Groundwater

A New Package in MODFLOW to Simulate Unconfined Groundwater Flow in Sloping Aquifers

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Abstract

The nonhorizontal-model-layer (NHML) grid system is more accurate than the horizontal-model-layer grid system to describe groundwater flow in an unconfined sloping aquifer on the basis of MODFLOW-2000. However, the finite-difference scheme of NHML was based on the Dupuit-Forchheimer assumption that the streamlines were horizontal, which was acceptable for slope less than 0.10. In this study, we presented a new finite-difference scheme of NHML based on the Boussinesq assumption and developed a new package SLOPE which was incorporated into MODFLOW-2000 to become the MODFLOW-SP model. The accuracy of MODFLOW-SP was tested against solution of Mac Cormack (1969). The differences between the solutions of MODFLOW-2000 and MODFLOW-SP were nearly negligible when the slope was less than 0.27, and they were noticeable during the transient flow stage and vanished in steady state when the slope increased above 0.27. We established a model considering the vertical flow using COMSOL Multiphysics to test the robustness of constrains used in MODFLOW-SP. The results showed that streamlines quickly became parallel with the aquifer base except in the narrow regions near the boundaries when the initial flow was not parallel to the aquifer base. MODFLOW-SP can be used to predict the hydraulic head of an unconfined aquifer along the profile perpendicular to the aquifer base when the slope was smaller than 0.50. The errors associated with constrains used in MODFLOW-SP were small but noticeable when the slope increased to 0.75, and became significant for the slope of 1.0.

Introduction

Groundwater flow in hillslope aquifers has some unique features that are not commonly seen in flow in horizontally extended aquifers (Tsai 2011; Iverson and Major 1986). One of such features is that the sediment strata in the hillslope region are not always horizontal, sometime the slope is very steep and changes dramatically over spatial scales of interest (Broda et al. 2012; Ye and Khaleel 2008). An aquifer with a nonhorizontal base is called a sloping aquifer hereinafter.

The natural groundwater movement is controlled by a variety of stratigraphic and structural units in sedimentary environments (Toth 2009). The mechanism of groundwater flow in a sloping aquifer was found to be different from that in a horizontal aquifer more than one hundred years ago (Dupuit 1863; Boussinesq 1877). The first approach to handle this kind of problems was proposed by Dupuit (1863), named as the Dupuit-Forchheimer method which assumed that the streamlines of groundwater flow can be taken as horizontal, and the hydraulic gradient was equal to the slope of the free surface and did not vary with depth, that is, $\mathrm{d}H/\mathrm{d}z = 0$, where H and z were the hydraulic head and the vertical coordinate, respectively. A careful check of the Dupuit-Forchheimer method showed that this method did not preclude vertical flow in the aquifer (or model-layer), but merely implied that the resistance to vertical flow was ignored instead of vertical flow itself, as demonstrated in details by Kirkham (1967) and Strack (1984). Nevertheless, the implication that $\mathrm{d}H/\mathrm{d}z = 0$ always held, regardless of the interpretation of the Dupuit-Forchheimer method. The Dupuit-Forchheimer method was demonstrated to be a good approximation for an unconfined aquifer whose base slope was less than 0.10 or sloping angle was less than 5.7° (Bear 1972). However, errors associated with this approach increased quite significantly with increasing base slopes (Schmid and Luthin 1964; Wooding 1966; Wooding and Chapman 1966; Childs 1971; Chapman 1980). To tackle the problems with greater base slopes (more than 0.1),

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Boussinesq (1877) extended the Dupuit-Forchheimer method by assuming that the streamlines were nearly parallel with the sloping base. This assumption usually involved two different kinds of coordinate systems: one had the x-axis parallel to the horizontal direction and the other had the x-axis parallel to the sloping base (called the s-axis hereinafter). Since the variables in the approach of Boussinesq (1877) involved two different coordinate systems, it was sometimes difficult to obtain the solutions directly. Childs (1971) and Wooding and Chapman (1966) derived two corresponding formulas in the x-z and the s-z coordinate systems, respectively. The x-z coordinate system was an orthogonal Cartesian coordinate system with the x-axis horizontal and the z-axis vertical. The s-z coordinate system was a skewed Cartesian coordinate system with the s-axis along the sloping base and the z-axis vertical. Up to present, these two formulas became the basis to solve problems related to the unconfined groundwater flow in sloping aquifers.

Early works on the subject mainly focused on the steady seepage between ditches or rivers in a sloping unconfined aquifer with recharge (Schmid and Luthin 1964; Wooding and Chapman 1966; Childs 1971; Chapman 1980). Subsequently, many hydrogeologists devoted significant efforts to develop analytical solutions of transient flow in sloping aquifers (Chauhan et al. 1968; Beven 1981; Brutsaert 1994; Verhoest and Troch 2000; Upadhyaya and Chauhan 2001; Zissis et al. 2001; Verhoest et al 2002; Stagnitti et al. 2004; Bansal and Das 2011; Asadi-Aghbolaghi et al. 2012; Bansal 2012). Among these analytical solutions, Upadhyaya and Chauhan (2001) and Asadi-Aghbolaghi et al. (2012) adopted the Dupuit-Forchheimer assumptions. Beven (1981), Brutsaert (1994), Verhoest and Troch (2000), Stagnitti et al. (2004) and Verhoest et al. (2002) derived solutions in the s-z coordinate system based on the Boussinesq assumption. Zissis et al. (2001), Bansal and Das (2011), and Bansal (2012) presented solutions in the x-z coordinate system, also based on the Boussinesq assumption. Regardless of the skewed or orthogonal coordinate system used, a linearization method was inevitably adopted in above analytical solutions to deal with the nonlinear governing equations of flow.

To check the accuracy of the linearization method used in above analytical solutions, carefully designed numerical solutions were needed. Chapuis (2011) employed a finite-element solution by Seep/W (Geo-Slope 2003) to assess the robustness of the steady-state analytical solutions. Mac Cormack (1969) (reprint Mac Cormack [2003]) developed a robust finite-difference computational scheme for transient compressible Navier–Stokes equations, which was conditionally stable and convergent. The numerical scheme of Mac Cormack (1969) was subsequently applied for unconfined flow in sloping aquifers (Zissis et al. 2001; Bansal 2012). The commonly used MODFLOW model (McDonald and Harbaugh 1988) can be employed to deal with unconfined flow in a sloping aquifer if one used a sufficiently large number of layers for vertical discretization to describe the sloping base. Unfortunately, this may be numerically infeasible because of a few limitations of graphically-aided commercial MODFLOW packages such as Visual MODFLOW. Firstly, the maximum number of layers used in MODFLOW-2000 (McDonald and Harbaugh 1988) was limited (usually less than 200 in Visual MODFLOW). Secondly, even one was able to use a large number of layers; the resulting small layer thickness could make it very time consuming to assign the inactive cells above the initial water table which may not be located in the first layer. Although both limitations may be resolved by modifying the original program of MODFLOW, another problem related to convergence cannot be handled easily. For example, we tried to use MODFLOW-2000 to simulate unconfined groundwater flow employing parameters in Figures 4 and 5. In doing so, we used more than 100 layers and considered inactive cells above the initial water table. As a result, we found that the simulation was either divergent or ended in physically unrealistic results. To overcome such difficulty, one alternative approach was to use either layers with variable thickness or the so-called nonhorizontal-model-layer (NHML) as specifically discussed by Harte (1994). By doing so, one can use very few or even one layer for the vertical discretization, thus substantially reduced the computational cost and avoided the convergence problem as commonly seen in above discretization with horizontal layers. However, such an approach only provided a good approximation to the flow problem when the sloping angle was very gentle (usually less than 5.7°) and the errors were expected to increase substantially when the sloping angle increased above 5.7°.

This study has three purposes. The first is to analyze the possible problems in existing analytical and numerical solutions of groundwater flow in an unconfined sloping aquifer, including the problem associated with MODFLOW-2000. The second is to propose a new numerical scheme that specifically tackles the characteristics of a sloping base and to develop a new package SLOPE for MODFLOW-2000 based on NHML. The third is to verify the Boussinesq assumption (which assumes that the streamlines are parallel with the sloping base) through a high-resolution numerical simulation considering the vertical flow on the basis of COMSOL Multiphysics. Our new numerical scheme improves the MODFLOW-2000 model for dealing with sloping angles that are less than 45°. This new scheme is incorporated into MODFLOW-2000 to become MODFLOW-SP. Another benefit of the new numerical scheme is that it permits the spatial variation of the sloping angles, which is particularly useful for dealing with curved aquifer bases.

Problems in Existing Solutions of Unconfined Flow in Sloping Aquifers

The study on groundwater flow in an unconfined sloping aquifer has become an active research area since the 1860 s (Dupuit 1863; Boussinesq 1877). Many

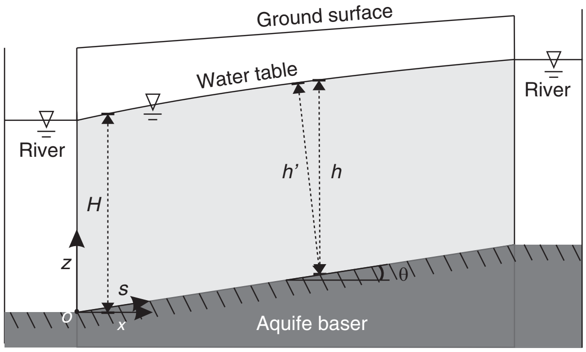

Figure 1. Schematic diagram of groundwater flow in an unconfined sloping aquifer.

approximate analytical and numerical solutions have been developed based on various types of assumptions which are inevitable for a few reasons. Firstly, the governing equations of groundwater flow for such problems are nonlinear, and linearization has to be performed to derive the analytical solutions. The second issue is related to the water table which is a free moving surface that is sometime difficult to deal with. The third is how to accurately approximate the effect of the sloping base on groundwater movement. In the following, we attempt to analyze the problems associated with existing solutions of unconfined flow in sloping aquifers.

A schematic diagram of groundwater flow in an unconfined sloping aquifer is depicted in Figure 1. The x-z coordinate system is an orthogonal Cartesian coordinate system with the x-axis horizontal and the z-axis vertical. The s-z coordinate system is a skewed Cartesian coordinate system with the s-axis along the aquifer base and the z-axis vertical. H is the hydraulic head (L) in the x-z coordinate system. h is the vertical length from the aquifer base to the water table (L). h' is the distance (L) between the aquifer base and water table along the direction perpendicular to the s-axis. On the basis of the Dupuit-Forchheimer assumption (the streamlines are assumed to be horizontal), the discharge per unit width, q (L^2/T), can be expressed as (Dupuit 1863)

$$q = -Kh\frac{\partial H}{\partial x} = -Kh\left[\frac{\partial h}{\partial x} + \tan(\theta)\right], \quad \text{where}$$
$$H = h + x\tan(\theta), \tag{1}$$

where K is hydraulic conductivity (L/T) and θ is the aquifer base angle (dimensionless) which is counter clockwise from the x-axis. Some other investigators approximate q as (Bear 1972; Dupuit 1863):

$$q = -Kh\frac{\partial H}{\partial s} \quad \text{or} \quad q = \frac{K\sec(\theta)(\partial H/\partial x)}{\left[1 + \tan(\theta)(\partial H/\partial x)\right]}. \tag{2}$$

The main difference between Equations 1 and 2 is the calculation of the hydraulic gradient. On the basis of the Boussinesq assumption that the streamlines are parallel to the sloping base, one has

$$q = -Kh'\frac{\partial H}{\partial s}. \tag{3}$$

Subsequently, there are two different approaches to approximate Equation 3. Wooding and Chapman (1966) proposed the following approximation using $h' \approx h\cos(\theta)$

$$q \approx -Kh'\left[\cos(\theta)\frac{\partial h'}{\partial s} + \sin(\theta)\right]. \tag{4}$$

The essence of this approximation is to regard h' as the projection of h along the direction perpendicular to the aquifer base. A careful check of Figure 1 reveals that this approximation works the best when the water table is parallel to the aquifer base, and it works poorly when the water table slope is very different from the slope of the aquifer base. Childs (1971) proposed an alternate approximation for Equation 3 as:

$$q \approx -\frac{Kh(\partial H/\partial x)}{\left[1 + \tan(\theta)(\partial H/\partial x)\right]}$$
$$= -\frac{K\cos^2(\theta)h(\partial H/\partial x)}{\left[1 + 0.5\sin(2\theta)(\partial H/\partial x)\right]}. \tag{5}$$

Since the denominator on the right side of Equation 5 contains a partial differential term, $\partial H/\partial x$ or $\partial h/\partial x$, Equation 5 is intrinsically nonlinear. Chapman (1980) assumed that when $0.5\sin(2\theta)\partial h/\partial x$ was much less than 1, which was true when $\partial h/\partial x$ was very small and/or the slope angle was very gentle, then Equation 5 can be simplified to:

$$q \approx -K\cos^2(\theta)h\left[\frac{\partial h}{\partial x} + \tan(\theta)\right] = -K\cos^2(\theta)h\frac{\partial H}{\partial x}. \tag{6}$$

The above different ways of calculating q, when combined with the mass balance principle, will lead to various forms of governing equations:

$$\frac{\partial q}{\partial x} + S\frac{\partial H}{\partial t} = Q, \tag{7}$$

where Q (L/T) is the net rate of the vertical accretion to the free surface, S is the storage coefficient (dimensionless). Substituting Equations 1, 4, and 5 into Equation 7 results in the following three types of governing equations:

$$\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right) + \tan(\theta)\frac{\partial h}{\partial x} + \frac{Q}{K} = \frac{S}{K}\frac{\partial h}{\partial t}, \tag{8}$$

$$\frac{\partial}{\partial s}\left(h'\frac{\partial h'}{\partial s}\right) + \tan(\theta)\frac{\partial h'}{\partial s} + \frac{Q}{K}\left[1 - \tan(\theta)\frac{\partial h'}{\partial s}\right]$$
$$= \frac{S}{K\cos(\theta)}\frac{\partial h'}{\partial t}, \tag{9}$$

$$\frac{\partial}{\partial x}\left(h\frac{\partial h}{\partial x}\right)+\tan(\theta)\frac{\partial h}{\partial x}+\frac{Q}{K\cos^2(\theta)}=\frac{S}{K\cos^2(\theta)}\frac{\partial h}{\partial t}. \tag{10}$$

These three governing equations become the basis for solving groundwater flow in an unconfined sloping aquifer. For example, Upadhyaya and Chauhan (2001) and Asadi-Aghbolaghi et al. (2012) obtained approximate analytical solutions based on Equation 8; Beven (1981), Brutsaert (1994), Verhoest and Troch (2000), Stagnitti et al. (2004), and Verhoest et al. (2002) derived approximate analytical solutions of Equation . Zissis et al. (2001), Bansal and Das (2011), and Bansal (2012) presented approximate analytical solutions of Equation 10.

There are two features associated with above three governing equations that deserve some discussion. The first is the nonlinearity, reflected in the first terms on the left sides of Equations 8 through 10. The nonlinearity imposes difficulty from an analytical perspective and some linearization methods have to be used. The second is the advective terms, which are the terms involving the first spatial derivative on the left sides of Equations 8 through 10, making such equations similar to the advection–diffusion equations (ADEs) commonly employed for studying solute transport (Bear 1972). The ADEs are fundamentally different from the conventional groundwater flow equations in horizontal aquifers, which are diffusion equations (Bear 1972). Such features will bring in potential errors in the analytical and numerical approaches.

For the analytical approaches, potential errors come from two sources. Firstly, linearization of the nonlinear governing equation will inevitably bring in some errors. For instance, one linearization method is to approximate $\partial(h\partial h/\partial x)/\partial x$ by $\overline{h}\left(\partial^2 h/\partial x^2\right)$, where $\overline{h}$ is the average saturated thickness of the aquifer (L). Secondly, the three forms of governing equations described above also involve various types of assumptions such as the Dupuit-Forchheimer assumption (Dupuit 1863) or the Boussinesq assumption (Boussinesq 1877) which will introduce errors also. In addition, Equations 9 and 10 assume that $h' \approx h\cos(\theta)$ and $0.5\sin(2\theta)\partial h/\partial x << 1$, respectively.

For the numerical approaches, in addition to problems discussed above for the analytical approaches, there is one more challenge related to the introduction of the advection terms in the governing equations which become ADEs, which might introduce numerical dispersion and artificial oscillation as commonly reported in solute transport literature (Zheng and Wang 1999; Bear 1972). Since the sloping angle has been incorporated explicitly into above governing equations, one can still use the horizontal-model-layer (HML) with a set of rectangular faces as usually done for studying groundwater flow in horizontal aquifers before. The benefit of doing so is to avoid the problems of designing a skewed grid system. Zissis et al. (2001) and Bansal (2012) employed a finite-difference scheme of Mac Cormack (1969) to solve Equation 10. This finite-difference scheme was a two-step explicit approach named predictor-corrector by Mac Cormack (1969), and was conditionally stable and convergent. One such condition was to use a sufficiently small time interval to ensure accuracy and convergence. To deal with groundwater flow in an unconfined sloping aquifer, the commonly used three-dimensional finite-difference model MODFLOW (McDonald and Harbaugh 1988) can be a powerful tool if one can adequately handle the characteristics of the sloping base. Two advantages of MODFLOW are particularly notable. The first is its capability to handle the free water table using the rewetting package (Niswonger et al. 2011). The second is its use of NHML to properly approximate the sloping base (Harte 1994). In fact, NHML is capable of dealing with variable sloping angles, making it very useful for studying realistic sloping aquifers over a large spatial scale which may see variable sloping angles at different locations. Notwithstanding above mentioned advantages, one may still face a few problems when using NHML of MODFLOW for sloping aquifers. One problem is that MODFLOW treats the streamlines between adjacent cells within one layer as horizontal, which may not be true. Some investigators such as Zheng (1994) realized that the assumption of horizontal flow lines in a distorted grid along the vertical dimension was problematic within the MODFLOW framework, where the distorted grid system may be employed to accommodate a slopping base. Zheng (1994) provided a methodology to correct this error. However, Zheng (1994) only concerned the particle tracking (or MODPATH) analysis and did not discuss the correction to the hydraulic head, which will be addressed in this study. The essence of NHML treatment is the Dupuit-Forchheimer assumption for unconfined flow, which is found to work satisfactorily only for gentle slopes (less than 0.10). Some studies such as Hoaglund and Pollard (2003) have adopted the Boussinesq assumption to improve MODFLOW in the skewed *s*-*z* coordinate system. However, such studies lead to a few additional challenges. Firstly, field data such as the observed hydraulic heads, recharge and discharge, pumping and observation well screens are often documented in the *x*-*z* coordinate system, and must be converted to the new *s*-*z* coordinate system before use. Secondly, the sloping angle of the base has to be constant across the entire spatial domain, which may not be the case for the actual field site.

This study attempts to overcome two challenges within the framework of MODFLOW, using the Boussinesq assumption instead of the Dupuit-Forchheimer assumption. This is because many previous investigations have shown that the Boussinesq assumption is a much better approximation than the Dupuit-Forchheimer assumption when the base slope is greater than 0.1 (Schmid and Luthin 1964; Wooding 1966; Wooding and Chapman 1966; Childs 1971; Chapman 1980). We will employ a *x*-*z* coordinate system instead of the *s*-*z* coordinate system of Hoaglund and Pollard (2003), and we will use NHML to handle spatially variable sloping angles of the aquifer base. In this study, we assume that the principal directions of horizontal anisotropy of hydraulic

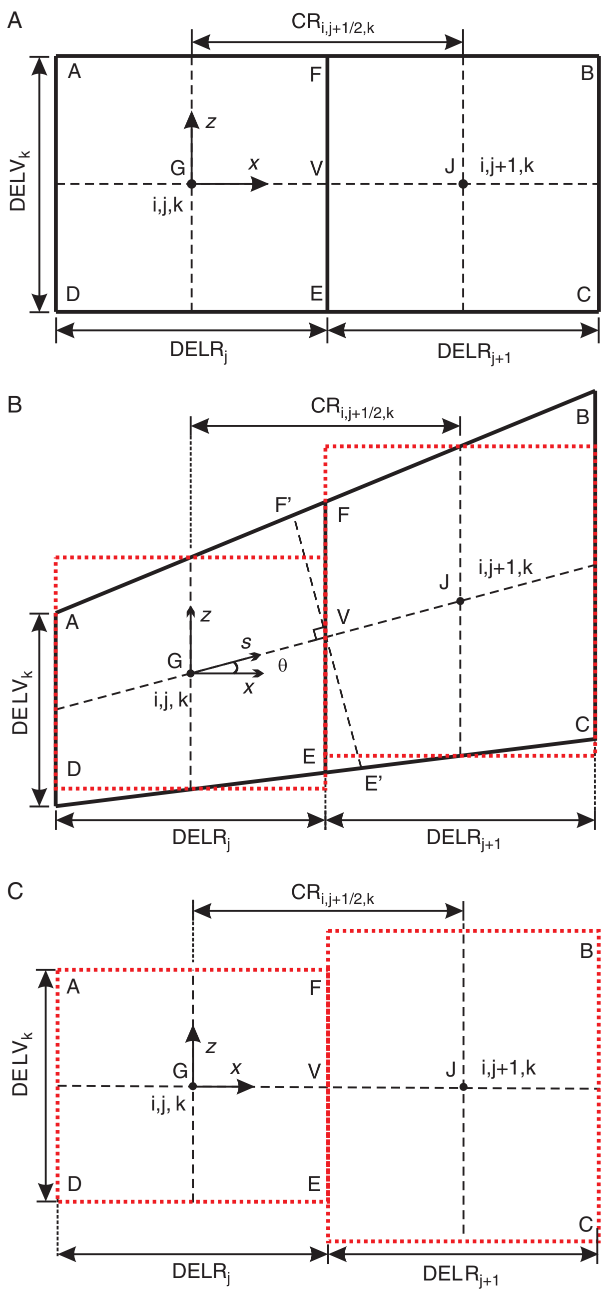

Figure 2. (A) Schematic diagram of HML grid system with rectangular face cells. (B) Schematic diagram of NHML grid system with deformed cells. (C) Schematic diagram of rearrangement NHML grid system in MODFLOW-2000.

conductivity are the same as the model-grid row and column directions. If this is not the case, one probably has to adopt the methodology proposed by Anderman et al. (2002) for further modification, which is out of scope of this study. The detailed procedures are described in the following sections.

Modeling Groundwater Flow in an Unconfined Sloping Aquifer Using MODFLOW-2000

Before introducing our new approach for studying groundwater flow in an unconfined sloping aquifer based on the framework of MODFLOW-2000, it is necessary to briefly explain the MODFLOW-2000 approach for such a problem. The orthogonal coordinate system in MODFLOW is usually defined in a way that the x and y axes are horizontal and along the column and row directions, and the z-axis is vertical. Based on the mass balance requirement, the continuity equation of the groundwater flow is

$$\sum Q_i = S_s \frac{\Delta H}{\Delta t} \Delta V, \tag{11}$$

where Q_i is water flux (L^3T^{-1}) into the cell of concern (i, j, k) including the discharge through the face between this cell and its neighboring cells and the source or sink inside this cell, where i, j, k are indexes of row, column, and layer of the cell, respectively; S_s is the specific storage (L^{-1}); ΔV is the volume of the cell (L^3); ΔH is the head change (L) over a time interval Δt(T). According to Darcy's law, the volumetric discharge between cells (i, j+1, k) and (i, j, k) as shown in Figure 2A is:

$$q_{i,j+1/2,k} = CR_{i,j+1/2,k}\left(H_{i,j,k} - H_{i,j+1,k}\right), \tag{12}$$

where $CR_{i,j+1/2,k} = KR_{i,j+1/2,k}\Delta c_i \Delta v_k / \Delta r_{j+1/2}$, and the suffix of parameter including 1/2 represents the equivalent value between the adjacent cells; $KR_{i,j+1/2,k}$ is the equivalent hydraulic conductivity along the row between cells (i, j+1, k) and (i, j, k); Δr_j, Δc_i and Δv_k are the dimensions of cell along the j, i, and k directions at cell (i, j, k), respectively, where $\Delta v_k = EF$ in Figure 2A; $\Delta r_{j+1/2}$ is the dimension along the j direction between cells (i, j+1, k) and (i, j, k). For three-dimensional flow, there are six adjacent aquifer cells around cell (i, j, k), denoted as ($i-1$, j, k), (i, $j-1$, k), (i, j, $k-1$), (i+1, j, k), (i, j+1, k), (i, j, k+1). The other expressions of volumetric discharge between cell (i, j, k) and the adjacent cells can be derived similarly, and the details can be seen in MODFLOW user's menu (McDonald and Harbaugh 1988). Substituting the volumetric discharge terms into Equation 11, the finite-difference scheme of the governing equation is developed as

$$\begin{aligned}
&CV_{i,j,k-1/2}H^m_{i,j,k-1} + CC_{i-1/2,j,k}H^m_{i-1,j,k} \\
&\quad + CR_{i,j-1/2,k}H^m_{i,j-1,k} + \left(-CV_{i,j,k-1/2}\right. \\
&\quad - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} \\
&\quad \left. - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k}\right) H^m_{i,j,k} \\
&\quad + CV_{i,j,k+1/2}H^m_{i,j,k+1} + CC_{i+1/2,j,k}H^m_{i+1,j,k} \\
&\quad + CR_{i,j+1/2,k}H^m_{i,j+1,k} = RHS_{i,j,k},
\end{aligned} \tag{13}$$

$$HCOF_{i,j,k} = P_{i,j,k} - \frac{SS_{i,j,k}\Delta r_j \Delta c_i \Delta v_k}{t^m - t^{m-1}}, \tag{14}$$

$$RHS_{i,j,k} = -Q_{i,j,k} - \frac{SS_{i,j,k}\Delta r_j \Delta c_i \Delta v_k h^{m-1}_{i,j,k}}{t^m - t^{m-1}}, \quad (15)$$

where $H^m_{i,j,k}$ is the hydraulic head (L) at cell (i, j, k) at time step m; CC, CR, and CV are branch conductances (L^3T^{-1}) between cell (i, j, k) and a neighboring cell oriented along columns, rows, and layers, respectively; $P_{i,j,k}$ is the sum of coefficients of head in source and sink terms (L^2T^{-1}); $Q_{i,j,k}$ is the sum of constants from source and sink terms (L^3T^{-1}); $SS_{i,j,k}$ is the specific storage at cell (i, j, k) (L^{-1}); and t^m is the time (T) at the step m. The $HCOF$ and RHS coefficients are composed of external source terms and storage terms, and their detailed expressions can be seen from the MODFLOW user's menu (McDonald and Harbaugh 1988).

It is apparent from the above formulation of MODFLOW that the streamlines between cells along the columns and rows are taken as horizontal, and it is accurate only for the HML grid systems and maybe acceptable for NHML grid systems when the slope of the layer is small (less than 0.1). Above formulation of MODFLOW (Equation 13) becomes increasingly less accurate when slope of the layer increases above 0.1.

In the following section, we will develop a new finite-difference scheme considering the slope of the aquifer base and a new package (SLOPE) for MODFLOW-2000 to reduce the errors associated with the formulation of Equation 13.

New Finite-Difference Scheme for Groundwater Flow in Unconfined Sloping Aquifers

For an unconfined sloping aquifer, the grid system of NHML is not horizontal like Figure 2A, while the lower and upper boundaries of each cell are sloping with the base like Figure 2B. In Figure 2B, cells ADEF and EFBC represent the discretization of the real aquifer, and the upper boundary of the cell (AF or FC in Figure 2B) represents the water table when the hydraulic head is less than the elevation of the top cell face. The corresponding red dash-line cells represent the discretization of the real aquifer in NHML of MODFLOW-2000. When the dimension of the horizontal spatial step approaches 0, the discretization of NHML can accurately represent the real aquifer. However, when the centers of two adjacent horizontal cells are not at the same level, as shown in Figure 2B, MODFLOW-2000 changes the actual arrangement of cells of G and J into a "modified" arrangement which realigns the centers of G and J into the same horizontal level, as shown in Figure 2C. All the subsequent calculation of flux in MODFLOW-2000 is based on the realigned grid system of Figure 2C. Such a realignment of cells shown in Figure 2C could bring in nonnegligible numerical errors, particularly when the vertical discrepancy between the centers of G and J increases (or the slope of the aquifer becomes greater). In this study, we assume that the groundwater flow direction is along the actual stream line GJ, and robustness of this assumption will be verified later. On the basis of Equation 4, the expression of the discharge per unit width (q) in the aquifer can be written as

$$q \approx -K \cdot E'F' \left[\cos(\theta)\frac{\partial h}{\partial s} + \sin(\theta)\right], \quad (16)$$

where $E'F'$ is the distance between the water table and the aquifer base along the direction perpendicular to the aquifer base (see Figure 2B). The point of V is in the middle of EF or $E'F'$, where EF is the distance between the water table and the aquifer base along the z-axis in Figure 2B. In the x-z coordinate system, Equation 16 becomes

$$q \approx -K \cdot EF \cdot \cos^2(\theta)\left[\frac{\partial h}{\partial x} + \tan(\theta)\right]. \quad (17)$$

Rewriting Equation 17 using the variables defined in MODLFOW-2000 leads to

$$q_{i,j+1/2,k} \approx -KR_{i,j+1/2,k}\Delta c_i \Delta v_k \cos^2(\theta_{i,j+1/2,k}) \times \left[\frac{h_{i,j+1,k} - h_{i,j,k}}{\Delta r_{j+1/2}} + \tan(\theta_{i,j+1/2,k})\right], \quad (18)$$

where $\theta_{i,j+1/2,k}$ is the aquifer sloping angle between cells (i, j, k) and $(i, j+1, k)$ and it can be determined easily using the coordinates of cells (i, j, k) and $(i, j+1, k)$:

$$\tan(\theta_{i,j+1/2,k}) = \frac{z_{i,j+1,k} - z_{i,j,k}}{y_{i,j+1,k} - y_{i,j,k}}, \quad (19)$$

$$\tan(\theta_{i+1/2,j,k}) = \frac{z_{i,j+1,k} - z_{i,j,k}}{x_{i+1,j,k} - x_{i,j,k}}, \quad (20)$$

where x, y, z are the coordinates of the center of the cell. One point needs to be emphasized is that the top face of the cell is the water table when the water table is lower than the elevation of the top cell face. Similarly, we can derive the volumetric discharges through cell (i, j, k) and other adjacent cells as:

$$q_{i,j-1/2,k} = -KR_{i,j-1/2,k}\Delta c_i \Delta v_k \cos^2(\theta_{i,j-1/2,k}) \times \left[\frac{h_{i,j,k} - h_{i,j-1,k}}{\Delta r_{j-1/2}} + \tan(\theta_{i,j-1/2,k})\right], \quad (21)$$

$$q_{i-1/2,j,k} = -KC_{i-1/2,j,k}\Delta r_j \Delta v_k \cos^2(\theta_{i-1/2,j,k}) \times \left[\frac{h_{i,j,k} - h_{i-1,j,k}}{\Delta c_{i-1/2}} + \tan(\theta_{i-1/2,j,k})\right], \quad (22)$$

$$q_{i+1/2,j,k} = -KC_{i+1/2,j,k}\Delta r_j \Delta v_k \cos^2\left(\theta_{i+1/2,j,k}\right) \times \left[\frac{h_{i+1,j,k}-h_{i,j,k}}{\Delta c_{i+1/2}} + \tan\left(\theta_{i+1/2,j,k}\right)\right], \quad (23)$$

$$q_{i,j,k-1/2} = -KV_{i,j,k-1/2}\Delta r_j \Delta c_i \frac{h_{i,j,k}-h_{i,j,k-1}}{\Delta v_{k-1/2}}, \quad (24)$$

$$q_{i,j,k+1/2} = -KV_{i,j,k+1/2}\Delta r_j \Delta c_i \frac{h_{i,j,k+1}-h_{i,j,k}}{\Delta v_{k+1/2}}. \quad (25)$$

Redefining the equivalent conductances as:

$$CR_{i,j+1/2,k} = \frac{KR_{i,j+1/2,k}\Delta c_i \Delta v_k \cos^2\left(\theta_{i,j+1/2,k}\right)}{\Delta r_{j+1/2}}, \quad (26)$$

$$CR_{i,j-1/2,k} = \frac{KR_{i,j-1/2,k}\Delta c_i \Delta v_k \cos^2\left(\theta_{i,j-1/2,k}\right)}{\Delta r_{j-1/2}}, \quad (27)$$

$$CC_{i+1/2,j,k} = \frac{KC_{i+1/2,j,k}\Delta r_j \Delta v_k \cos^2\left(\theta_{i+1/2,j,k}\right)}{\Delta c_{i+1/2}}, \quad (28)$$

$$CC_{i-1/2,j,k} = \frac{KC_{i-1/2,j,k}\Delta r_j \Delta v_k \cos^2\left(\theta_{i-1/2,j,k}\right)}{\Delta c_{i-1/2}}. \quad (29)$$

One notable point is that the hydraulic head involved in Equations 18, 21 through 25 is "h", which is the vertical length from the aquifer base to the water table, whereas the hydraulic head needed for MODFLOW-2000, H, is in respect to the x-axis. Therefore, the following straightforward conversion is required before the use of MODFLOW-2000:

$$\frac{H_{i,j+1,k}-H_{i,j,k}}{\Delta r_{j+1/2}} = \frac{h_{i,j+1,k}-h_{i,j,k}}{\Delta r_{j+1/2}} + \tan\left(\theta_{i,j+1/2,k}\right), \quad \frac{H_{i,j,k}-H_{i,j-1,k}}{\Delta r_{j-1/2}} = \frac{h_{i,j,k}-h_{i,j-1,k}}{\Delta r_{j-1/2}} + \tan\left(\theta_{i,j-1/2,k}\right), \quad (30)$$

$$\frac{H_{i,j,k}-H_{i-1,j,k}}{\Delta c_{i-1/2}} = \frac{h_{i,j,k}-h_{i-1,j,k}}{\Delta c_{i-1/2}} + \tan\left(\theta_{i-1/2,j,k}\right), \quad \frac{H_{i+1,j,k}-H_{i,j,k}}{\Delta c_{i+1/2}} = \frac{h_{i+1,j,k}-h_{i,j,k}}{\Delta c_{i+1/2}} + \tan\left(\theta_{i+1/2,j,k}\right). \quad (31)$$

Substituting Equations 30 and 31 into Equation 11, one has:

$$CV_{i,j,k-1/2}H^m_{i,j,k-1} + CC_{i-1/2,j,k}H^m_{i-1,j,k} + CR_{i,j-1/2,k}H^m_{i,j-1,k} + \left(-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k}\right)H^m_{i,j,k} + CV_{i,j,k+1/2}H^m_{i,j,k+1} + CC_{i+1/2,j,k}H^m_{i+1,j,k} + CR_{i,j+1/2,k}H^m_{i,j+1,k} = RHS_{i,j,k}. \quad (32)$$

Despite the same apparent forms of Equations 32 and 13, the definitions of conductance terms of *CR* and *CC* in Equation 32 (see Equations 26 through 29) are different from their counterparts in Equation 13. In another word, the errors between MODFLOW-2000 and MODFLOW-SP caused by the vertical discretization are the same, and the main errors for the sloping aquifer come from the calculation of the horizontal conductance terms. In addition, we can see that the errors based on the Dupuit-Forchheimer assumption instead of the Boussinesq assumption are related to the angle of the sloping aquifer by comparing Equations 26 and 12. The error increases with the increasing angle, and becomes maximum when the angle is 90°.

MODFLOW is designed in a modular fashion and the modules are grouped into packages which can be modified straightforwardly for specific needs (McDonald and Harbaugh 1988). In this study, we incorporated above mathematical models into MODFLOW-2000 to generate a new package named SLOPE. This new package is combined with MODFLOW-2000 to create MODFLOW-SP for the following analysis.

Comparison of MODFLOW-SP with the Mac Cormack (1969) Scheme

In this section, the newly developed MODFLOW-SP will be tested against the numerical solution of Mac Cormack (1969), which has been used to examine the effectiveness and validity of the linearization technique used in the analytical solutions of Zissis et al. (2001) and Bansal (2012). The conceptual model and the hydraulic parameters used are referenced from Bansal (2012). An unconfined aquifer overlays an impermeable sloping base with an upward sloping angle of θ. The aquifer is bounded by two rivers with constant water levels, h_L(left river) and h_R(right river), and the groundwater flow is assumed to be one-dimensional along the aquifer base. The initial condition of aquifer is $h = 0.5$ m. The aquifer is homogeneous and isotropic, and the horizontal distance between two rivers L is 100 m. The water levels of two rivers are $h_L = 3.0$ m and $h_R = 5.0$ m. Source and sink terms are not considered. Hydraulic conductivity and specific yield of the aquifer are 2.5 m/day and 0.2, respectively. To test the MODFLOW-SP model, three sets of bed slope values are used, such as 0, 0.27, and 0.75.

The conceptual model described above is a typical one-dimensional groundwater flow in an unconfined aquifer. Bansal (2012) presented an analytical solution considering the time-dependent water level of the river. For the purpose of comparison, we define the following dimensionless variables: $h_D = h/L$, $x_D = x/L$, and $t_D = tK/(SL)$. One can see that K and S are combined into the dimensionless time term. Figure 3A represents the dimensionless hydraulic heads vs. the dimensionless times, where Mac Cormack, MODLFOW, and MODFLOW-SP represent the solutions of Mac Cormack (1969), MODLFOW-2000 and MODFLOW with the SLOPE package, respectively. Some observations can be made. Firstly, the solutions by Mac Cormack and MODFLOW-SP are almost the same, regardless of the aquifer slopes used. We have further compared the results of MODFLOW-SP with those of Mac Cormack for sloping angles up to 45°, and find that the MODFLOW-SP solutions agree with those of Mac Cormack remarkably well. This implies that MODFLOW-SP is robust and free from numerical errors at least for sloping angles up to 45°, as the Mac Cormack solution has been regarded as the benchmark by many previous studies (Zissis et al. 2001; Bansal 2012). Secondly, the difference between MODFLOW and MODFLOW-SP is nearly negligible when the slope is less than 0.27 (or sloping angle less than 15.0°) during the transient flow stage, while it is noticeable when the slope increases above 0.27 to 0.75 (or sloping angle increases above 15.0° to 36.9°). Such a difference disappears eventually when flow reaches steady state. Thirdly, the hydraulic head of MODFLOW-SP is smaller than that of MODFLOW-2000 in the transient stage, and the groundwater flow simulated by MODFLOW-2000 approaches steady state earlier. Fourthly, the curves of MODFLOW-2000 and MODFLOW-SP are the same for SLOPE of 0.

Above observations will be briefly elaborated as follows. In terms of the second observation, the reason that the MODFLOW-2000 and MODFLOW-SP solutions become the same under steady-state flow can be seen from the governing equations used by MODFLOW-2000 and MODFLOW-SP for one-dimensional problem (see Equations 8 through 10). For example, for steady-state flow without the sink/source term, Equation 10 becomes $\partial(h\partial h/\partial x)/\partial x + \tan(\theta)\partial h/\partial x = 0$, which can be rewritten as $\partial(h\partial H/\partial x)/\partial x = 0$, if recognizing that $H = h + x\tan(\theta)$ (see Equation 1). Therefore, the governing equation becomes identical to the one used in MODFLOW-2000 for the problem of concern. As for the third observation, the reason is also obvious, since the MODFLOW-2000 uses $CR_{i,j+1/2,k}$ to calculate the flux instead of GJ, as shown in Figure 2B.

To further check the difference of the solutions between the MODFLOW-2000 and MODFLOW-SP, we define the following dimensionless error criterion

$$E = \frac{h_{\text{MODFLOW}} - h_{\text{MODFLOW-SP}}}{h_R - h_L}, \tag{33}$$

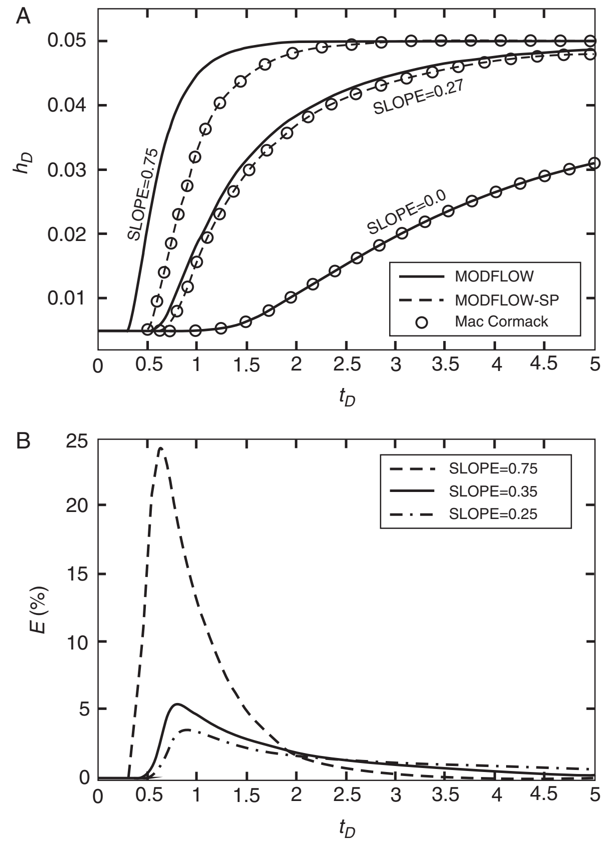

Figure 3. (A) Comparisons of the dimensionless hydraulic head in the *s-z* coordinate system for different aquifer slope values. (B) Dimensionless errors between MODFLOW, and MODFLOW-SP for different aquifer slope values.

where h_{MODFLOW} and $h_{\text{MODFLOW-SP}}$ represent the vertical distances from the aquifer base to the water table calculated by MODFLOW-2000 and MODFLOW-SP, respectively. Figure 3B shows the E changes with the dimensionless time for different aquifer base slope values. We can see that the errors are smaller than 5% when the slope is less than 0.27, and the maximum error nearly approaches 25% when the slope is 0.75.

As commonly used in many previous studies (Zissis et al. 2001; Bansal 2012; Chapman 1980), the following two constrains have been incorporated in MODFLOW-SP: the Boussinesq assumption (Boussinesq 1877) is satisfied and the term of $0.5\sin(2\theta)\partial h/\partial x$ in Equation 5 is small enough to be ignored. However, there is no detailed investigation on these two constrains, and it is unclear how to precisely quantify the errors associated with them. The objective of the following section is to test the validity of these two constrains.

Comparison with the COMSOL Solution

The two constrains used in MODFLOW-SP are widely employed to study groundwater flow in an unconfined sloping aquifer, where the essence of these constrains is to simplify the two-dimensional flow into one-dimensional flow by ignoring resistance to vertical

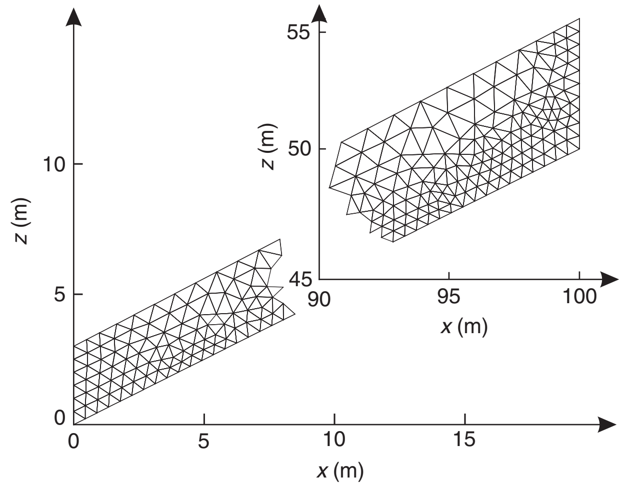

Figure 4. Part of the grid system of the aquifer domain used in the COMSOL Multiphysics simulation.

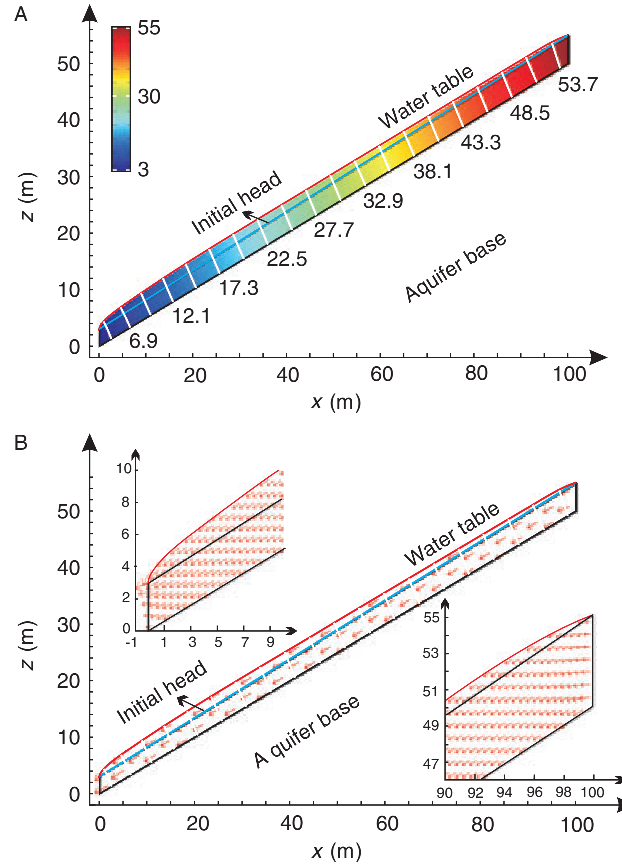

Figure 5. (A) Hydraulic head contour of the unconfined aquifer domain at t=100 h. (B) Velocity distribution of the unconfined aquifer domain at t=100 h.

flow and avoiding the moving boundary problem of the water table. In this section, a two-dimensional flow model will be introduced to check the robustness of these two constrains by including resistance to vertical flow.

MODFLOW-2000 is a three-dimensional finite-difference model whose grid system has to satisfy a condition that the initial water table should be in the first layer of the model. When the water table is not horizontal like the one discussed in the above section, the thickness of the first layer must be sufficiently large to accommodate the spatially variable water table to avoid numerical divergence problems. Therefore, it is difficult to establish a numerical model with very fine layer thickness to describe the groundwater flow in an unconfined sloping aquifer if using the HML discretization scheme of MODFLOW-2000. To resolve this issue, we will employ COMSOL Multiphysics software to simulate groundwater flow in an unconfined sloping aquifer for the purpose of comparing with the MODFLOW-SP solutions under realistic flow conditions. COMSOL Multiphysics is a robust finite-element software package that can handle the type of governing equations of this study, and it has been tested in many previous investigations in hydrogeology (You et al. 2011; You and Zhan 2012). The grid system of COMSOL is composed of a set of triangle elements, and it is easy to refine the grid mesh near the slope base to precisely describe the sloping geometry. In addition, there is a package in COMSOL named the "deformed mesh" (ALE), which can be used conveniently to simulate the moving water table. The conceptual model used in COMSOL is the same as the one discussed in the above section. Figure 4 is an enlarged portion of the grid system for clarification.

Figure 5A and 5B shows the head contour and velocity distribution at $t = 100$ h, at which flow has already approached the steady-state condition. From these two figures, we can see that the groundwater flow direction is almost parallel to the aquifer base except in a narrow region near the left or right boundary. Near the right boundary, the flow direction changes quickly within a very short distance from horizontal (or perpendicular to the constant head right boundary) to the direction parallel to the aquifer base. Similar finding can be seen near the left boundary. This observation confirms the validity of the Boussinesq assumption for majority of the flow domain except for the narrow regions near the left and right boundaries.

To test the contribution of the $0.5 \sin(2\theta)\partial h/\partial x$ term in Equation 5, we have studied the head-time distribution at several selected locations for three different aquifer base slopes of 0.50, 0.75, and 1.0. Figure 6A through 6D shows the comparison of the head calculated by MODFLOW-SP and COMSOL. For the MODFLOW-SP simulation, we find that the difference resulted from one or three layers of the vertical discretization is negligible. This finding is not surprising if one carefully checks the formulations of Equations 26 through 32 since the primary improvement of MODFLOW-SP over MODFLOW-2000 is to correct the horizontal hydraulic conductance terms, not the vertical hydraulic conductance terms.

In these figures, COMSOL E, V, F, E', F' represent the heads calculated by COMSOL at locations E, V, F, E', F' as shown in Figure 2B, where point V is the common middle point of EF or $E'F'$. E-V-F is a vertical profile, while E'-V-F' is a profile perpendicular

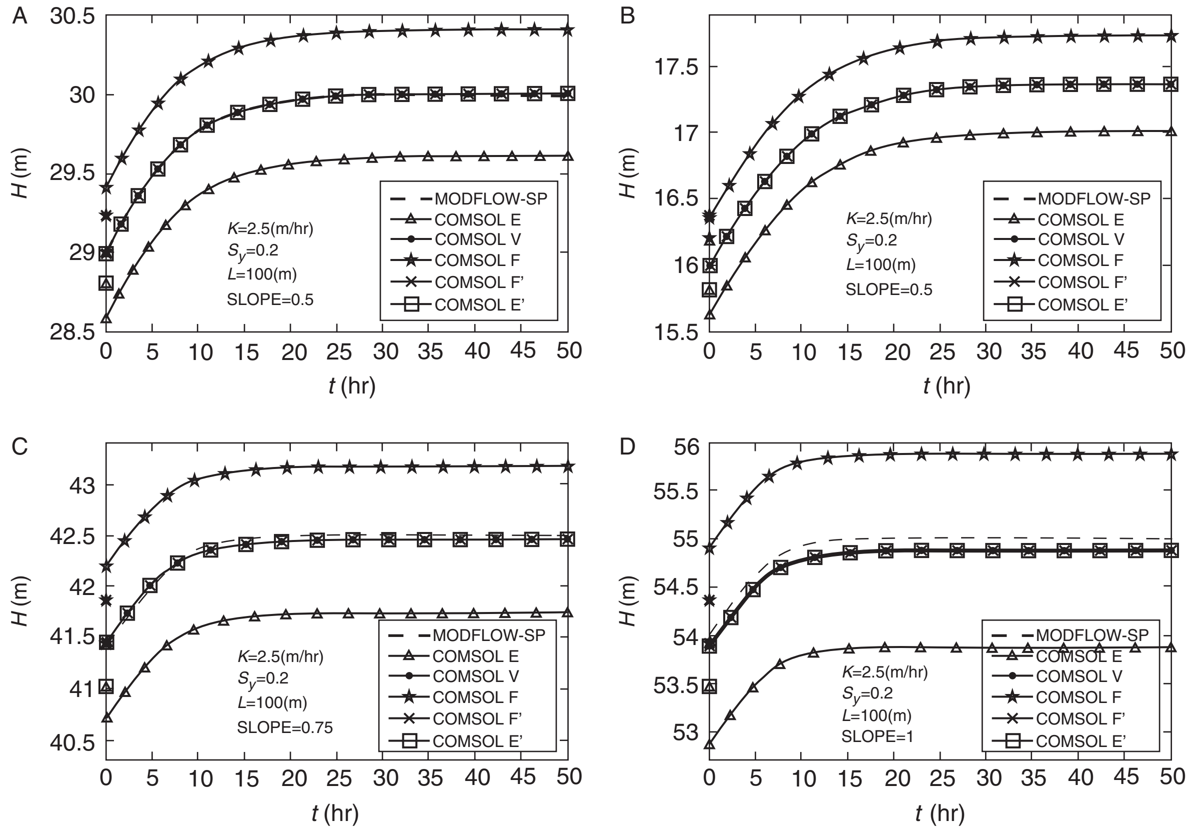

Figure 6. (A) Comparisons of the hydraulic head in the *x-z* coordinate system between the MODFLOW-SP and COMSOL at $x = 50$ m with slope of 0.50. (B) Comparisons of the hydraulic head in the *x-z* coordinate system between the MODFLOW-SP and COMSOL at $x = 25$ m with slope of 0.50. (C) Comparisons of the hydraulic head in the *x-z* coordinate system between the MODFLOW-SP and COMSOL at $x = 50$ m with slope of 0.75. (D) Comparisons of the hydraulic head in the *x-z* coordinate system between the MODFLOW-SP and COMSOL at $x = 50$ m with slope of 1.0.

to the aquifer base. One can see that the head increases considerably along the vertical profile E-V-F, while the head remains constant along the vertical profile E'-V-F'. In addition, the initial conditions of the hydraulic head are the same at locations E, V, and F, and the hydraulic heads at these locations become different within a short period of time. In contrary, the initial conditions of the hydraulic head are different at locations E', V, and F', while the hydraulic heads at these locations become almost the same within a short period of time. These observations imply that the groundwater flow directions become along the aquifer base within a short period of time even if the initial flow is not along the aquifer base. Figure 6A and 6B shows the head-time distributions at different locations of $x = 50.0$ m and $x = 25.0$ m, respectively. In these two figures, the solution calculated by MODFLOW-SP agrees very well with the solution by COMSOL at points E', V, F'. Therefore, when the Boussinesq assumption is satisfied and the term of $0.5 \sin(2\theta)\partial h/\partial x$ in Equation 5 can be neglected, the hydraulic head of one-dimensional flow represents the E'-V-F' profile, not the E-V-F profile. Figure 6A, 6C, and 6D represents the head-time distributions for different base slopes of 0.50 (26.6°), 0.75 (36.9°), and 1.0 (45.0°), respectively at $x = 50.0$ m. One can see that the difference between the solution by MODLOW-SP and COMSOL at location V is small enough to be ignored when the slope is 0.50. The difference slightly increases when the slope is 0.75, and it becomes quite distinctive and nonnegligible when the slope reaches 1.0.

In summary, our observations show that the two constrains mentioned before in MODFLOW-SP are acceptable when the aquifer slope is smaller than 0.50; the errors are small but noticeable for the slope of 0.75; while the errors are quite obvious and nonnegligible when the slope becomes 1.0. Furthermore, MODFLOW-SP provides very good prediction of hydraulic heads along the E'-V-F' profile.

Summary and Conclusions

In this study, the assumptions involved in existing analytical and numerical solutions of groundwater flow in an unconfined sloping aquifer are carefully analyzed. The problems and potential numerical errors associated with MODFLOW-2000 are also discussed in great details. We propose a new numerical scheme based on the NHML grid system considering the characteristics of the sloping base using two constrains: the Boussinesq assumption and the negligible $0.5 \sin(2\theta)\partial h/\partial x$ term in Equation 5, where θ, h, and x are the aquifer sloping angle, the distance from the aquifer base to the water table along the vertical direction, and horizontal distance from the left boundary, respectively. This new numerical scheme is specifically programed in a SLOPE package that is integrated into the MODFLOW-2000 program to create MODFLOW-SP which can handle the problems related to sloping aquifers. The solutions by MODFLOW-SP agree with a widely used numerical benchmark solution of Mac Cormack (1969) very well. The difference between MODFLOW-2000 and MODFLOW-SP is small but maybe nonnegligible when the aquifer slope is 0.27 (or the sloping angle is 15.0°), while the difference is obvious when the aquifer slope is 0.75 (or the sloping angle is 36.9°). To test the robustness of above two constrains, the results of MODFLOW-SP are compared against those of COMSOL Multiphysics for a two-dimensional model considering the vertical and horizontal flow with a very fine grid mesh. Under the steady-state flow condition, the groundwater flow direction is almost parallel to the aquifer base except in narrow regions near the left and right boundaries. MODFLOW-SP can be used to predict the hydraulic head along the E'-V-F' profile very well (see Figure 2B). The errors associated with above two constrains used in MODFLOW-SP are negligible when the slope is smaller than 0.50 (or sloping angle of 26.6°). Such errors are small but noticeable when the slope is 0.75 (or sloping angle of 36.9°), and they become significant when the slope is 1.0 (or sloping angle of 45.0°).

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