A CONVERGENT EXPLICIT GROUNDWATER MODEL

Victor M. Ponce

Professor, Department of Civil and Environmental Engineering,

San Diego State University, San Diego, California 92182-1324 USA

Ampar V. Shetty

Scientist 'C', National Institute of Hydrology, Roorkee, India.

Sezar Ercan

Hydrologist, State Hydraulics Works, Ankara, Turkey.

ABSTRACT: A groundwater model is developed by using an explicit formulation of the two-dimensional diffusion equation of flow in porous media for a homogeneous isotropic aquifer. Appropriate sources/sinks and head/flux or permeable/impermeable boundaries can be specified. The model is stable for cell Reynolds number $D \leq 1$. Numerical tests under a wide range of conditions show that the model is convergent only for $D = 1$. Hypothetical tests show that the model is able to simulate groundwater flow with excellent stability, convergence, and mass-conservation properties.

INTRODUCTION

A stable-and-convergent numerical groundwater model is developed herein. Stability being a necessary condition for model operation, the emphasis is on convergence, i.e., whether the numerical model can reproduce the differential equation with sufficient accuracy.

A significant feature of the model is its simplicity, which makes it attractive and useful for a wide variety of applications, including water quality. The numerical model is an explicit formulation of the two-dimensional (x-y) diffusion equation of flow in porous media for a homogeneous isotropic aquifer. Sources (percolation from rainfall and/or irrigation) and sinks (pumping) are accounted for in the formulation. Boundary conditions are specified as head or flux, and permeable or impermeable.

A specific focus of the model development is the assessment of stability and convergence. Explicit models are subject to a strict stability criterion, which must be satisfied if the model is to simulate natural conditions in a realistic way (O'Brien et al. 1949; Douglas 1956). As shown herein, the model must also satisfy a convergence criterion if accuracy is to be maintained. The satisfaction of both stability and convergence requires that the cell Reynolds number D be equal to 1.

After more than 20 years of implicit model development of groundwater flow, the choice of an explicit model at this juncture requires further explanation. It is well known that implicit models are unconditionally stable. Lesser known is the fact that implicit models are subject to a convergence criterion which effectively places an upper limit on the time step. Examples of lack of convergence in surface-water and sediment-transport modeling have been documented by Ponce et al. (1978; 1979). Thus, when their additional complexity is factored in, implicit models may not be necessarily better than explicit models.

MODEL FORMULATION

The three-dimensional diffusion equation for flow through porous media is (Rushton and Redshaw 1979; Kresic 1997):

$$\frac{\partial}{\partial x}(K_x \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(K_y \frac{\partial h}{\partial y}) + \frac{\partial}{\partial z}(K_z \frac{\partial h}{\partial z}) + W = S_s \frac{\partial h}{\partial t} \tag{1}$$

in which h = piezometric head [L]; K_x, K_y, and K_z are the hydraulic conductivities along the x, y, and z coordinate axes, respectively [L T^{-1}]; W = volumetric flux per unit volume, representing sources (+) or sinks (-) [T^{-1}]; S_s = specific storage of the porous material [L^{-1}]; and t = time.

In two dimensions in plan, Eq. 1 simplifies to:

$$\frac{\partial}{\partial x}(K_x \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(K_y \frac{\partial h}{\partial y}) + W = S_s \frac{\partial h}{\partial t} \tag{2}$$

Assuming a homogeneous isotropic aquifer of hydraulic conductivity K:

$$K(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}) + W = S_s \frac{\partial h}{\partial t} \tag{3}$$

Defining the hydraulic diffusivity of the aquifer (Freeze and Cherry 1979) as

$$\nu = \frac{K}{S_s} \tag{4}$$

leads to

$$\nu(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}) + \frac{\nu W}{K} = \frac{\partial h}{\partial t} \tag{5}$$

Equation 5 represents two-dimensional flow in a homogeneous isotropic aquifer of properties K and ν and source/sink term W. A simple and appropriate finite-difference scheme of first order in time and second order in space is (Fig. 1):

$$\frac{h_{j,k}^{n+1} - h_{j,k}^{n}}{\Delta t} = \nu\,\frac{h_{j+1,k}^{n} - 2h_{j,k}^{n} + h_{j-1,k}^{n}}{(\Delta x)^2} + \nu\,\frac{h_{j,k+1}^{n} - 2h_{j,k}^{n} + h_{j,k-1}^{n}}{(\Delta y)^2} + (\frac{\nu}{K})W_{j,k} \tag{6}$$

The spatial interval is set as $\Delta s = \Delta x = \Delta y$. Following Roache (1972), we define a type of cell Reynolds number as the ratio of physical and numerical diffusivities. This leads to:

$$D = \frac{\nu}{\frac{(\Delta s/2)^2}{\Delta t}} = 4\nu\,\frac{\Delta t}{(\Delta s)^2} \tag{7}$$

Eq. 6 reduces to

$$h_{j,k}^{n+1} = D\overline{h}_{j,k}^{\,n} + (1-D)h_{j,k}^{n} + (\frac{\nu\Delta t}{K})W_{j,k} \tag{8}$$

in which

$$\overline{h}_{j,k}^{\,n} = \frac{h_{j+1,k}^{n} + h_{j-1,k}^{n} + h_{j,k+1}^{n} + h_{j,k-1}^{n}}{4} \tag{9}$$

The time-averaged source term in velocity units is

$$W_{j,k} = \frac{r_{j,k}}{b} \tag{10}$$

in which $r_{j,k}$ = percolation rate [L T^{-1}] (due to rainfall and/or irrigation) at spatial node (j,k), and b = aquifer depth [L].

The time-averaged sink term in discharge units is

$$W_{j,k} = -\frac{p_{j,k}}{b(\Delta s)^2} \tag{11}$$

in which $p_{j,k}$ = pumping rate [L^3 T^{-1}] at spatial node (j,k).

Since transmissivity

$$T = Kb \tag{12}$$

and diffusivity

$$\nu = \frac{T}{S} \tag{13}$$

in which S = storage coefficient (Freeze and Cherry 1979), Eq. 8 reduces to

$$h_{j,k}^{n+1} = D\overline{h}_{j,k}^{\,n} + (1-D)h_{j,k}^{n} + (\frac{\Delta t}{S})r_{j,k} - \left[\frac{\Delta t}{S(\Delta s)^2}\right]p_{j,k} \tag{14}$$

With Eqs. 7 and 13, Eq. 14 reduces to

$$h_{j,k}^{n+1} = D\overline{h}_{j,k}^{\,n} + (1-D)h_{j,k}^{n} + \left[\frac{D(\Delta s)^2}{4T}\right] r_{j,k} - (\frac{D}{4T})p_{j,k} \tag{15}$$

For the special case $D = 1$, Eq. 15 reduces to

$$h_{j,k}^{n+1} = \overline{h}_{j,k}^{\,n} + \left[\frac{(\Delta s)^2}{4T}\right] r_{j,k} - (\frac{1}{4T})p_{j,k} \tag{16}$$

Equation 15 calculates piezometric head at the unknown node $(j, k, n+1)$ based on the average piezometric head $\overline{h}_{j,k}^{\,n}$ at the four known nodes adjacent to (j, k, n), the percolation rate $r_{j,k}$, the pumping rate $p_{j,k}$, the space interval Δs, and the transmissivity T (Fig. 1).

BOUNDARY CONDITIONS

The boundary conditions can be of Dirichlet or Neumann type (Kinzelbach 1986). Dirichlet conditions specify the head h; Neumann conditions specify the flux, i.e., the head gradient $\partial h/\partial x$ orthogonal to the boundary. In general, Dirichlet conditions lead to a permeable boundary, since the flux is usually finite. Neumann conditions are type A (permeable) or type B (impermeable). A Neumann type A condition specifies a finite gradient, i.e., $\partial h/\partial x \neq 0$; conversely, a Neumann type B condition specifies a zero gradient, i.e., $\partial h/\partial x = 0$.

Neumann type A boundaries may be specified by linear extrapolation from the two immediately neighboring interior nodes. Linear extrapolation results in a finite gradient, which amounts to a permeable boundary. Neumann type B boundaries may be specified by relocation of the neighboring interior node. Relocation results in a zero gradient, which amounts to an impermeable boundary.

Mixed Neumann type A/type B conditions, appropriate for semipermeable boundaries or temporally varying inflows, can be specified as follows:

$$h_{j,k}^{n+1} = (1+\alpha)h_{j-1,k}^{n+1} - \alpha h_{j-2,k}^{n+1} \qquad (17)$$

in which j = boundary node, and α = weighting factor, varying in the range $0 \leq \alpha \leq 1$, such that $\alpha = 0$ represents an impermeable boundary and $\alpha = 1$ a permeable boundary.

MODEL TESTING

The computations were performed using a SUN Sparc Ultra 10 Unix workstation. The model was subjected to the following four tests to examine its numerical properties:

1. *Permeable hot-start test*

   This condition tests the model's ability to return to the steady-equilibrium baseline condition following the specification of (a) a depleted water table as initial condition, (b) permeable boundaries, and (c) no pumping.

2. *Permeable cold-start test*

   This condition tests the model's ability to achieve a steady-equilibrium cone of depression following the specification of (a) the baseline steady-equilibrium initial condition, (b) permeable boundaries, and (c) pumping.

3. *Impermeable hot-start test*

   This condition tests the model's ability to return to a steady-equilibrium non-baseline condition following the specification of (a) a depleted water table as initial condition, (b) impermeable boundaries, and (c) no pumping.

4. *Impermeable cold-start test*

   This condition tests the model's ability to simulate the linear depletion of the aquifer following the specification of (a) the baseline steady-equilibrium initial condition, (b) impermeable boundaries, and (c) pumping.

Convergence testing

First, the groundwater model was tested for convergence (O'Brien et al. 1949). For this purpose, a permeable hot-start test was used, wherein the head recovery to steady-equilibrium baseline condition is a proof of the model's convergence.

The test prototype specification was a 100-km^2 square aquifer (10 km $\times$ 10 km) of transmissivity T = 0.01 m^2 s^{-1} and storage coefficient S = 0.1. Given Eq. 13, the hydraulic diffusivity is $\nu = 0.1$ m^2 s^{-1}. The space interval was set as $\Delta s = 100$ m, i.e., a total of 101 $\times$ 101 = 10201 grid nodes, labeled (0,0) to (100,100).

Stability requires that $D \leq 1$. Therefore, $D = 1$ is the maximum cell Reynolds number that can be used in practice. For $D = 1$, the time interval is fixed at (Eq. 7):

$$\Delta t = \frac{(\Delta s)^2}{4\nu} \tag{18}$$

A series of sixteen (16) runs were performed to test the convergence of the groundwater model under varying cell Reynolds number D and reference head h_{ref} (steady-equilibrium baseline condition). The initial condition was specified as h_0 = (h_{ref} - 100) in a square area of 5 km $\times$ 5 km located in the middle of the computational field (51 $\times$ 51 = 2601 grid nodes).

Four cell Reynolds numbers (D = 1.0, 0.5, 0.25, and 0.125) and four reference heads

(h_{ref} = 100, 200, 400 and 800 m) were chosen for the test series. The aquifer bottom was set at $h_{bottom} = 0$ m. From Eq. 18, the time interval for $D = 1.0$ is $\Delta t = 6.944$ hr. Therefore, the time intervals to be used in the test series are: Δt = 6.944, 3.472, 1.736, and 0.868 hr, corresponding to D = 1.0, 0.5, 0.25, and 0.125, respectively.

Figures 2 (a) to (d) show head recovery at centerfield node (50, 50) for reference heads h_{ref} = 100, 200, 400, and 800 m, and cell Reynolds numbers D = 1.0, 0.5, 0.25, and 0.125. For values other than $D = 1$, a head recovery deficit is present, signaling the model's inability to return to steady-equilibrium baseline condition, i.e., lack of convergence. Table 1 shows head recovery deficit h_{def} as a function of reference head h_{ref} and cell Reynolds number D.

The following conclusions are drawn from Fig. 2 and Table 1:

1. The head recovery deficit $h_{ref} = 0$, i.e., the head recovery is complete, only for $D =$ 1.

2. Head recovery deficit increases nonlinearly with decreases in cell Reynolds number from 1.0 to 0.125.

3. Head recovery deficit increases linearly with increases in reference head from 100 to 800 m.

4. The condition $D = 1$ is not only the most accurate but also the most economical. For smaller values of D, the model is less convergent and the run takes more processor and total time to complete.

The permeable/impermeable hot/cold tests were carried out by specifying the same geometry and aquifer properties as for the convergence test runs. The cell Reynolds number was set at $D = 1$, which leads to $\Delta t = 6.944$ hr.

For the "hot" tests, the reference head is set at $h_{ref} = 500$ m and the initial condition is specified as $h_0 = (h_{ref}$ - 100) in a square area of 5 km $\times$ 5 km located in the middle of the computational field. The aquifer bottom is set at $h_{bottom} = 0$ m. Then, the steady-equilibrium aquifer volume is 50,000 hm^3.

For the "cold" tests, the reference head $h_{ref} = 500$ m is specified as initial condition at every node and the aquifer bottom is set at $h_{bottom} = 0$ m. Thus, the steady-equilibrium aquifer volume is 50,000 hm^3. A battery of 17 pumps is symmetrically positioned across the field, at a distance of 1,414.2 m apart, making the shape of an X (Fig. 3), and each pumping $p = 250$ L s^{-1}.

Permeable hot-start test

The initial aquifer volume is 47,399 hm^3. The piezometric level returned to steady-equilibrium condition ($h = 500$ m at every node) in an asymptotic fashion after 15.85 yr of simulation (Fig. 4). The simulation was strongly stable and convergent. The calculated aquifer volume, after attainment of the steady-equilibrium condition, was 50,000 hm^3.

Permeable cold-start test

The initial aquifer volume is 50,000 hm^3. The piezometric level reached a steady-equilibrium condition, with the maximum depletion ($h = 441.662$ m) at the centerfield node (50,50), in an asymptotic fashion after 12.43 yr of simulation (Fig. 5). The simulation was strongly stable. The calculated aquifer volume was 48,218 hm^3. The volume conservation, calculated by taking the initial aquifer volume, subtracting the pumped volume and adding the boundary inflows, was 99.98 percent at the end of the 20-yr simulation.

Impermeable hot-start test

The initial aquifer volume is 47,399 hm^3. The piezometric level reached a steady-equilibrium condition (h = 473.462 m at every node) in an asymptotic fashion after 8.34 yr of simulation (Fig. 6). The simulation was strongly stable. The calculated aquifer volume, after achievement of the steady-equilibrium condition, was 47,349 hm^3. The volume conservation, calculated as the ratio of calculated to initial aquifer volume, was 99.89 percent at the end of the 20-yr simulation.

Impermeable cold-start test

The initial aquifer volume is 50,000 hm^3. The piezometric level decreased in a linear fashion, with the maximum depletion (h = 203.905 m) at the center-field node (50,50) after 20 yr of simulation (Fig. 7). The simulation was strongly stable. The calculated aquifer volume at the end of the 20-yr simulation was 22,687 hm^3, i.e., 45.37% of the initial aquifer volume.

SUMMARY AND CONCLUSIONS

A stable-and-convergent two-dimensional groundwater model of a homogeneous isotropic aquifer has been developed and tested under a wide range of flow conditions. The model is explicit and can account for sources/sinks and head/flux or permeable/impermeable boundaries. A significant feature of the model is that it sets the cell Reynolds number D = 1 to satisfy both stability and convergence.

Testing of the model under hypothetical conditions showed that the model is stable, convergent, and mass-conservative. The permeable hot-start test converged to the steady-equilibrium baseline condition after 15.85 yr. The permeable cold-start test converged to a steady-equilibrium cone of depression after 12.43 yr. The impermeable hot-start test converged to a steady-equilibrium non-baseline condition after 8.34 yr. The impermeable cold-start test properly simulated the linear depletion of the aquifer.

APPENDIX I. REFERENCES

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APPENDIX II. NOTATION

b = aquifer depth;

D = cell Reynolds number, Eq. 7;

h = piezometric head;

j = spatial index, x-direction;

k = spatial index, y-direction;

K = hydraulic conductivity;

K_x = hydraulic conductivity, x-direction;

K_y = hydraulic conductivity, y-direction;

K_z = hydraulic conductivity, z-direction;

n = temporal index;

p = pumping rate, in discharge units;

r = percolation rate, in velocity units;

S = storage coefficient;

S_s = specific storage;

t = temporal variable;

T = transmissivity, Eq. 12;

W = volumetric flux per unit volume;

x = spatial variable;

y = spatial variable;

Δs =space interval;

Δt =time interval, Eq. 18;

Δx =space interval, x-direction;

Δy = space interval, y-direction; and

ν = hydraulic diffusivity, Eqs. 4 and 13.

FIGURE CAPTIONS

Fig. 1 Notation for finite-difference scheme.

Fig. 2 (a) Head recovery at centerfield node (50,50) for $h_{ref} = 100$ m.

Fig. 2 (b) Head recovery at centerfield node (50,50) for $h_{ref} = 200$ m.

Fig. 2 (c) Head recovery at centerfield node (50,50) for $h_{ref} = 300$ m.

Fig. 2 (d) Head recovery at centerfield node (50,50) for $h_{ref} = 400$ m.

Fig. 3 Pump locations for cold-start tests.

Fig. 4 Head at centerfield node (50,50) for permeable hot start test.

Fig. 5 Head at centerfield node (50,50) for permeable cold start test.

Fig. 6 Head at centerfield node (50,50) for impermeable hot start test.

Fig. 7 Head at centerfield node (50,50) for permeable cold start test.