COMPARISON OF ALTERNATIVE NUMERICAL MODELS TO REPRESENT PERMEABILITY ANISOTROPY IN FRACTURED-SEDIMENTARY ROCK


Abstract

Ground-water flow through the folded and faulted sedimentary rocks in the Shenandoah Valley in Virginia is simulated using the U.S. Geological Survey ground-water flow and transport model SUTRA. Hydraulic connections along bedding planes within the rocks are represented by specifying variable-direction anisotropy based on a three-dimensional structural model that depicts the strike and dip of the bedding throughout the model domain. The directions of maximum and medium permeability conform to the strike and dip of the bedding, respectively, while the minimum permeability direction is normal to the strike and dip of the bedding.

Simulation studies of inclined fractured-rock aquifers typically utilize finite-difference models that are formally limited to an orthogonal grid oriented with the principal axes of the permeability tensor. Bedrock structure can be represented in these models by (1) aligning the grid rows parallel to the strike of the bedding and specifying horizontal anisotropy to decrease permeability in the grid-column direction, or (2) aligning the grid layers to the dip of the bedding to represent flow within bedding-plane fractures. Under approach (1) the simulated permeability tensor is horizontal and does not account for the dip of the rock. Under approach (2) the axis of minimum permeability is vertical, rather than perpendicular to the bedding.

Results of SUTRA models of the Shenandoah Valley are compared to evaluate differences in predicted ground-water flow paths and delineated capture zones to a production well. The base model (A) has spatially-variable three-dimensional anisotropy, while three alternative were prepared by adjusting the permeability tensor to represent the bedrock structure as (B) horizontally isotropic, (C) horizontally anisotropic with a uniform strike, and (D) horizontally anisotropic with spatially-variable strike. Alternative numerical models, which do not explicitly represent the generalized three-dimensional anisotropy, cannot accurately reproduce all features of the flow paths and the capture zone to the production well.
Introduction

Ground water flows through fractures in sedimentary rocks that underlie the 7120-km² Shenandoah Valley. The valley is underlain by Cambrian to Devonian sedimentary rocks that were contractionally deformed and folded during the Alleghanian orogeny about 300 m.y. ago. The Massanutten synclinorium occupies the central part of the valley and contains a section of strata as much as 5 km thick with a core of clastic rocks that form Massanutten Mountain. The clastic rocks are underlain by carbonate rocks that outcrop on the eastern and western sides of the synclinorium (Figure 1). The valley is bounded to the east by Neoproterozoic metamorphic rocks of the Blue Ridge anticlinorium and to the west by the North Mountain Fault. Bedding is the dominant foliation in the sedimentary rocks and generally strikes N 30° E. Rocks on the western limb of the synclinorium generally dip gently southeast, whereas the rocks on the eastern limb dip to the northwest, are near vertical, or locally are overturned. The east and west limbs converge in the core beneath Massanutten Mountain and are nearly flat-lying. The bedding is intersected by cross and longitudinal joints related to folding that are steep and strike northwest and northeast, respectively.

Ground-water flow in the Shenandoah Valley was simulated with three-dimensional models constructed using SUTRA with an irregularly-connected mesh of quadrilateral elements with maximum lateral lengths of 1 km. Steady-state simulations were used to compute the hydraulic-head distribution and to estimate the rate of ground-water flow because the aquifer system is assumed to be near equilibrium, as indicate by long-term well hydrographs and the relatively small rate of ground-water withdrawals. The models represent the aquifer system in fractured bedrock with a constant saturated thickness and represent downward flow from the saturated overburden as recharge to the underlying fractured bedrock.

Figure 1 Bedrock geology in Shenandoah Valley.
Conceptual fracture framework

Ground-water in the Shenandoah Valley flows through a diffuse, regional flow system that consists of a three-dimensional network of fractures formed by bedding and joints. The direction of maximum hydraulic conductivity is typically oriented within bedding planes, while the direction of minimum hydraulic conductivity is perpendicular to the bedding. This arrangement causes anisotropic hydraulic behavior that has been observed in tracer and aquifer tests (Jones, 1991; Burbey, 2003). The regional flow system locally is disrupted by faults and karst. Faults offset bedding, fractures associated with some faults provide conduits for vertical flow (Harlow and others, 2005), and some faults are barriers to flow. Dissolution along fractures in carbonate rocks creates narrow karst channels, sinkholes are areas of recharge, and springs are points of discharge. The faults and karst features create local flow systems that are hydraulically connected to the diffuse, regional flow system, and they can either direct or divert water to or from the regional system. The ground-water model in this study was designed to only represent the diffuse, regional flow system, a decision supported by water-quality data from springs which indicate that ground-water discharge is generally near saturation with respect to calcite (L. Niel Plummer, U.S. Geological Survey, oral commun., 2007), as expected in areas dominated by diffuse flow. Ground water in areas dominated by discrete flow is typically under saturated with respect to calcite because travel times are too short to allow dissolution reactions to reach saturation (White, 1988).

Representation of bedrock structure

Simulation studies of inclined fractured-rock aquifers typically utilize finite-difference (FD) models (such as MODFLOW) that are formally limited to an orthogonal grid oriented with the principal axes of the hydraulic-conductivity tensor. Bedrock structure can be represented in these models by (1) aligning the grid rows parallel to the strike of the bedding and specifying horizontal anisotropy to decrease hydraulic conductivity in the grid-column direction, or (2) aligning the grid layers to the dip of the bedding to represent flow along bedding. Under approach (1) the simulated hydraulic-conductivity tensor is horizontal and does not account for the dip of the rock. Under approach (2) the axis of minimum hydraulic conductivity is vertical, rather than perpendicular to the bedding. Moreover, application of this latter approach to represent folds is complicated because the dip direction is not constant.

The accuracy of simulations using an orthogonal FD grid with MODFLOW is limited by the assumption that the principal directions of the conductivity tensor are parallel to the coordinate axes used to define the grid. Significant errors in flow can result if the orientation of the conductivity tensor does not coincide with the model coordinate axis (Hoaglund and Pollard, 2003). The resulting errors in flow are a function of the dip, the direction of the hydraulic gradient, and anisotropy (ratio of bedding-parallel to cross-bedding hydraulic conductivity). The errors are small (< 20 percent) for dip angles less than 10º, but can reach 100 percent for dip angles greater than 50º (Hoaglund and Pollard,
Weiss (1985) had previously developed a FD numerical method to address this issue by using a non-orthogonal, curvilinear coordinate system, but the method has not been incorporated in widely-used FD models such as MODFLOW. Anderman and others (2002) added a package to MODFLOW to represent variable-direction anisotropy within a two-dimensional plane. Although this same method could be extended, in principal, to three dimensions, it is not currently available in MODFLOW.

In finite-element (FE) models, such as SUTRA (Voss and Provost, 2002), the principal directions of the conductivity tensor can be specified independently of the model coordinate axes and the finite-element mesh. As a result, FE models are particularly applicable to the simulation of flow through folded, fractured-rock where directions of strike and dip are variable. Bedrock structure can be represented by varying the orientation of the conductivity tensor in each element to reflect variations in the strike and dip of the bedding. In this study, SUTRA was used to simulate ground-water flow using strike and dip values computed from bedding form-surfaces that were interpolated from generalized structural cross-sections.

**Computation of conductivity tensor**

A series of geologic sections were constructed, northwest to southeast, across the Shenandoah Valley, from the Potomac River at the north to the southern watershed divide, two of which are shown on Figure 2. The sections extend from the North Mountain thrust fault at the west boundary to its base at a depth of about 5 km below sea level; the eastern boundary is the drainage divide in the Blue Ridge. The sections show the distribution of major rock units, form lines of bedding, and mapped thrust faults. Contacts at land surface were projected to depth using the dip values of the bedding, and the thicknesses of units at the surface were used to project the geometry into the subsurface. Form lines of bedding illustrate the folded strata and are generalized due to the scale and spacing of the cross sections. Form lines on each section were connected along strike to create “form surfaces”, which provide hydraulic continuity. The resulting stack of form surfaces provides a three-dimensional representation of bedding. Due to complexity, the form surfaces are generalized on the clastic rocks that underlie Massanutten Mountain and the carbonate rocks to the east of it.
Anisotropy in clastic, carbonate, and western-toe carbonate rocks was represented in the base model A (variable strike and dip) by aligning the principal directions of the conductivity tensor with the bedding, so the components of the conductivity tensor are parallel to the principal fracture orientations. The directions of maximum and medium hydraulic conductivity ($K_{\text{max}}$ and $K_{\text{med}}$) are assumed to lie within each form surface, along strike and down dip (respectively), while the minimum hydraulic conductivity ($K_{\text{min}}$) is oriented perpendicular to the form surface (i.e., parallel to the joint sets). The conductivity tensor for metamorphic rock was horizontally isotropic with the $K_{\text{min}}$ direction oriented vertically. Values of $K_{\text{max}}$, $K_{\text{med}}$ and $K_{\text{min}}$ were estimated through model calibration. Power functions were specified to decrease in hydraulic conductivity with increasing depth below land surface using separate decay factors $\lambda$ for carbonate and noncarbonate rocks.

The predominant strike direction of the bedding in model A is N 30° E, but the strike directions in the model range from N 30° W to S 30° W (Figure 3A). The directions N 30° E (yellow) and S 30° W (blue) are parallel and distinguish bedding that is inclined southeastward from bedding that is inclined northwestward, respectively. These areas cover most of the model domain and are associated with clastic and carbonate rocks. Narrow bands of equal-strike direction correspond to undulations in the bedding. The area with a strike direction of E 90° (green) is defined in SUTRA for areas that are isotropic ($K_{\text{max}} = K_{\text{med}}$) and corresponds to the metamorphic rock. Dip angles range from 0° to 60° E and are generally steepest in carbonate rocks along the flanks of the basin (Figure 3B). Dip angles of 0° (red) are assigned to metamorphic rocks and areas where the bedding is horizontal.
Three alternative SUTRA models of the Shenandoah Valley based on different conceptual models of bedrock structure in carbonate and clastic rocks were prepared by specifying the conductivity tensor as horizontally isotropic (model B), horizontally anisotropic with a uniform strike (model C), and horizontally anisotropic with spatially-variable strike (model D). Bedrock structure is essentially ignored in alternative model B. Alternative model C is equivalent to using an orthogonal FD grid with grid rows parallel to the strike of the bedding and specifying horizontal anisotropy to decrease hydraulic conductivity in the grid-column direction. Alternative model D is equivalent to using the variable-direction anisotropy (LVDA) package in MODFLOW to represent bedrock structure.

Model calibration

The ground-water flow models were calibrated through nonlinear regression using UCODE (Poeter and Hill, 1998) to optimize hydraulic conductivity values using measured ground-water levels in 354 wells and discharges at 23 gaging stations in the Shenandoah Valley. The optimized parameters included $K_{\text{max}}$ of each of the four rock classes, the $K_{\text{max}}$$:K_{\text{min}}$ ratios of carbonate and metamorphic rock, and two decay factors used in the power functions. Residual plots for heads simulated by model A indicate good model fit.
with little bias and a standard error in head of 18.8 m, about 3 percent of the 646-m measurement range. Simulated flows were within 35 percent of the observed values with a slight bias toward under prediction at higher flows, which could result from either lack of detail in the simulated stream network, or omission of discrete features that increase ground-water discharge.

The optimized $K_{\text{max}}$ values of the four rock units in model A differ by less than a factor of four, with the largest values estimated for carbonate rocks (3.3 m/d) and the smallest value estimated for clastic rock (0.9 m/d). The estimated $K_{\text{max}}$:$K_{\text{min}}$ ratios for both clastic rocks (5000) and metamorphic rocks (4100), however, are much larger than for the carbonate rocks (50), restricting the simulated flow across the bedding in clastic rock and within the vertical plane in metamorphic rock. The estimated λ value for clastic and metamorphic rocks (3.4e-03 m$^{-1}$) is also larger than the value estimated for carbonate rocks (4.9e-04 m$^{-1}$), which results in a steeper decline of hydraulic conductivity with depth than in carbonate rocks. As a result, most of the simulated flow is relatively shallow in the clastic and metamorphic areas. Simulated flow in carbonate rock areas is deeper and less restricted by the bedding because the estimated values for λ and the $K_{\text{max}}$:$K_{\text{min}}$ ratio are lower than for the clastic and metamorphic rocks. The estimated $K_{\text{max}}$:$K_{\text{med}}$ ratio for carbonate rocks (2.4) is larger than 1.0, however, which limits flow in the direction of dip.

**Comparison of alternative models**

The three alternative models were calibrated through nonlinear regression with UCODE using the same parameter set and observations included in the calibration of variable-strike-and-dip model A. The model fit for the alternative models is slightly better than in model A and is mostly the result of improving the fit to head observations in carbonate rocks. The parameter values estimated for clastic and metamorphic rocks with the alternative models are generally similar to those estimated with model A. The estimated $K_{\text{max}}$ values for carbonate rocks are lower than those estimated for clastic and metamorphic rocks, however, which is not consistent with field observations. As a result, the range of $K_{\text{max}}$ values estimated with the alternative models (0.8 to 1.7 m/d) is narrower than that estimated with model A (0.9 to 3.3 m/d).

The most significant differences in the parameter sets are the values estimated for carbonate rocks. The $K_{\text{max}}$ values estimated with the alternative models are less than one-half the value estimated with model A, and the estimated λ values result in less decline of hydraulic conductivity with depth. The estimated $K_{\text{max}}$:$K_{\text{med}}$ ratios for the carbonate rocks (3.4 to 6.5) are larger because the anisotropy ratio represents the contrast in hydraulic conductivity between directions parallel and perpendicular to strike within a horizontal plane, rather than along strike and dip as in model A. The estimated $K_{\text{max}}$:$K_{\text{min}}$ ratios for the carbonate rocks have values close to 1.0, so flow is nearly isotropic in the vertical plane throughout the model domain. In contrast, vertical flow in model A is limited to areas where the bedding of the carbonate rocks is inclined. The $K_{\text{max}}$:$K_{\text{min}}$ ratio estimated in model B (6.3; horizontally isotropic) is less than the ratio estimated in model A and restricts vertical flow. As a result of these differences in estimated parameter values,
simulated flow in models C and D penetrates deeper into the aquifer system over broader areas than in model A, while simulated flow in model B is shallower.

**Ground-water age distributions**

Ground-water age was computed through steady-state simulations in which the solute concentration was interpreted as age. The initial concentration (age) and concentration of recharge were specified as zero, and a zero-order solute production of unit strength (1 concentration unit/year) was used to represent aging. Longitudinal and transverse dispersivities were specified as 500 m and 10 m, respectively, to facilitate convergence of the transport solution and reduce numerical oscillations. Simulated ages are inversely proportional to the value of effective porosity specified in the models (1.3x10^{-3}), which was estimated by adjusting the flow-weighted average age of ground-water discharge in model A to the 20-yr residence time previously computed for the Potomac watershed by Michel (1992), who used long-term records of tritium content in surface water. The simulated age distributions are qualitative and are used only to distinguish younger waters from older waters, because of uncertainty regarding the variability of effective porosity within rock units and with depth below land surface.

The simulated distribution of ground-water age in model A (variable strike and dip) indicates that most shallow ground water is less than 3 years old in the carbonate rock areas, and less than 10 years old in the metamorphic rock areas (Figure 4A). Older water (more than 30 years old) discharges beneath the major stream channels. In carbonate areas the depth of recent flow (less than 3 years) is typically within 150 m of land surface, except in areas with high relief where the bedding is steeply dipping. In these areas, such as the western basin boundary along the North Mountain fault and the periphery of Massanutten Mountain, the depth of recent flow is as much as 500 m. Ground water that penetrates to these depths flows northeastward along the strike of the bedding and discharges in the northern parts of the basin. Simulated ground-water ages increase with depth towards the bottom of the basin where the older waters have simulated ages greater than 100 years. Unfortunately, it is not possible to compare the simulated results with observed data because information concerning ground-water age at discrete depth intervals within the aquifer system is not available.
The ground-water age distribution simulated with model B (horizontally isotropic) is similar, but 30-yr old water does not penetrate as deep as in model A because the $K_{\text{max}}:K_{\text{min}}$ ratio (6.3) restricts vertical flow. In contrast, the 30-yr old water in model C (uniform strike) penetrates deeper than in model A because the hydraulic conductivity decreases more slowly with depth and flow is isotropic in the vertical plane (Figure 4B). This effect is most pronounced in carbonate rock beneath Massanutten Mountain in the center of the valley where the ground-water age is more than 100 years in model A and only 30 years in model C. Water flows downward with the dip of the bedding in model A, but the depth of penetration is limited in the center of the valley where the bedding becomes horizontal. In contrast, the degree of vertical hydraulic connection is uniform throughout the domain of model C, which does not represent the dip of the bedding. The ground-water age distribution simulated with model D (variable strike) closely matches that of model C.

**Capture zones of a municipal well field**

Capture zones of the Martinsburg well field in Berkeley County WV were delineated through backwards tracking in reverse-flow simulations. Reverse-flow simulations are achieved by multiplying all specified heads and all sources by negative one (-1). This means that water production wells become injection wells in the reverse-flow simulation and recharge rates are specified as negative values. Further, the drain boundaries representing discharge to streams are replaced by specified head boundaries with negative head values. These changes have the effect of routing flow in a reverse direction from inflow points at production wells and along streams to discharge points at land surface. Inflow from the well was labeled with a conservative tracer of unit strength and tracked
backwards through steady-state transport simulations to delineate approximate capture zones. Longitudinal and transverse dispersivities were specified as 500 m and 10 m, respectively, as in the simulations of ground-water age presented above.

This procedure is similar to backward tracking using particles (Zheng and Bennett, 2002), but, the simulation of dispersion results in larger areas being delineated. The dispersion coefficient represents heterogeneity in aquifer hydraulic conductivity that creates uncertainty in the position of the capture zone. A normalized concentration distribution can be strictly interpreted as a location probability distribution (Neupauer and Wilson, 2004) for a similar simulation with somewhat different boundary conditions. Qualitatively, the present simulated concentration distributions may be interpreted as relative certainties that water recharging parts of the capture zone will reach the well. Water recharging at locations of higher concentrations are more likely to reach the well at the field site than water recharging at locations of lower concentrations.

The capture zone delineated with model A (Figure 5A) is irregular in shape and displays more evidence of the underlying bedrock structure than the zones delineated with the three alternative models, which are smoother. The shading of the capture zones indicates the relative likelihood that recharge within the capture zone will be discharged by the well. The width of the capture zone is related to the specified value of transverse dispersivity (10 m), and would be greater for larger dispersivity values that reflect more heterogeneity in hydraulic conductivity. Flow vectors simulated with model A (not shown) indicate more flow to tributary streams that flow perpendicular to the N 30° E strike of the bedding and less flow to the larger stream reaches that are aligned parallel to strike. This result is consistent with the pattern of base flow observed by Lewis (1992) in the Newark Basin.

There is more flow to larger streams reaches and less to tributaries in the alternative models, which is opposite to the flow pattern simulated by model A. The capture zone delineated by model C (uniform strike) generally follows the strike of the bedding (Figure 5B, but there is more cross-strike flow than in model A because the estimated $K_{\text{max}}:K_{\text{med}}$ ratio (6.5) provides larger hydraulic conductivity perpendicular to the bedding than the $K_{\text{max}}:K_{\text{min}}$ ratio (50) in model A. The capture zone delineated with model D is similar to that of model C. The depth of the capture zone delineated by variable-strike-and-dip model A is limited by the dip of the bedding (Figure 5A), which is inclined southeastward. In contrast, the capture zones delineated with the three alternative models extend to the bottom of the modeled domain (Figure 5B). Although most of the flow to the production wells in all four models is through the upper 300 m of the model domain, it is unreasonable to assume that water from depths of 5 km will discharge to the wells, as predicted by the three alternative models.
Figure 5. Capture zones to the Martinsburg municipal well field in Berkley County WV delineated with models variable strike and dip (A) and uniform strike (C).

Conclusions

Variable-strike-and-dip model A provides a distinctive characterization of the flow system in the Shenandoah Valley that reflects the underlying bedrock structure. Representation of changes in the strike and dip of bedding limits the depth of simulated flow where bedding is near horizontal and enhances simulated discharge to streams channels aligned perpendicular to strike. These features produce a physically realistic flow system that is consistent with conceptual models for flow through inclined fractured rock.

The alternative models do not explicitly represent changes in the strike or dip of bedding and simulate flow systems that do not reflect the underlying bedrock structure. These models produced physically unrealistic depictions of the flow system with nearly isotropic flow in the vertical plane throughout the model domain. As a result, ground-water flow penetrated deeper into the aquifer system over broader areas than in the original model and simulated ground-water ages were younger, particularly in the center of the valley beneath Massanutten Mountain, which forms the core of the synclinorium. Capture zones to a municipal well field delineated with the alternative models did not reflect the underlying bedrock structure and extended to the bottom of the 5-km deep basin, which is physically unrealistic. In contrast, the depth of the capture zone delineated with the original model was limited by the dip of the bedding and reflects the orientation of the underlying bedding. The three alternative models do produce a slightly improved model fit to the head and discharge observations used in model calibration, so the available data are not sufficient to rigorously determine which model of the flow system is best. Differences in simulated ground-water ages indicate that age data could be used for this purpose.
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References


**Biography**

Richard Yager is a research hydrologist with the US Geological Survey and has been involved with ground-water modeling studies for over 25 years in western New York. He graduated from Cornell University with a BS in Civil Engineering (1973) and MS in Agricultural Engineering (1981). His research interests include application of nonlinear regression to parameter estimation in model calibration, and flow and transport modeling in fractured rock terrains. He is currently involved in ground-water modeling studies in Rockland County NY.