0 cm/day for clay 100.0 cm/day for sand 300.0 cm/day for gravel			
Saturated moisture content (θ_s) and residual moisture content, respectively	0.45-0.15 for clay 0.40-0.08 for sand 0.42-0.05 for gravel			
Brooks and Corey (1964) parameters (h_b and λ_p)	−50 cm, 0.6 for clay −15 cm, 1.0 for sand −8 cm, 1.2 for gravel			
Specific storage (S_s)	1.0×10^{-6} cm^{-1} for all materials			
Bottom boundary condition	Prescribed fixed pressure head (0.55 m)			
Top boundary conditions for four recharge periods	2.5 cm/day rainfall for 1 day (1st period) 0.2 cm/day potential evaporation for 30 days (2nd period) 2.5 cm/day rainfall for 1 day (3rd period) potential evapotranspiration for 45 days (4th period)			
Evapotranspiration parameters change linearly as time progresses	0th day	30th day	60th day	90th day
Potential transpiration (cm/day)	0.0	0.0	0.45	0.60
Root depth (cm)	0.0	35	35	35
Root pressure (cm)	−8,000	−8,000	−12,000	−15,000
Root activity at bottom	0.2	0.2	0.2	0.2
Root activity at top	0.9	0.9	0.9	0.9
Potential evaporation (cm/day)	0.2	0.2	0.2	0.2
Surface resistance (1/cm)	0.6	0.6	0.6	0.6
Atmospheric pressure potential (cm)	−100,000	−100,000	−100,000	−100,000
Initial condition	Hydrostatic equilibrium with horizontal water table at depth of 2.0 m			
Grid characteristics	22 cells in x-direction; dx values in cm: 22.5, 22.5, 15, 15, 15, 15, 11.25, 11.25, 7.5, 7.5, 7.5, 7.5, 7.5, 7.5, 11.25, 11.25, 15, 15, 15, 15, 22.5, and 22.5 26 cells in z-direction; dz values in cm: 3.0, 3.0, 3.0, 4.5, 4.5, 6.0, 6.0, 6.0, 6.0, 9.0, 9.0, 9.0, 9.0, 12.0, 15.0, 15.0, 12.0, 9.0, 6.0, 6.0, 6.0, 9.0, 9.0, 9.0, 9.0, and 15.0			
Time increment (dt)	Varies from 0.00001 to 0.15 day			
Maximum simulation time	77 days			

A thick deposit of clayey silt underlies the aquifer. The water table was located 2.3 m below land surface at the time the pumping test started. The pumped well has an inner diameter of 0.15 m with a 4.0 m screen located at the bottom of the aquifer. Water levels were measured by piezometers installed at different radial distances and terminated at different depths. The test lasted for 24 h at a discharge rate of 60 L/min. The instrumentation and test procedures are described in detail by Nwankwor et al. (1984, 1992).

The hydrologic properties developed by Akindunni and Gillham (1992) were used in this application. In their study, an h versus θ relationship was obtained from the laboratory drainage experiment reported by Nwankwor et al. (1984). Best-fit values for the van Genuchten (1980) parameters α and n were determined to be 6.095 and 1.9 m^{-1}, respectively. A K versus θ relationship was obtained from the laboratory experiment of Abdul (1985) by fitting data to the function

$$K_x(\theta) = K_y(\theta) = a\theta^b \tag{13}$$

Values of $a=43.17$ and $b=4.72$ were obtained by Akindunni and Gillham (1992).

The saturated principal hydraulic conductivity in the horizontal direction was obtained by Akindunni and Gillham (1992) from the results of a permeameter test reported by Sudicky (1986), while the vertical hydraulic conductivity was determined from the relation

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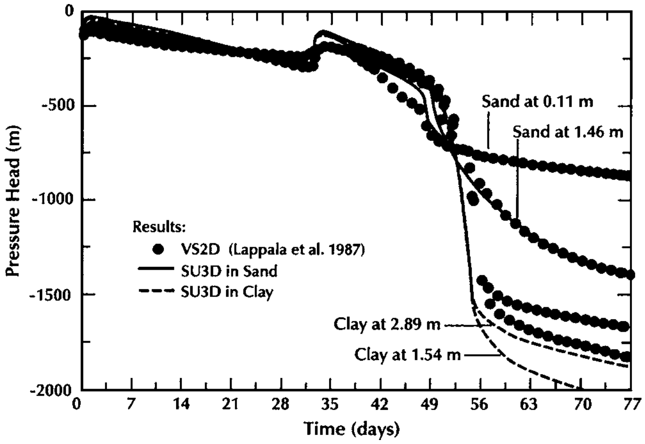

Fig. 6. Comparison of SU3D with VS2D from Lappala et al. (1987)

$$K_z = \frac{d}{\sum_{i=1}^{j} \frac{d_i}{K_i}} \tag{14}$$

where d is the length of the soil column for which hydraulic conductivity K_i was determined; d_i is the thickness of the layer; and j is the total number of layers used for evaluating the vertical hydraulic conductivity K_z. Anisotropy was determined to be

$$K_z(\theta) = 0.64 K_x(\theta) \tag{15}$$

Akindunni and Gillham (1992) calibrated the value of the principal hydraulic conductivity at saturation to improve the fit between the field data and their numerical results. The experimental horizontal saturated hydraulic conductivity value of 5.0×10^{-5} m/s was increased to 6.6×10^{-5} m/s, but this adjusted value was well within the range measured using slug tests (Nwankwor et al. 1984). Accordingly, the saturated hydraulic conductivities were taken as 6.6×10^{-5} m/s in the horizontal directions and 4.2×10^{-5} m/s in the vertical direction by Akindunni and Gillham (1992), which were the values used in this study.

The saturated moisture content of 0.37 and the residual moisture content of 0.07 used in this study were obtained from the water content profiles of Nwankwor et al. (1984). The specific storage, S_s, was obtained from Akindunni and Gillham (1992) as 3.25×10^{-4} m^{-1}. The top and the bottom boundary conditions are

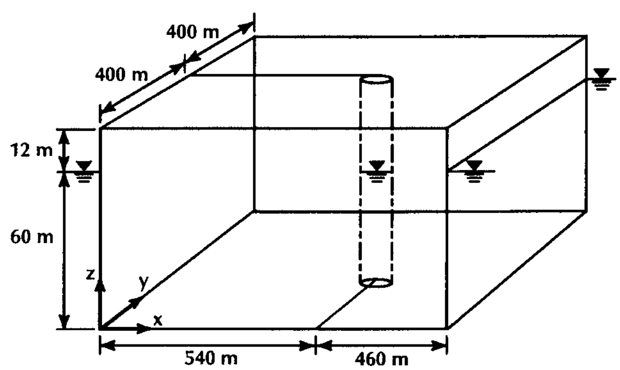

Fig. 7. Definition sketch for 3D pumping problem solved using 3DFEMWATER, modified from Yeh et al. (1992)

Table 5. Parameters Used in 3D Steady-State Pumping Problem Solved Using 3DFEMWATER, from Yeh and Cheng (1994)

Parameter	Value or expression
Flow domain	1,000 m $\times$ 800 m $\times$ 72 m (Fig. 7)
Relative hydraulic conductivity $[K_r = K(h)/K_s]$	Eq. (12)
Moisture content $[\theta(h)]$	Eq. (11)
Saturated hydraulic conductivity (K_s)	K_x=5 m/d, K_y=0.5 m/d, K_z=2 m/d
Saturated moisture content (θ_s)	0.25
Residual moisture content (θ_r)	0.0125
h_a	0
α	2.0
β	0.5
Bottom boundary condition	Impervious no-flow boundary
Top boundary condition	Land surface at 72 m above bottom of aquifer
Left and right boundary conditions	Hydraulically connected river (specified head H=60 m)
Front and back boundary conditions	Impervious no-flow boundary
Initial pressure heads	Hydrostatic equilibrium with horizontal water table 60 m above bottom of aquifer
Grid characteristics	27 $\times$ 17 $\times$ 100=45,900 cells withdx changing from 20 to 50 m, dy= 47 m, and dz changing from 0.25 min unsaturated zone to 20 m in saturated zone
Well location	x=540 m, y=400 m
Well pumping simulated by assuming	Well head=60 m at t=0
	Well head=30 m at t>0

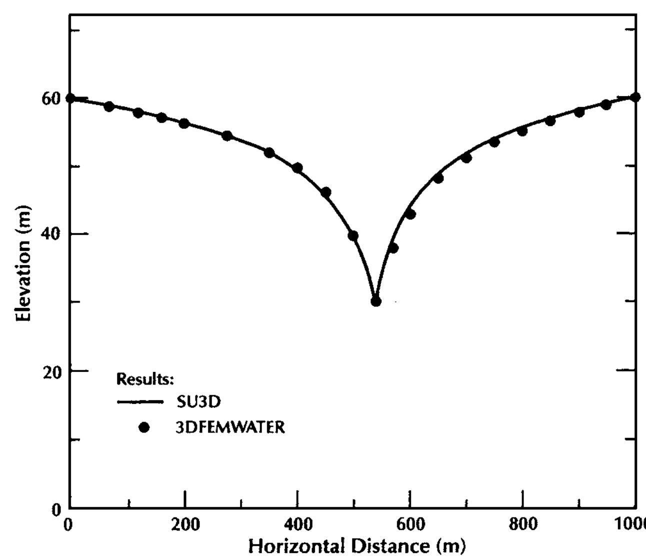

Fig. 8. Water table position at steady state for 3D pumping problem solved using SU3D and 3DFEMWATER, from Yeh and Cheng (1994)

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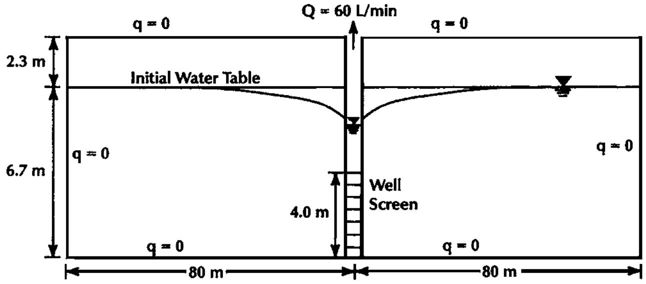

Fig. 9. Cross section of unconfined aquifer-pumping-problem of Nwankwor et al. (1992)

no-flow boundaries. The initial pressure heads were chosen to be in hydrostatic equilibrium with a horizontal water table at 2.3 m below land surface.

The domain was discretized for this study into a 3D variably sized grid. Finer discretization was used close to the well around the top of the screen. It was also necessary to extend the fine discretization to some distance above the top of the capillary fringe to ensure that a reasonable number of nodes were specified within the zone where the magnitude of specific water capacity and hydraulic conductivity varied significantly with changes in pressure head. The external boundary was kept at 100 m as a no-flow boundary condition to ensure that all the flow originated from the discretized flow domain. Only one quadrangle of the aquifer was modeled because of radial symmetry of the cone of depression around the pumped well. The quadrangle of the model domain was discretized into 49 layers, 49 rows, and 49 columns totaling 117,649 cells with various sizes of dx, dy, and dz, ranging from 0.08 m to 10 m (Table 6). The time increment, dt, was varied from 0.001 min to 1.0 min. The values of the parameters used in SU3D to reproduce the results of Nwankwor et al. (1984) are summarized in Table 7.

Table 7. Parameters Used to Reproduce Results of Unconfined-Aquifer Pumping Test of Nwankwor et al. (1984)

Parameter	Value or expression
Flow domain	$100 \times 100 \times 9$ m
Hydraulic conductivity $[K(h)]$	Eq. (13)
Moisture content $[\theta(h)]$	Van Genuchten (1980) relation
Saturated hydraulic conductivity (K_s)	$K_x = K_y = 6.6 \times 10^{-5}$ m/s $K_z = 4.2 \times 10^{-5}$ m/s
Saturated moisture content (θ_s)	0.37
Residual moisture content (θ_r)	0.07
van Genuchten (1980) parameters	$n = 6.095$ and $\alpha = 1.9$ m^{-1}
Specific storage (S_s)	3.25×10^{-4} m^{-1}
Bottom boundary condition	Impervious no-flow boundary
Top boundary condition	No-flow boundary
Initial pressure heads	Hydrostatic equilibrium with horizontal water table at 6.7 m
Grid characteristics	$49 \times 49 \times 49 = 117{,}649$ cells with various sizes of dx, dy, dz (Table 6)
Time increment (dt)	Varies from 0.001 to 1 min
Maximum simulation time	1,440 min (24 h)

Drawdowns versus time calculated using SU3D at horizontal distances of 5 and 15 m from the pumped well at a depth of 7 m below land surface are in good agreement with the field data reported by Nwankwor et al. (1992) (Fig. 10). The results indicate that SU3D can simulate the delayed yield effect observed in the

Table 6. Discretization Used in SU3D to Reproduce Unconfined-Aquifer Pumping Test Results of Nwankwor et al. (1984)

Row numbers	Δy (m)	Column numbers	Δx (m)	Layer numbers	Δz (m)
1	0.08	1	0.08	1–23	0.1
2	0.1	2	0.1	24–41	0.15
3–6	0.15	3–6	0.15	42–49	0.5
7–8	0.2	7–8	0.2		
9–10	0.25	9–10	0.25		
11–15	0.3	11–15	0.3		
16	0.4	16	0.4		
17–19	0.5	17–19	0.5		
20	0.6	20	0.6		
21–24	0.7	21–24	0.7		
25–30	0.8	25–30	0.8		
31–32	0.9	31–32	0.9		
33–35	1	33–35	1		
36–37	2	36–37	2		
38–40	3	38–40	3		
41	4	41	4		
42	5	42	5		
43	6	43	6		
44	7	44	7		
45	8	45	8		
46	9	46	9		
47–49	10	47–49	10		

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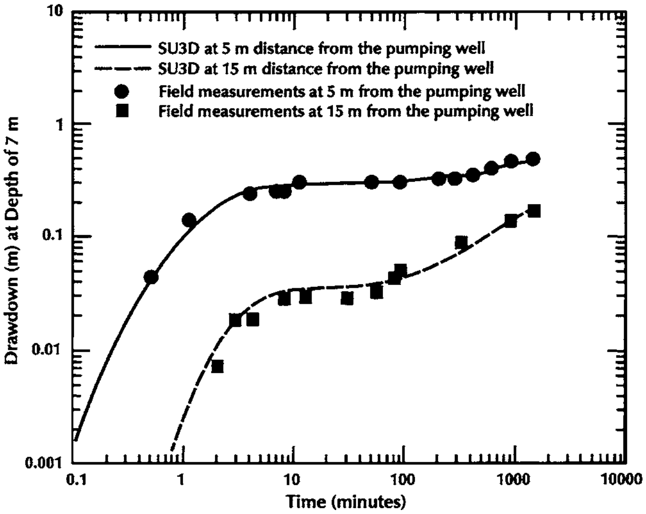

Fig. 10. Comparison of SU3D with pumping test results of Nwankwor et al. (1992)

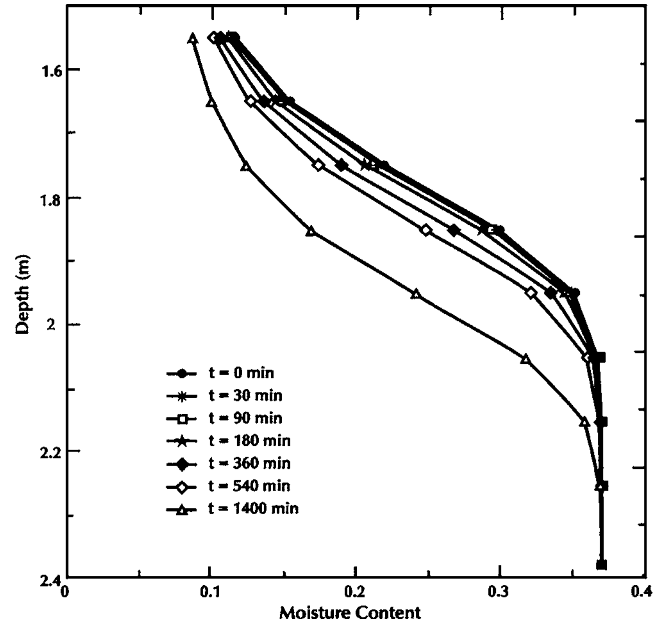

Fig. 12. Simulated moisture content versus depth and time in unsaturated zone above initial water table at 15 m from the pumping well

time-drawdown curves in the field study of Nwankwor et al. (1992). Moisture content versus depth in the unsaturated zone above the initial water table was simulated for selected times and horizontal distances of 5 and 15 m from the pumped well (Figs. 11 and 12). These results illustrate the changes in moisture content that occur in the unsaturated zone in response to water table drawdowns during pumping.

Summary

This paper presents verification and application for a 3D variably saturated numerical groundwater flow model (SU3D) (Dogan and Motz 2005). This model can simulate most hydrologic events with the exception of surface runoff, which is assumed to be a loss term from rainfall after ponding starts. The mixed form of the modified Richards equation is solved using the modified Picard iteration scheme based on Celia et al. (1990). The resultant system of equations is solved using the preconditioned conjugate gradient method, which is very robust and converges to a solution relatively quickly if a good preconditioner matrix is provided. Sink and source terms that include pumping, recharge, and drains can be simulated in SU3D. Rainfall and evaporation are simulated as upper boundary conditions. Actual transpiration calculations can be done using two options, and the model has a subprogram to calculate potential evapotranspiration from climatologic data (Dogan 1999)). SU3D (Dogan and Motz 2005) has been successfully applied to match the results of five analytical and numerical examples and a field-scale unconfined-aquifer pumping test. The results of these simulations indicate that SU3D can be used to solve hydrogeological problems in one, two, and three dimensions.

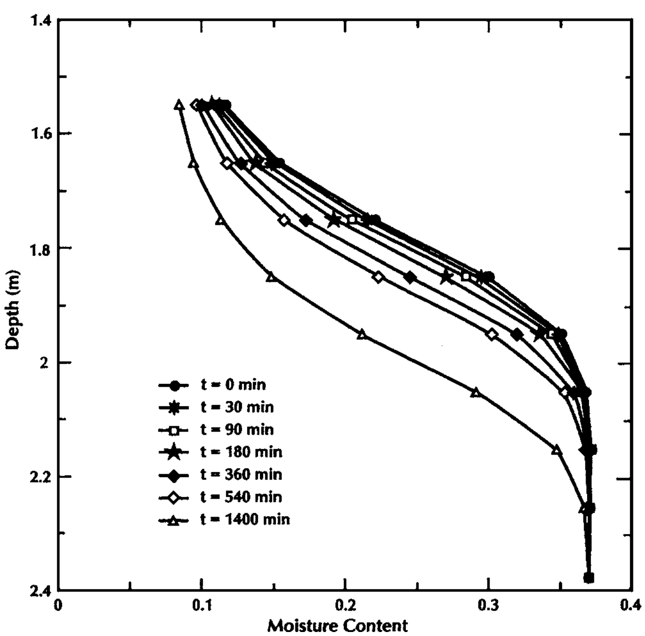

Fig. 11. Simulated moisture content versus depth and time in unsaturated zone above initial water table at 5 m from pumping well

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Notation

$C(h)$ = specific moisture capacity (L^{-1});
dt = time increment (T);
dz = vertical nodal spacing (L);
E_p = potential evaporation (LT^{-1});
h = pressure head (L);

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h_b = Brooks and Corey (1964) parameter (L);
$h_{p\,\max}$ = maximum ponding depth (L);
h_s = bubbling (or air entry) pressure head (L);
h_0 = parameter in van Genuchten and Nielsen's (1985) closed-form equation;
K = hydraulic conductivity (LT^{-1});
$K(h)$ = hydraulic conductivity as function of pressure head h (LT^{-1});
K_r = relative hydraulic conductivity;
K_s = saturated hydraulic conductivity (LT^{-1});
m = fitting parameter in moisture-retention curve;
n = fitting parameter in moisture-retention curve and ($m = 1 - 1/n$);
Q_{ext} = volumetric source or sink term ($L^3L^{-3}T^{-1}$);
S_s = specific storage (L^{-1});
S_w = saturation ratio;
T_p = potential transpiration (LT^{-1});
α = soil pore-size distribution parameter representing rate of reduction in hydraulic conductivity and moisture content (L^{-1});
α_v = van Genuchten (1980) soil parameter that is measure of first moment of pore-size density function (L^{-1});
β = parameter in van Genuchten and Nielsen's (1985) closed-form equation $= (|h_0/h_s|)^n$;
β_0 = parameter in van Genuchten and Nielsen's (1985) closed-form equation $= (h_0/h_s)^n$;
η = porosity;
θ = moisture content;
θ_r = residual water content;
θ_s = saturated moisture content; and
λ_p = pore-size distribution index in Brooks and Corey (1964) equation.

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