ground water

Dip and Anisotropy Effects on Flow Using a Vertically Skewed Model Grid

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Abstract

Darcy flow equations relating vertical and bedding-parallel flow to vertical and bedding-parallel gradient components are derived for a skewed Cartesian grid in a vertical plane, correcting for structural dip given the principal hydraulic conductivities in bedding-parallel and bedding-orthogonal directions. Incorrect-minus-correct flow error results are presented for ranges of structural dip ($0 \leq \theta \leq 90$) and gradient directions ($0 \leq \varphi \leq 360$). The equations can be coded into ground water models (e.g., MODFLOW) that can use a skewed Cartesian coordinate system to simulate flow in structural terrain with deformed bedding planes. Models modified with these equations will require input arrays of strike and dip, and a solver that can handle off-diagonal hydraulic conductivity terms.

Introduction: Structure, Scaling, and Anisotropy

In regional ground water models of structural terrain, the principal conductivity directions may not be aligned with the model axes, and the intralayer distances separating solution points may not correspond to map distances. As a result, the directional components of an arbitrary flow direction, and the intralayer distances upon which these calculations are based, may become functions of the angle of dip. Modeling these systems, where bedding and/or bedding-plane partings are known to influence ground water flow (Burton et al. 2002), requires the physical rotation with dip of the transverse anisotropy in hydraulic conductivity, and depending on the model grid, may require the rescaling of intra-aquifer distances along dip. Bedding-parallel hydraulic conductivities, K_x, are determined from the analyses of in situ aquifer tests and/or lab tests in the plane of bedding. Intralayer distances between solution points (nodes) in the model are determined in the horizontal plane, usually from maps. Typically, the modeler assigns both the bedding-parallel hydraulic conductivity and the map distances to a layer within the model, assuming the principal conductivity directions in the plane of bedding, and the locations corresponding to the nodes of the grid, both lie in the horizontal plane. Bedding-orthogonal hydraulic conductivities, K_y, are determined from the analyses of in situ packer tests and/or lab tests in the plane perpendicular to bedding. Interlayer distances are commonly determined from vertical stratigraphic separations between aquifers; the vertical spacing between nodes may either be fixed or vary according to the thickness of the aquifer. Typically, the modeler assigns both the vertical stratigraphic separations and the bedding-orthogonal hydraulic conductivity to the vertical direction in the model, assuming the vertical direction corresponds to the principal conductivity direction perpendicular to the plane of bedding. However, in structural terrains at the scale of a ground water or reservoir model, the principal conductivity directions may not be aligned with the model axes and thus the directional components of an arbitrary flow direction become functions of the angle of dip, rotating the principal directions with the regional and/or local fold-controlled bedding. Depending on the choice of model grid, the intralayer distances also may become functions of the angle of dip. The typical approach then fails to characterize the flow properly within the medium and error is introduced to the model calculated heads and flows. This paper outlines corrections that can be made to ground water models to rescale intralayer distances and characterize the transverse anisotropy related to the structural dip of bedding.

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Model coordinate systems commonly require solution of the ground water flow equations in grid directions that are scaled along dip, and/or are not coincident with the principal hydraulic conductivity directions. MODFLOW (McDonald and Harbaugh 1988) allows for two basic approaches in defining a model grid, the grid overlay method and the boundary-matching approach (Jones et al. 2002). The grid overlay method results in uniform grids that do not necessarily match hydrostratigraphic boundaries, but are orthogonal in the vertical as well as horizontal plane. Orthogonality in the vertical plane allows for standard rotation transformations for the transverse anisotropy, although these transformations are not part of standard MODFLOW. The boundary-matching approach "ensure[s] that each upper and lower boundary [of the hydrostatigraphy] is precisely matched by a layer boundary in the MODFLOW grid." (Jones et al. 2002, p. 195). Use of the boundary-matching approach results in layer-centered nodes that parallel the bounding hydrostratigraphy, which usually results in a curvilinear coordinate system for the model.

Weiss (1985) presents an analysis of the hydraulic effects from changes in the aquifer elevation of nodes "that follow dip and local changes in aquifer thickness" (Weiss 1985, p. 254). Using a nonorthogonal, curvilinear coordinate system, he modeled a synclinal fold involving three isotropic aquifers and concluded that "elevation changes cause only small changes in flow pattern and head distribution from those of similar horizontal systems" (Weiss 1985, p. 272). Although he presents, in an appendix to the paper, the full ground water flow equation for transverse anisotropy in the nonorthogonal, curvilinear coordinate system, he does not present an analysis of the effect of the transverse anisotropy on either head or flow simulation. To isolate the effect of transverse anisotropy on flow, we present the error associated with Darcy flow equations for different conditions of gradient, structural dip, and degree of anisotropy. This paper presents corrections to the Darcy flow equations relative to a skewed Cartesian coordinate system (Butkov 1968) that commonly results from applying the boundary-matching approach to standard MODFLOW models designed for dipping beds. The nonorthogonal, layer-centered nodes are similar to those of Weiss (1985), but we neglect the effects related to curvature, i.e., the effects from local changes in the dip angle and/or aquifer thickness.

Methods

Darcy flow equations relating vertical and bedding-parallel flow to vertical and bedding-parallel gradient components, using bedding-parallel and bedding-orthogonal principal hydraulic conductivities, were derived as a function of structural dip, from known hydraulic conductivity tensor relationships.

Hydraulic Conductivity Ellipsoid and the Skewed Cartesian Grid

One quarter of a hydraulic conductivity ellipsoid is shown in Figure 1, with two equal principal hydraulic conductivities in the plane of dipping strata (K_x in direction

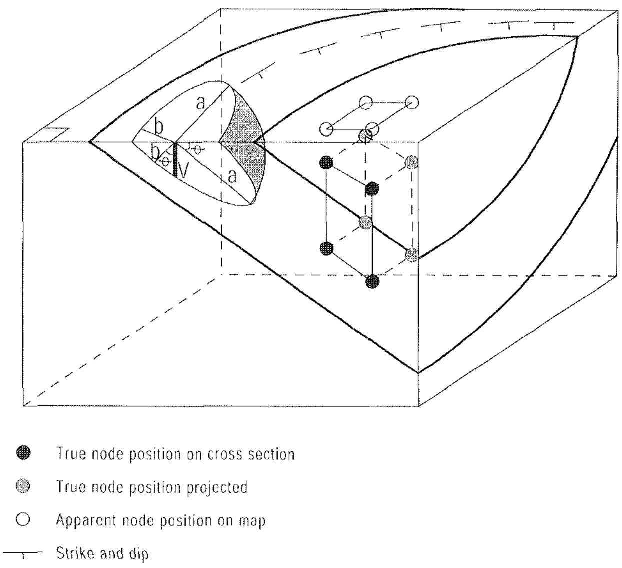

Figure 1. Block diagram showing relationship between true (stratally centered) and apparent (mapped) node positions, strike and dip of bedding. *a* is direction of bedding parallel hydraulic conductivity; *b* is direction of bedding perpendicular hydraulic conductivity; *V* is direction of vertical hydraulic conductivity between nodes. Eight nodes are connected in a prism in the *a* and *V* directions as they would be related in finite-difference approximations. The map or apparent positions of the eight nodes are connected in a rectangle.

"a") and an unequal principal hydraulic conductivity perpendicular to the plane of bedding (K_y in direction "b"). The condition shown is bedding-parallel isotropy (one principal direction in the direction of strike equal to the other in the direction of dip) and bedding-orthogonal anisotropy (the principal directions in the plane of bedding unequal to the principal direction perpendicular to bedding). The figure also shows layer-centered nodes that parallel the bounding hydrostratigraphy as commonly applied in MODFLOW models using the boundary-matching approach. These "true" nodes have "apparent" positions as they would appear mapped in a grid coverage for the horizontal domain. Eight neighboring true nodes, four in each stratum, are connected as they would be related in finite-difference approximations between them. The four nodes connected within a stratum are connected in the principal directions within the plane of bedding. However, the four nodes connected between strata are connected vertically in the direction "V" of the ellipsoid, not in the direction perpendicular to bedding. The coordinate system is thus nonorthogonal with layer-centered nodes that follow dip, similar to the curvilinear coordinate system of Weiss (1985), but neglecting curvature.

Results

Figure 2 shows the skewed Cartesian coordinate system (Butkov 1968), in a vertical plane oriented in an internodal direction (Figure 1), that would result in MODFLOW from using the boundary-matching approach to follow a dipping bed. The coordinate system is nonorthogonal with layer-centered nodes that follow dip, similar to the curvilinear coordinate system of Weiss (1985), but neglecting

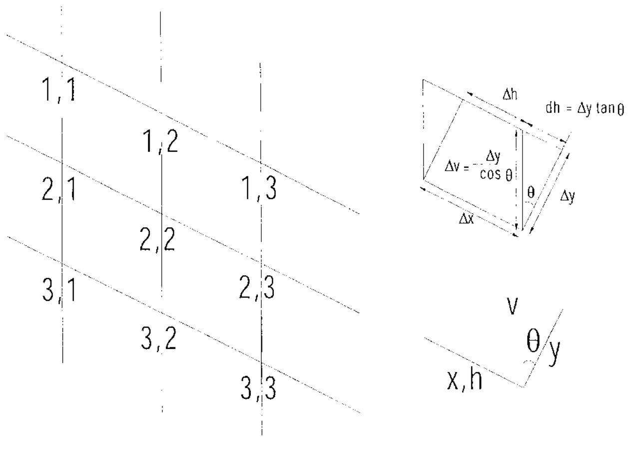

Figure 2. Skewed cartesian coordinate system (Butkov 1968) used in MODFLOW. The vertical plane, oriented in an internodal direction, shows *h* and *v* independent axes, corresponding to the bedding-parallel and vertical directions, respectively, and *x* and *y* independent axes, corresponding to the bedding-parallel and bedding-orthogonal principal hydraulic conductivities. The *h* and *x* directions are shared while the *v* direction is offset from the *y* direction by the apparent dip angle, θ.

curvature. The coordinate system is a skewed Cartesian system (Butkov 1968) with h and v independent axes corresponding to the bedding-parallel and vertical directions, respectively. The relationship of the coordinate system to a standard Cartesian coordinate system, with x and y independent axes corresponding to the bedding-parallel and bedding-orthogonal principal hydraulic conductivities, is also shown. The h and x directions are shared. However, the v direction is offset from the y direction by the apparent dip angle, θ, corresponding to the h-axis internodal direction. For the purpose of discussion and derivation, θ will be referred to as the dip. However, when correcting an actual ground water model, the apparent dip corresponding to each specific h-axis internodal direction must be calculated from the true dip angle, and the angle between the h-axis internodal direction and the strike direction using the standard formulas from structural geology.

A model using the skewed Cartesian coordinate system (Butkov 1968) but without correcting for dip introduces into the flow solution two types of error related to the dip angle: (1) it neglects the deviation of the vertical coordinate axis with the bedding-orthogonal principal hydraulic conductivity, and (2) it solves h-axis gradient and flow-vector calculations using the apparent internodal map distances supplied by the user, as opposed to the true internodal distances within bedding planes. Correcting the first type of error requires transformations between coordinate systems. Correcting the second type of error requires rescaling the h-axis-scaled flow and gradient calculations into the horizontal map dimensions with projection.

The corrections to the flow equations for the skewed grid accommodating structural dip, θ, involve (1) the transformation of the arbitrary flow vector (arbitrary direction) from the orthogonal coordinate system into the skewed coordinate system; (2) the rescaling of the skewed h-axis flow vector, converting its dimensions from the h-axis distances to map distances with projection onto the horizontal; (3) consideration of the relationship between the principal components of flow and the gradient vector in the orthogonal coordinate system; (4) the rescaling of the skewed h-axis component of the gradient, converting its dimensions from the h-axis distances to map distances with projection onto the horizontal; and (5) the transformation of the resultant gradient vector out of the skewed coordinate system into the orthogonal coordinate system.

The transformation of the arbitrary flow vector from the orthogonal coordinate system into the skewed coordinate system is given by

$$\begin{Bmatrix} q_h' \\ q_v' \end{Bmatrix} = \begin{bmatrix} 1 & -\tan\theta \\ 0 & \dfrac{1}{\cos\theta} \end{bmatrix} \begin{Bmatrix} q_x \\ q_y \end{Bmatrix} \qquad (1)$$

where the primes indicate that the flow vector, q′, is scaled in the skewed coordinate system. The rescaling of the skewed h-axis flow vector, converting its dimensions from the h-axis distances to map distances with projection onto the horizontal, yields

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} \cos\theta & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -\tan\theta \\ 0 & \dfrac{1}{\cos\theta} \end{bmatrix} \begin{Bmatrix} q_x \\ q_y \end{Bmatrix} \qquad (2)$$

The relationship between the principal components of flow and the gradient vector in the orthogonal coordinate system is given by

$$\begin{Bmatrix} q_x \\ q_y \end{Bmatrix} = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial x} \\ \dfrac{\partial H}{\partial y} \end{Bmatrix} \qquad (3)$$

The rescaling of the skewed horizontal component of the gradient onto map coordinates, converting its dimensions from the h-axis distances to map distances with projection onto the horizontal, and the transformation of the resultant gradient out of the skewed coordinate system into the orthogonal coordinate system is given by

$$\begin{Bmatrix} \dfrac{\partial H}{\partial x} \\ \dfrac{\partial H}{\partial y} \end{Bmatrix} = \begin{bmatrix} 1 & 0 \\ -\tan\theta & \dfrac{1}{\cos\theta} \end{bmatrix} \begin{bmatrix} \cos\theta & 0 \\ 0 & 1 \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix} \qquad (4)$$

Combining Equations 2, 3, and 4 yields a relationship between an arbitrary flow vector and the gradients in the skewed (i.e., model) coordinate system:

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} \cos\theta & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -\tan\theta \\ 0 & \dfrac{1}{\cos\theta} \end{bmatrix} \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ -\tan\theta & \dfrac{1}{\cos\theta} \end{bmatrix} \begin{bmatrix} \cos\theta & 0 \\ 0 & 1 \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix} \qquad (5)$$

The matrix multiplication yields

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} K_x \cos^2\theta + K_y \sin^2\theta & -K_y \tan\theta \\ -K_y \tan\theta & \dfrac{K_y}{\cos^2\theta} \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix} \qquad (6)$$

The correction for structural dip given by Equation 6 cannot be accommodated in most ground water flow models by input modification alone. Though the formulas on the main diagonal as input can modify the component of the gradient coincident with the solved component of the flow, the presence of off-diagonal terms requires modification of the solution algorithm to handle flow terms with mixed gradient components. Most model codes are designed with the assumption that coordinate axes of the model are aligned with the principal directions and with orthogonal gradient components (i.e., solving Equation 3). Uncorrected, these models can solve an incorrect equation for flow using principal conductivities and skewed gradient components:

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix} \qquad (7)$$

The error introduced to ground water models by structural dip, θ, can be analyzed by comparing the two solutions for *v*-axis and *h*-axis flows, subtracting Equation 6 (correct) flow solutions from Equation 7 (errant) flow solutions, for dips ranging between 0 and 90 degrees under a given condition of gradient (given gradient magnitude and direction). For a gradient magnitude of 1, the gradient directions can be conveniently expressed in the orthogonal coordinate system, specified by an angle φ where bedding-parallel gradients are given by $\varphi = 0°$ and $\varphi = 180°$ and bedding-orthogonal gradients are given by $\varphi = 90°$ and $\varphi = 270°$ as illustrated in Figure 3. The relationship between the orthogonal-coordinate-system gradient components and the skewed-coordinate-system gradient components are given by the inverse of Equation 4:

$$\begin{Bmatrix} \dfrac{\partial H}{\partial h} \\ \dfrac{\partial H}{\partial v} \end{Bmatrix} = \begin{bmatrix} \dfrac{1}{\cos\theta} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \sin\theta & \cos\theta \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial x} \\ \dfrac{\partial H}{\partial y} \end{Bmatrix} \qquad (8)$$

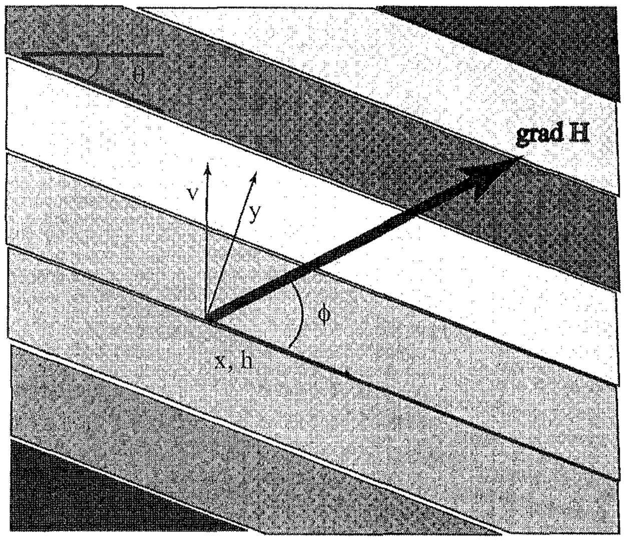

Figure 3. Relationship between structural dip (θ) and the orientation of an arbitrary head gradient measured from bedding (φ).

which reduces Equation 6 (the correct flows) to

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} K_x \cos\theta & -K_y \sin\theta \\ 0 & \dfrac{K_y}{\cos\theta} \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial x} \\ \dfrac{\partial H}{\partial y} \end{Bmatrix} \qquad (9)$$

and reduces Equation 7 (the errant flows) to

$$\begin{Bmatrix} q_h \\ q_v \end{Bmatrix} = \begin{bmatrix} \dfrac{K_x}{\cos\theta} & 0 \\ K_y \sin\theta & K_y \cos\theta \end{bmatrix} \begin{Bmatrix} \dfrac{\partial H}{\partial x} \\ \dfrac{\partial H}{\partial y} \end{Bmatrix} \qquad (10)$$

Assuming a gradient magnitude of 1 and different bedding-parallel (K_x) to bedding-orthogonal (K_y) hydraulic conductivity ratios, Equation 9 (correct) flows were subtracted from Equation 10 (errant) flows and expressed as a flow error percent by dividing by the magnitude of the correct flow vector (Equation 9, $\sqrt{q_h^2 + q_v^2}$). Figure 4 shows the range of the flow errors analyzed through 360° of different gradient directions (φ) and through 90° of dip (θ).

Discussion

The plots of Figure 4 show that the flow errors, introduced by not correcting the flow equations for structural dip, are significant. For isotropic conditions as well as for two anisotropic conditions with order-of-magnitude changes in the K_x to K_y ratios, flow errors along the *h*-axis usually reach 100% error within 50° of dip. The error range is smaller for smaller dips, generally <20% within 10° of dip. Flow errors along the *h*-axis are significant for isotropic conditions, and become increasingly significant with increasing K_x to K_y ratios. Flow errors along the *v*-axis

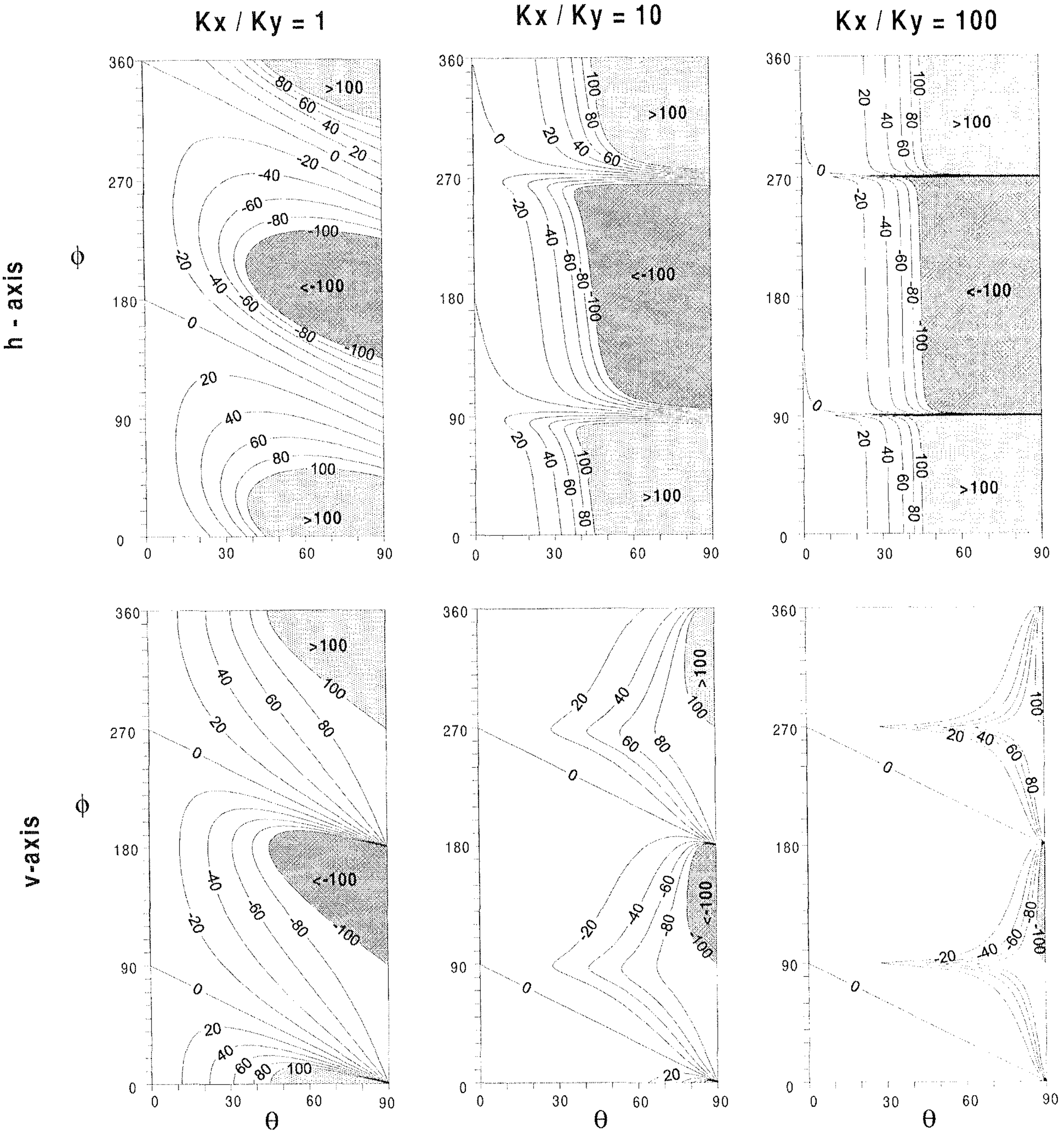

Figure 4. Errors (incorrect minus correct) of the *h*-axis and *v*-axis components of flow q_h and q_v in the skewed (*h, v*) coordinate system, as a percentage of the correct "magnitude" $\sqrt{q_h^2 + q_v^2}$. This expression represents the average size of q_h and q_v, and is not the physical length of the flow vector (unless θ = 0). Each panel shows the error as a function of structural dip (θ) and orientation of the head gradient measured from bedding (φ), with values ≤ –100% dark shaded and >100% light shaded. The upper panels are for the *h*-axis flow component, and the lower panels are for the *v*-axis component. The three columns are for amounts of anisotropy between the bed-parallel (K_x) and bed-orthogonal (K_y) hydraulic conductivities.

are significant for isotropic conditions, but become less significant with increasing K_x to K_y ratios.

Our results suggest that failure to consider the effects of structural dip on model grid rescaling and rotation of the direction of transverse anisotropy results in large errors in model calculated flows. Weiss (1985) presents the derivation of the full ground water flow equation for transverse anisotropy in the nonorthogonal, curvilinear coordinate system, a coordinate system that usually results from using the boundary-matching method in MODFLOW models. Kladias and Ruskauff (1997) outline how to incorporate spatially variable (heterogeneous) anisotropy within the plane of the layer in MODFLOW. Their modification generalizes the column-to-row anisotropy factor into an array, prescribing a unique value for each cell in the model. This approach does not allow the orientation of the principal axes to change spatially. The U.S. Geological Survey is currently researching ways to incorporate generalized heterogeneous anisotropy within the plane of the layer in MODFLOW, where both the anisotropic factor and orientation of principal axes can change spatially (Hill 2002). Cross-sectional models constructed within a single layer would thus be able to handle structural dip. However two- or three-dimensional, multiple layered models exploiting the boundary-matching method would still not be able to handle structural dip until a correction for generalized heterogeneous anisotropy is implemented in the vertical plane. Implementing Equation 6 corrections into MODFLOW is not trivial, requiring a solver routine that can handle the off-diagonal terms.

If implemented in MODFLOW or another model that similarly uses a boundary-matched grid, the flow equation corrections of Equation 6 will require apparent dips for each *h*-axis internodal direction. Therefore, these corrections will similarly require two significant variables for each cell in the model, namely strike and dip (or dip and dip direction) of bedding, derived from one traditional geologic field measurement and compiled into model arrays. Generating arrays of these variables as input to ground water and/or reservoir models will require strike and dip measurements to be geographically located within the model domain, preferably in a GIS.

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