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Grid Cell Distortion and MODFLOW's Integrated Finite-Difference Numerical Solution

by Dave M. Romero and Steven E. Silver

Abstract

The ground water flow model MODFLOW inherently implements a non-generalized integrated finite-difference (IFD) numerical scheme. The IFD numerical scheme allows for construction of finite-difference model grids with curvilinear (piecewise-linear) rows. The resulting grid is comprised of model cells in the shape of trapezoids and is distorted in comparison to a traditional MODFLOW finite-difference grid. A version of MODFLOW-88 (herein referred to as MODFLOW IFD) with the code adapted to make the one-dimensional DELR and DELC arrays two dimensional, so that equivalent conductance between distorted grid cells can be calculated, is described. MODFLOW IFD is used to inspect the sensitivity of the numerical head and velocity solutions to the level of distortion in trapezoidal grid cells within a converging radial flow domain. A test problem designed for the analysis implements a grid oriented such that flow is parallel to columns with converging widths. The sensitivity analysis demonstrates MODFLOW IFD's capacity to numerically derive a head solution and resulting intercell volumetric flow when the internal calculation of equivalent conductance accounts for the distortion of the grid cells. The sensitivity of the velocity solution to grid cell

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distortion indicates criteria for distorted grid design. In the radial flow test problem described, the numerical head solution is not sensitive to grid cell distortion. The accuracy of the velocity solution is sensitive to cell distortion with error less than one percent if the angle between the non-parallel sides of trapezoidal cells is less than 12.5 degrees. The error of the velocity solution is related to the degree to which the spatial discretization of a curve is approximated with piecewise linear segments. Curvilinear finite-difference grid construction adds versatility to spatial discretization of the flow domain. MODFLOW-88's inherent IFD numerical scheme and the test problem results imply that more recent versions of MODFLOW 2000, with minor modifications, have the potential to make use of a curvilinear grid.

Introduction

The ground water flow model MODFLOW (McDonald and Harbaugh 1988) inherently implements a non-generalized integrated finite-difference (IFD) numerical scheme (Romero and Maddock 2003). The inherent IFD numerical scheme allows for adding versatility to the spatial discretization of the flow domain. Specifically, rectangular model grid cells typically associated with finite-difference numerical schemes can be distorted into trapezoids to create a curvilinear finite-difference grid. This paper presents an evaluation of the effect of grid cell distortion on the MODFLOW IFD numerical solution of head and calculation of intercell ground water flow. The evaluation entails inspecting the relationship between the level of spatial resolution in a curvilinear grid of a fixed radial (converging) flow domain and the cell dimensions used to derive the equivalent conductance between cells. A sensitivity analysis reveals MODFLOW IFD's capacity to numerically derive a head solution and resultant intercell volumetric flow when the internal calculation of equivalent conductance between adjacent cells is affected by the variable width of the cells. Sensitivity of the head solution and ground water velocity to resolution of the converging grid indicates criteria for grid design. A previous test problem (Romero and Maddock 2003) is adapted to relate numerical solution error to the angle of trapezoidal cell convergence within a curvilinear grid so that criteria for spatial refinement can be established. Guidelines of curvilinear grid development are discussed.

MODFLOW Adapted For IFD Use

MODFLOW IFD herein refers to the existing version of MODFLOW-88 (McDonald and Harbaugh 1988) adapted to allow for flow in a curvilinear grid; the adaptations convert the one-dimensional DELR and DELC arrays into two-dimensional arrays and rewrite the equivalent conductance calculation in its unreduced form (Romero and Maddock 2003). The changes are minor and make the code capable of solving the governing ground water flow equation within a finite-difference grid in which the rows can be curved into piecewise linear segments. Curved rows in the grid imply that individual column widths are variable. An example of a curvilinear grid is shown on Figure 1.

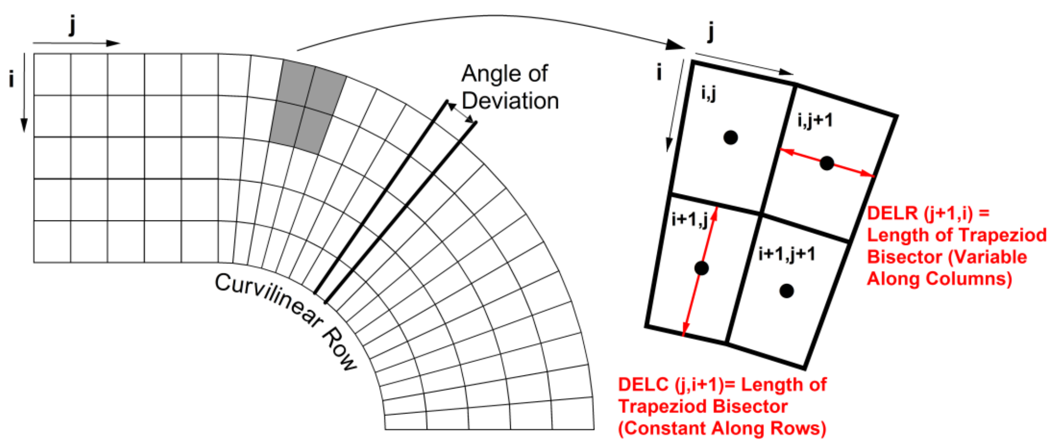

Figure 1. Example of curvilinear finite-difference grid and illustration of row and column widths.

MODFLOW IFD is capable of simulating ground water flow through either a rectilinear or a curvilinear grid. The flow domain for a modeling problem can be created out of both rectangular and trapezoidal cells to construct a grid like that shown in Figure 1. The cell distortion method employed in the model is analogous to that of the Generalized Finite-Difference Package (Harbaugh 1992) except that a model grid, rather than conductance between model cells, is input to the model. MODFLOW IFD then calculates the conductance based on the dimensions of the grid cells. Another analogous method makes use of MODFLOW to simulate cylindrical flow to a well, except that code is specifically for cylindrical flow problems (Reilly and Harbaugh 1993).

The theory previously presented (Romero and Maddock 2003; Narasimhan and Witherspoon 1976) demonstrates that model simulations with MODFLOW IFD can be considered a method of generalized finite differences or, more appropriately, a method of non-generalized integrated finite differences. MODFLOW IFD source code, code documentation and user documentation are freely available at www.balleau.com.

Other model grid refinement studies focus on variable density flow and transport (Schincariol et al. 1994; Frolkovic and Schepper 2000; Kolditz et al. 1997) or particle tracking (Zheng 1994). This paper describes a grid refinement test that compares MODFLOW IFD calculated head and velocity to the solution derived analytically. A grid refinement study with MODFLOW IFD that involves a calculated velocity field with transport or particle tracking would require development of a method to link the curvilinear grid of flow with the rectilinear grid of codes such as MT3DMS (Zheng and Wang 1999), MODPATH (Pollock 1994) or PATH3D (Zheng 1991). That linkage is not yet implemented.

MODFLOW IFD Equivalent Conductance

Expanding the capability of MODFLOW to simulate flow through a curvilinear grid requires adapting the equivalent conductance calculation between model grid cells to account for trapezoidal shaped cells; the adaptation does not change the MODFLOW equation used for calculating equivalent conductance, but it rewrites the equation in an unreduced form (Romero and Maddock 2003). MODFLOW uses one-dimensional arrays (DELR and DELC) to store the width of each column and row of a rectilinear grid. One-dimensional arrays are sufficient for constructing a rectilinear grid because individual row and column widths are constant. The MODFLOW IFD numerical formulation uses two-dimensional arrays to represent the average length of flow in the column and row directions of trapezoidal shaped cells. Figure 1 shows a schematic of four trapezoidal cells that could be used to represent two segments of a curvilinear grid. The MODFLOW index convention for rows (i) and columns (j) is shown so that each cell can be referenced. The length DELR(j+1,i) is equal to the average of the two bases of the trapezoid that encloses node i,j+1 and length DELC(j,i+1) is equal to the height of the trapezoid that encloses node i+1,j. Cell dimensions throughout the IFD model grid are represented this way and the equivalent conductance calculation between model cells is rewritten, in its unreduced form, to account for column-width variability (Romero and Maddock 2003). If the model grid cells were rectangular, then DELR and DELC shown in Figure 1 would be the same as in standard MODFLOW and the grid would be rectilinear. Figure 1 also shows the angle of deviation associated with a trapezoidal shaped cell. Cell shape variability can be described with either the widths of the adjacent cells (length of cell-to-cell bisectors) or the angle of deviation associated with the non-parallel sides of the trapezoid.

As with the standard version of MODFLOW, the computation of ground water velocity through a curvilinear grid must be calculated external to a model simulation. MODFLOW and MODFLOW IFD solve for head and calculate intercell volumetric flow rates. The volumetric flow rate in each model formulation is derived from the head difference and the equivalent conductance between adjacent cells. Computation of ground water velocity requires dividing the intercell volumetric flow rate by the area of the cell face through which it flows. A point of interest in the calculation of velocity within a curvilinear grid is that the cell face can be the common area between two grid cells with different average widths. A test problem is developed to inspect how the MODFLOW IFD numerical solution is affected by width changes between adjacent cells. The term *grid cell distortion* herein refers to the level of width change between adjacent model grid cells. In Figure 1, there is no grid cell distortion in the rows as MODFLOW IFD does not currently account for it. *Grid cell distortion* is distinguished from *grid distortion* in that a curvilinear grid with high resolution representing the domain of interest can be made to have a small amount of grid cell distortion, while the grid as a whole exhibits significant distortion in comparison to a rectilinear grid.

Test Problem Description

The effect of grid cell distortion on the numerical solution is examined by spatially discretizing the same flow domain for multiple cases with increased levels of refinement. For each more-refined spatial discretization of the flow domain, the numerical solution is compared with the known analytical solution (Crank 1967). The flow domain over which the grids are constructed is shown on Figure 2. The model simulations are homogeneous and isotropic with a head (h) gradient of 0.667 over a length (radius = r) of 4.57 meters (m).

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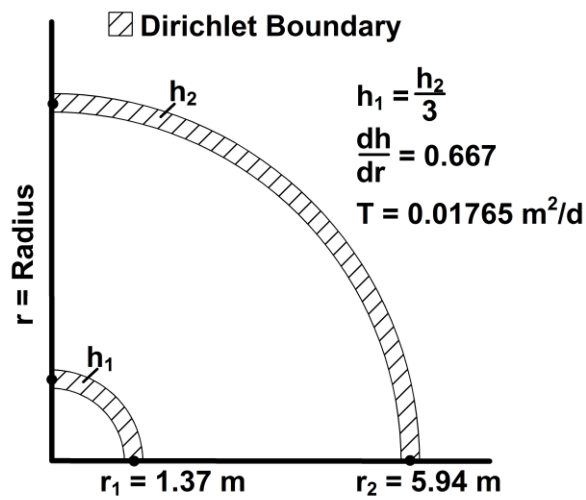

Figure 2. Flow domain simulated for test problem.

The system for describing the level of spatial refinement within a grid is based on the number of columns in the grid that are used to represent flow converging over 90 degrees. Figure 3 shows the flow domain discretized with multiple levels of refinement. In the first discretization, a 90 degree angle (the entire flow domain) is spanned with one column; in the second, 90 degrees is spanned with two 45 degree columns and so forth so that the angle spanned by a

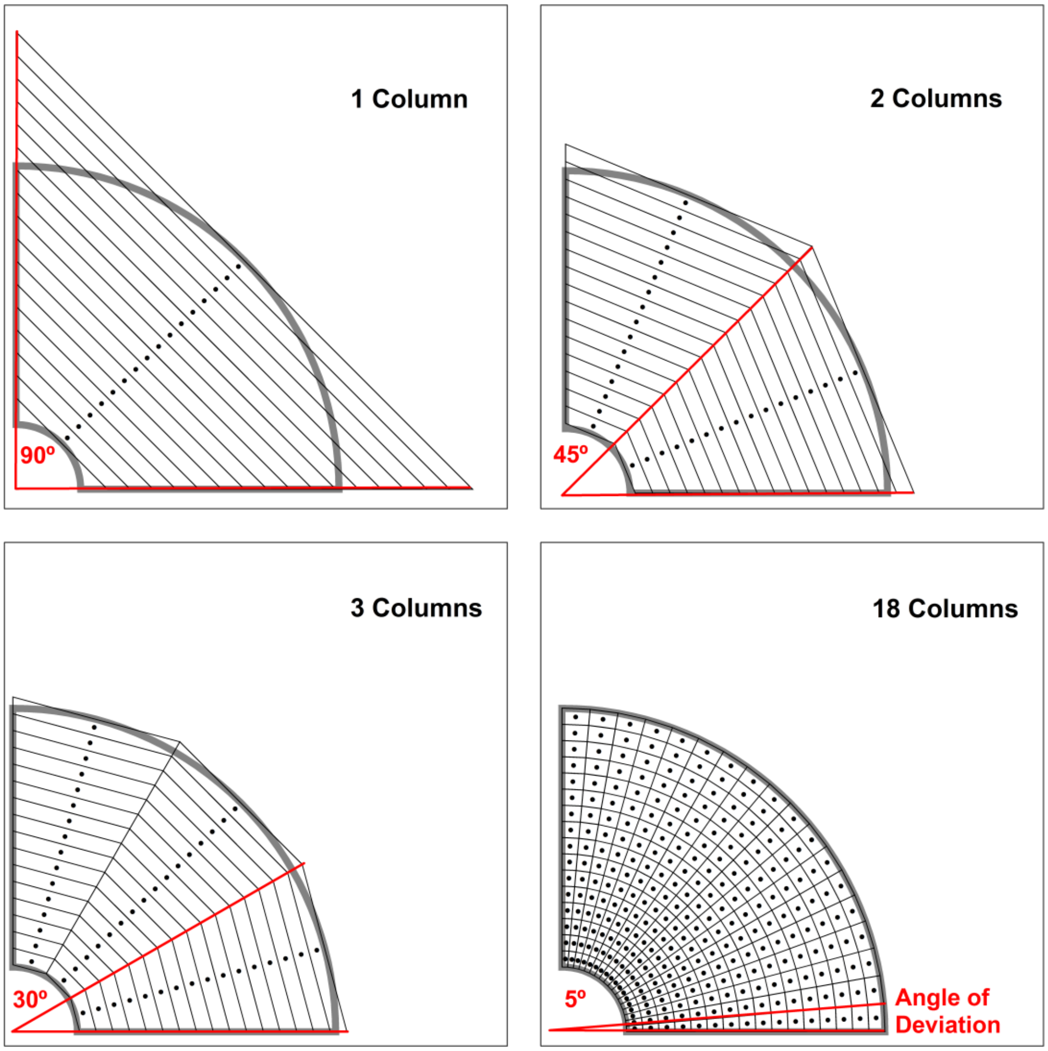

Figure 3. Illustration of system for describing multiple levels of spatial refinement for test problem.

single column is described as 90 degrees divided by the total number of columns in the flow domain. Figure 3 illustrates how increasing grid resolution reduces grid cell distortion between adjacent cells. Each grid contains 16 rows. For each case of spatial discretization, the block-centered grid nodes are placed at the same radial location so that any differences in the numerical solution between grids are attributed to the distortion of the grid, not to the location of the node where the solution is calculated. The coefficients in MODFLOW's numerical formulation are conductance-based and equivalent conductance between adjacent cells is affected by grid cell distortion. The test problem inspects MODFLOW IFD's capacity to numerically derive a head solution and associated intercell volumetric flow compared to the analytical solution when the internal calculation of equivalent conductance is affected by grid cell distortion.

Results and Discussion

The numerical solutions are compared to the analytical solution of the steady-state radial flow problem developed by Crank (Crank 1967). Figure 4 shows a comparison between analytical and numerical solutions for head (Figure 4a) and velocity (Figure 4b) along the radius of the flow domain for different levels of grid refinement. The values h_1 and r_1 are as defined on Figure 2. For the purpose of presentation, normalized velocity is shown. Normalized velocity is calculated by dividing each of the velocity values on Figure 4b by 3.59 meters per second, which is the smallest velocity resulting from the test problem.

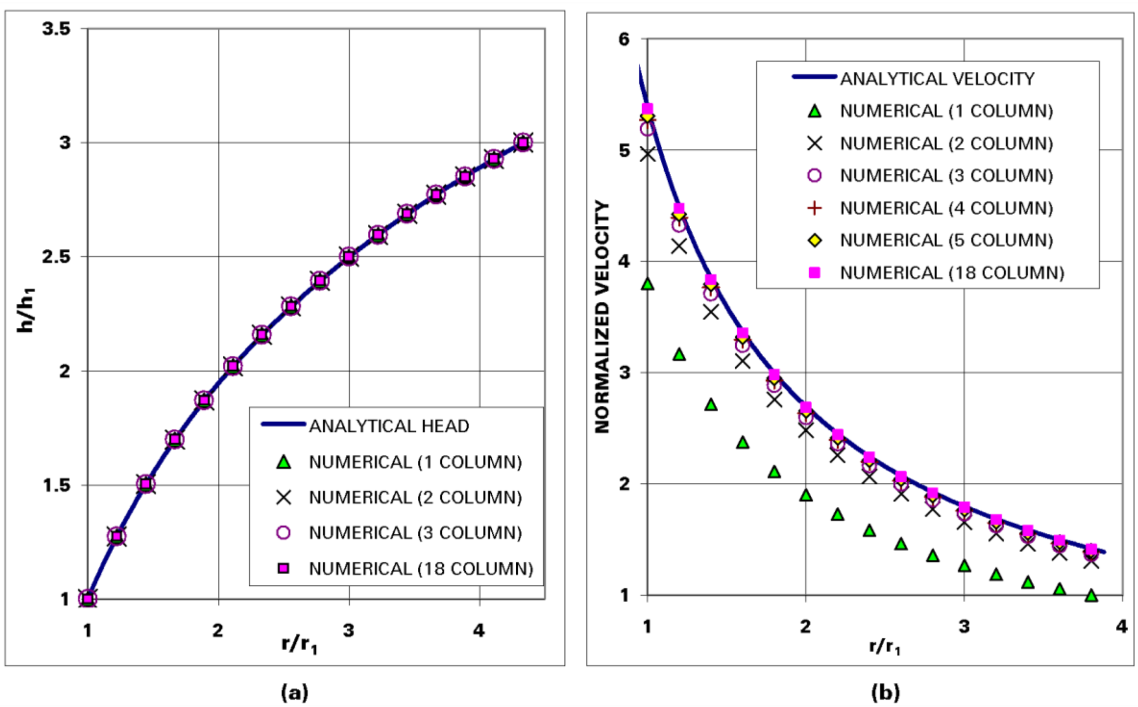

Figure 4. Comparison between analytical and numerical solutions for head (a) and velocity (b) along the radius of the flow domain for various levels of grid refinement.

The head solution is unaffected by grid cell distortion. The velocity solution is affected with significant improvement in accuracy as the grid is refined and grid cell distortion is reduced. Constructing a spatial grid with one or two columns is considered an inadequate spatial representation of the curve in the flow domain; however the cases are included to inspect the associated solution error. Figure 5 shows the sensitivity of the numerical velocity calculation to curvilinear grid spatial refinement.

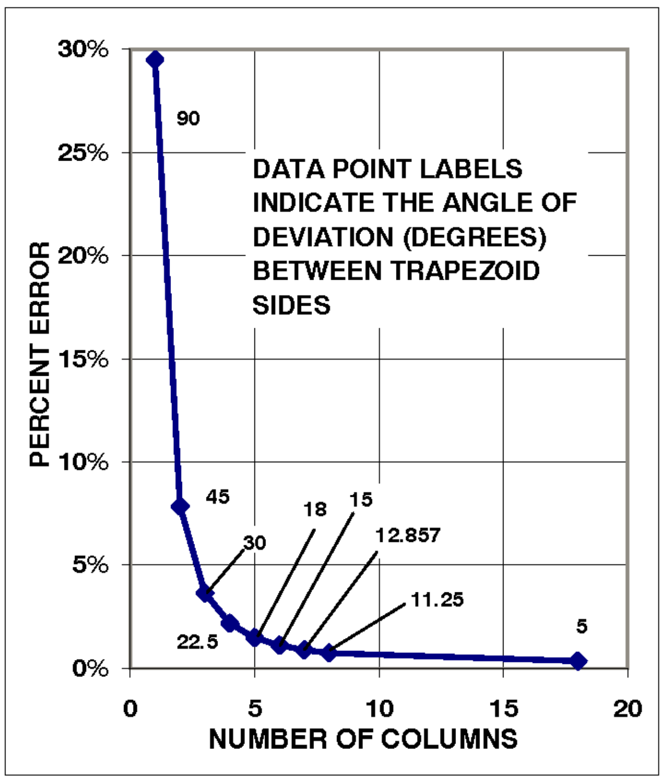

Figure 5. Sensitivity of numerical velocity percentage error to grid refinement.

The percent error is derived as the analytical calculation of velocity divided into the difference between the analytical and numerical velocity calculations. The percent error of the numerical velocity calculation is less than one percent if the flow domain is constructed with a curvilinear grid containing at least seven columns per 90 degrees or an angle less than 12.5 degrees deviation per column (rounding down to the nearest half degree). Users of the program may require more or less than one percent error in the velocity calculation for their purpose and may adjust the grid resolution and grid cell distortion accordingly.

The error of the calculated velocity solution is related to the degree to which the spatial discretization of a curve is approximated by piecewise linear segments or grid cell distortion as defined above. The relationship between the numerical error and the approximated curve stems from using the Divergence Theorem (Davis 1964) when the IFD numerical scheme is formally derived from the analytical governing flow equation. Details of the derivation and a description of this relationship are in Romero and Maddock (Romero and Maddock 2003).

The grid orientation for the test problem is such that the direction of flow is radial along grid columns. Tests designed to demonstrate the validity of the numerical solution when flow is not parallel to grid columns are planned, but are not presented here. However, the IFD numerical method has been mathematically proven (Narasimhan and Witherspoon 1976), so a grid with flow that is not parallel to the row or column directions is expected to work as well as does MODFLOW, so long as the grid exhibits enough spatial refinement such that the average length of flow between two piecewise linear cells adequately represents the actual length of flow. This point is illustrated in Romero and Maddock (Romero and Maddock 2003). The grid construction criterion developed here provides a means to quantify that adequacy. In the generalized case, the IFD numerical scheme is defined to work within a grid constructed from cells that have as many sides as the user wishes. Grids of that type do not have rows and columns as described in the curvilinear finite-difference grid used in MODFLOW IFD (Figure 1) and the direction of flow relative to any grid direction has no relevance with regard to accuracy of the numerical solution. MODFLOW IFD is the special non-generalized integrated finite-difference case in which model cells are always constructed out of cells with six sides. Standard MODFLOW is even more non-generalized than MODFLOW IFD because its grid cells are always constructed from cells with six orthogonal sides.

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Implications of Curvilinear Grid Development

MODFLOW IFD model simulations within a curvilinear grid require construction of a grid with rows and columns. Grid cells within a model layer can be in the shape of rectangles or trapezoids, thereby removing the constraint of spatially orthogonal rows and columns. Distortion of individual rows is not implemented here. Imposing a constraint on the distortion of trapezoidal shaped cells for integrated finite-difference calculations is analogous to the common practice of constructing finite element grids comprised of triangles that satisfy the geometric DeLaunay criterion (DeLaunay 1934). Grid refinement tests with finite element grids have shown that triangles with angles less than about 22.5 degrees can cause problems with the numerical solution (Neuman 1996).

In addition to the versatility added to grid construction with the implementation of MODFLOW IFD, the principal directions of hydraulic conductivity within the numerical model are affected. MODFLOW was developed under the assumption that the governing flow equation is oriented along the principal directions of hydraulic conductivity (McDonald and Harbaugh 1988). It follows that these directions in the modeled flow domain are parallel to the row and column directions of the model grid. If the grid is curvilinear, then the principal directions subject to anisotropy will meander with the curve of the grid. Figure 6 shows an example of meandering principal directions of hydraulic conductivity.

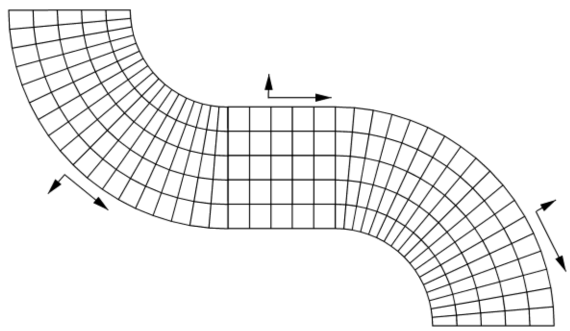

Figure 6. Illustration of meandering column to row anisotropy factor subject to principal directions of hydraulic conductivity.

Others have recently added the capability of variable principal hydraulic conductivity directions to a rectilinear grid in MODFLOW 2000 (Anderman et al. 2002; Minnema et al. 2003). Those methods alter the principal directions using operator and matrix splitting techniques implemented during the numerical solution process. Rather than altering the numerical solution process, the MODFLOW IFD approach alters the grid to reflect changes in the principal directions of hydraulic conductivity.

MODFLOW is one of the most widely used groundwater flow models in the fields of consulting and research. MODFLOW's inherent IFD numerical scheme and the illustrated test problem indicate that with minor modifications, all versions of MODFLOW may have the potential to make use of curvilinear grids incorporated with the ground water flow process. The code adaptations required to enable MODFLOW-88 to use its IFD method in curvilinear grids are minor and do not affect the numerical scheme or the solvers used to derive a solution. Users of standard MODFLOW can readily make use of the MODFLOW IFD implementation; rather than specifying DELR and DELC arrays to define the grid of the flow domain, a user inputs the x- and y-locations that define the corners of the rectangle or trapezoid that encloses each block-centered node for the topmost layer of the model grid. All other model input is the same as in the standard version of MODFLOW-88. If this same translation could be added to MODFLOW 2000(Harbaugh et al. 2000), then versatility in grid construction would potentially be made available as an option to the many existing users of the program. MODFLOW's robust numerical scheme does not have to be limited to a rectilinear grid.

Conclusions

MODFLOW IFD is capable of numerically deriving an accurate head solution and resultant intercell volumetric flow within a curvilinear grid constructed out of trapezoids. In the test problem defined herein, the IFD head solution is not affected by the level of refinement of angular displacement in the curvilinear grid. The velocity solution is affected, but associated error in the calculation from intercell volumetric flow is reduced to less than one percent if the angle between sides of trapezoidal cells is less than 12.5 degrees. The test problem is a hydrologic system in which flow directions are parallel to the direction of grid columns; however, the validity of the IFD numerical scheme in generalized grid cases supports the expectation that the solution will be valid for all flow directions.

MODFLOW's inherent integrated finite-difference method adds versatility to grid construction. A curvilinear grid creates a meandering column to row anisotropy factor that follows the directional change of the grid. Curvilinear grids with column to row anisotropy can have utility in either regional basins or local scale models where the principal directions of hydraulic conductivity are expected or known to change.

Minor modifications to MODFLOW-88's source code are required to enable utilization of its IFD numerical scheme and the associated changes to user input are transparent. MODFLOW-88's inherent IFD numerical formulation and the test problem results indicate that more recent versions of MODFLOW 2000 have the potential to make use of curvilinear grids incorporated within the ground water flow process.

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