Groundwater

Methods Note/

Axisymmetric Modeling Using MODFLOW-USG

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Abstract

Axisymmetric groundwater models are used for simulating radially symmetric conditions. Groundwater simulators built specifically to model axisymmetric conditions are most commonly used for simulating aquifer tests. Although some numerical models capable of simulating flow and solute transport that are developed in the cartesian coordinate system framework offer flexibility to simulate axisymmetric conditions, most of the numerical groundwater models, such as the MODFLOW family of codes, are based on structured grids in which axisymmetric flows cannot be directly simulated. Researchers in the past have provided methods to manipulate aquifer properties to mimic axisymmetric conditions. This study presents a methodology that takes advantage of the unstructured grids of MODFLOW-USG to simulate axisymmetric models within the MODFLOW framework. To develop axisymmetric models, the intercell interface area arrays of MODFLOW-USG were calculated to accurately represent coaxial cylindrical model cells. Three examples are presented to demonstrate the application of MODFLOW-USG for axisymmetric modeling: a pumping well with delayed yield effects, a vadose zone flow model simulating an infiltration basin, and a density-dependent saltwater intrusion problem for a circular island. Results were verified against analytical solutions and published numerical codes.

Introduction

Groundwater models simulating cylindrical flow domains that are symmetric around the axis of the modeled domain are referred by several names including axisymmetric (axially symmetric) models, radial flow models, cylindrical models, R-Z models, or R-Theta models. Groundwater flow equations for axisymmetric models are written using cylindrical polar coordinates (r, θ, z) and are solved for radial flow within a cylindrical domain.

Axisymmetric models are suitable for idealized situations in which the impact of stresses on the groundwater system is radially symmetric. Analytical models for aquifer flow like the Theis solution are classic examples of radial flow systems. Some numerical models are developed to exclusively simulate axisymmetric flow in a pumping well. Mansour et al. (2007) present an axisymmetric finite-difference flow model capable of solving heterogenous aquifer under confined or unconfined conditions designed to simulate pumping tests.

Fully three-dimensional (3D) models can be developed to solve radially symmetric problems, but axisymmetric models offer an advantage in efficiency and accuracy as fully 3D models are sometimes impractical to simulate if near-well and far-well processes are to be evaluated. In fully 3D models grid refinement can lead to a large number of model cells, which in turn can substantially increase the simulation run time. Axisymmetric models essentially reduce a 3D problem to two-dimensions resulting in fewer model cells and hence, improve efficiency. In contrast with 3D models, depending on the need for accuracy, high degree of grid refinement in the radial and vertical direction can be afforded in axisymmetric models reducing discretization issues associated with 3D numerical models.

Idealized conditions of axisymmetric models, however, are rarely encountered in the field scale applications

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of groundwater models. Therefore, most of the groundwater flow and transport simulators are based on the cartesian coordinate system to enable the development of 3D models. Some groundwater models offer an option to simulate groundwater flow conditions in an "axisymmetric mode." Examples of such numerical modeling codes include the proprietary codes MODFLOW-SURFACT (HydroGeoLogic 1998; Panday and Huyakorn 2008) and FEFLOW (Diersch 2002).

One of the most widely used groundwater flow codes is MODFLOW and its derivatives commonly called the MODFLOW family of codes. Most MODFLOW and related codes that are available in the public domain cannot model axisymmetric problems. Researchers have proposed various ways to circumvent the lack of axisymmetric modeling option in MODFLOW. Reilly and Harbaugh (1993) created a program called RADMOD, a preprocessor to create MODFLOW input files. RADMOD creates MODFLOW input files by manipulating cell-to-cell conductance values. That approach, however, makes the application of RADMOD limited to confined aquifers due to a-priori conductance calculations. The generalized finite-difference package used by RADMOD was supported in the early versions of MODFLOW but was not supported by MODFLOW-2000 and later versions. Samani et al. (2004) developed relationships between cylindrical coordinate system and cartesian coordinate system and a scaling methodology to convert between the two systems. The conversion was referred to as the log scaling method (LSM) and LSM was incorporated into MODFLOW-2000 source code to be able to simulate axisymmetric models. Langevin (2008) proposed a methodology to adapt MODFLOW to axisymmetric modeling without the need to modify the source code of MODFLOW. Langevin (2008) presented a strategy to modify input parameters, in particular, horizontal and vertical hydraulic conductivity, specific storage, and porosity. The parameter manipulation methodology acts as a surrogate to represent increased flow area in model cells with increased radial distance. Logarithmic weighting of interblock transmissivity (option available in MODFLOW) was used and Langevin (2008) showed the importance of logarithmic weighting against harmonic weighting for simulating axisymmetric models. Both confined and unconfined flow could be simulated with this approach. With the approach proposed by Langevin (2008) lateral heterogeneity could not be represented in the model, only layered heterogeneity could be represented; this is not, however, a serious limitation because lateral heterogeneity in an axisymmetric model would represent circular bands of heterogeneity that is typically not evaluated. Louwyck et al. (2014) presented an approach very similar to Langevin (2008), and additionally, had the capability to incorporate radial heterogeneity in the axisymmetric model. This was achieved by manipulating aquifer parameters values and setting width and length for all model cells equal to unity and using harmonic mean.

The current study presents another methodology to simulate axisymmetric models by taking advantage of

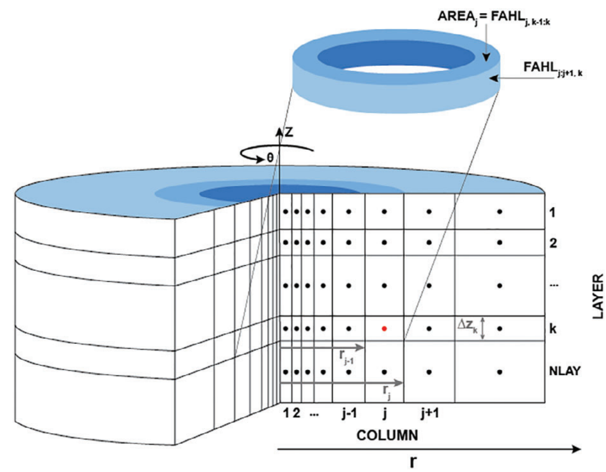

Figure 1. Schematic showing conceptual grid design for an axisymmetric model using MODFLOW-USG. Refer to Equations 1 to 3 for an explanation of the terms AREA, FAHL, r_{j-1}, r_j, and Δz_k.

unstructured grids of MODFLOW-USG (Panday 2017; Panday et al. 2017). Unstructured grids offer the flexibility of designing model grid cells of any shape. Taking advantage of the grid flexibility, MODFLOW-USG models can be fed appropriate intercell area values for a cross sectional model to simulate axisymmetric conditions as detailed in the next section. Three examples are then presented to verify and demonstrate the applicability of MODFLOW-USG for simulating axisymmetric conditions, including: (1) a pumping well, (2) vadose zone flow, and (3) saltwater intrusion on a circular island. The latest version in the MODFLOW family of codes, MODFLOW 6 (Langevin et al. 2017), offers unstructured grid functionality akin to MODFLOW-USG. Therefore, the methods described below can also be applied to MODFLOW 6 for developing axisymmetric models.

Methods

MODFLOW-USG is a finite volume unstructured grid code that does not impose any restrictions on the shape of individual model cells. The shape of individual model cells is not explicitly defined in the input files but is mathematically represented with user-defined intercell connectivities, distances and interface areas. Thus, an axisymmetric model can be conceptualized using coaxial cylindrical model cells. A schematic of such a model grid is shown in Figure 1. The associated grid cells can be represented as cylinders (at the axis of rotation) and donuts (or rings) within the unstructured discretization framework of MODFLOW-USG, implemented in the unstructured discretization (DISU) input file, also known as the DISU package of MODFLOW-USG. As noted in Figure 1, this grid is generated as a cross-section containing several columns or layers of cells which are rotated about the vertical z-axis.

Radial discretization was assumed the same in all model layers, that is, model cells were assumed to be stacked across all layers. MODFLOW-USG imposes no restrictions on the stacking of model cells, however, model cells were stacked in the examples presented below for simplicity. The total number of model cells (NODES) in the axisymmetric models was calculated as the number of model cells in the radial direction in each layer (NCOL) multiplied by the number of model layers (NLAY). The radial distance between model cells (Δr) may vary or held constant depending on the modeling requirements, though typically a finer discretization is applied nearer to the vertical z-axis for better resolution about the point of interest. Similarly, the vertical distance between model cells (Δz) can potentially vary, but a uniform thickness was used for all layers in the examples presented below.

Coaxial cylindrical cells were defined by means of two area input arrays in the model, the AREA and the FAHL[6] arrays as required by the DISU package[7] of MODFLOW-USG. The AREA array contains the horizontal area of model cells and the FAHL array contains the area of the interface between two connected cells. Note that the AREA array entry for a cell is the same as its vertical connection area entry within the FAHL array. The AREA input was calculated as the horizontal area of a model cell. The horizontal area for the model cell representing column j, can be calculated as shown in Equation 1.

$$\mathrm{AREA_j} = \pi\left(\mathrm{r_j^2} - \mathrm{r_{j-1}^2}\right) \tag{1}$$

where $\mathrm{r_j}$ and $\mathrm{r_{j-1}}$ are the distances of the outer cell boundaries of columns j and j−1, respectively, as shown in Figure 1. Equation 1 essentially calculates the area of concentric rings by subtracting the area of the concentric circle formed by the inner edge of a model cell in column j, from the area of the concentric circle formed by the outer edge of a model cell in column j.

Two area calculations were needed to represent cell interface areas in the FAHL array of the DISU package: (1) cell interface area calculated in the radial direction as shown in Equation 2; and (2) cell interface area in the vertical direction as shown in Equation 3. Note that the calculation in Equation 3 is the same as Equation 1 as both the calculations essentially represent horizontal area of a model cell.

$$\mathrm{FAHL_{j:j+1,k}} = 2\,\pi\;\mathrm{r_j}\Delta z_{\mathrm{k}} \tag{2}$$

$$\mathrm{FAHL_{j,k-1:k}} = \pi\left(\mathrm{r_j^2} - \mathrm{r_{j-1}^2}\right) \tag{3}$$

where, $\Delta \mathrm{z_k}$ is the model cell dimension in the vertical direction. The calculations detailed above for the AREA and FAHL arrays of MODFLOW-USG's DISU package are the only calculations needed to create axisymmetric models with MODFLOW-USG. A preprocessing program was developed to write the DISU file of MODFLOW-USG by reading user-defined NLAY, NCOL, and horizontal and vertical cell spacing. Detailed input instructions for the DISU file and other input files are available in the documentation of MODFLOW-USG.

With this methodology of creating axisymmetric models, the simulator MODFLOW-USG can be used as-is, that is, no code modifications are needed to the program. A priori calculations of model parameters are also not needed. In fact, once the model domain is appropriately discretized using the methodology discussed above, heterogeneity may be introduced and changed as needed without the need to recalculate any surrogate parameters needed by other methodologies proposed in the past.

The methodology presented here can be extended to make more complex radial sections (pie shaped grids) in a model, as the model requirements may be, by manipulating the area calculations and defining intercell connections appropriately. This study, however, only discusses the application of MODFLOW-USG to create axisymmetric models.

Example Problems

Pumping Well

A pumping well was simulated in an unconfined aquifer system with delayed yield response as the first example. An analytical solution provided by Neuman (1974) forms the basis of this simulation. MODFLOW-USG was used to create an axisymmetric model to simulate the drawdown caused by a pumping well. Results of the MODFLOW-USG axisymmetric model were compared to the analytical solution provided by Neuman (1974). The analytical solution was solved using the software AQTESOLV. A fully 3D model was also developed using MODFLOW-USG and drawdown results from the 3D model were compared to the axisymmetric model to assess the impact of representing a 3D numerical discretization with a radially symmetric discretization.

The example simulated a partially penetrating pumping well with a pumping rate of 113.27 m^3/day (4000 ft^3/day) in an unconfined aquifer. The aquifer was assumed homogeneous and isotropic. The initial saturated thickness was set to 15.24 m (50 ft) with a hydraulic conductivity of 6.096 m/day (20 ft./day), specific yield of 0.1, and specific storage of $3.281 \times 10^{-5}\ \mathrm{m^{-1}}$ ($10^{-5}\ \mathrm{ft^{-1}}$). The pumping well was assumed to be screened within the bottom 3.048 m (10 ft) of the 15.24 m (50 ft) thick unconfined aquifer.

The axisymmetric numerical model was discretized vertically into 25 layers (NLAY = 25) with each layer 0.6096 m (2 ft) thick. Horizontal discretization varied from 0.0762 m to 152.4 m (0.25 to 500 ft), with the smallest grid spacing assigned near the pumping well and increased grid spacing assigned away from the well. The axisymmetric model was discretized into 22 model cells in the radial direction (NCOL = 22) in each model layer with the total radial distance from the pumping well equal to 609.6 m (2000 ft). A prescribed flux boundary representing the pumping well was imposed on the vertical set of model cell representing the center of the radially symmetric model. Well boundary was imposed on model layers 21 through 25 representing the bottom 3.048 m (10 ft) of the aquifer. No-flow boundary was assumed on the lateral, top, and bottom boundaries.

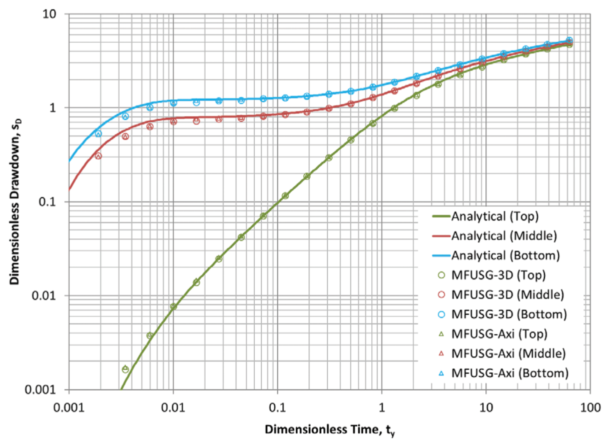

Figure 2. Drawdown for a pumping test comparing MODFLOW-USG axisymmetric model (MFUSG-Axi) results shown as triangles with analytical solution shown as lines and MODFLOW-USG three-dimensional model (MFUSG-3D) results shown as circles.

For the fully 3D numerical model, vertical and horizontal grid spacing was set the same as the axisymmetric model. The 3D model was discretized into 25 layers, 43 rows, and 43 columns, with the total model domain extent of 1219.2 m (4000 ft) in both the x- and y-directions and 15.24 m (50 ft) in the vertical z-direction. Well boundary was implemented at the center of the model domain, that is, row number 22 and column number 22. Akin to the axisymmetric model, well boundary was imposed from model layers 21 to 25.

Transient drawdown was recorded at the top, middle, and bottom of the 15.24 m thick aquifer at a distance of 12.192 m (40 ft) from the pumping well. Dimensionless drawdown, s_D and dimensionless time, t_y were calculated as shown in Equations 4 and 5 (Neuman 1974):

$$s_D = \frac{4\pi Ts}{Q} \tag{4}$$

$$t_y = \frac{Tt}{S_y r^2} \tag{5}$$

where T is the transmissivity of the aquifer [L^2/T]; s is the drawdown [L]; Q is the pumping rate [L^3/T]; t is the elapsed time [T]; S_y is the specific yield [−]; and r is the radial distance [L].

Results obtained from the MODFLOW-USG axisymmetric model were compared to the analytical solution and the MODFLOW-USG 3D model as shown in Figure 2. As seen in Figure 2, drawdown results show good agreement between the axisymmetric numerical model, and the analytical and 3D models. Excellent agreement between the model results in all cases signifies that axisymmetric models can be appropriately simulated using MODFLOW-USG with the approach presented here.

Vadose Zone Flow

The second example simulates the saturation profile underneath an infiltration basin as a result of water seeping through a thick vadose zone. The vadose zone considered in this example is a sandy aquifer with a lower conductivity confining unit in the middle. A circular infiltration basin is considered that infiltrates water at a rate that is higher than the vertical conductivity of the confining unit. This condition creates a subsurface mound on top of the confining unit underneath the infiltration basin. The mound of water spreads horizontally over the confining unit until the point that the infiltration rate at the extreme edge of the mound is as small as the conductivity of the confining unit. The formation of a subsurface mound and the study of the extent of its spread presents an ideal scenario for an axisymmetric model. The system was simulated with two models, both using MODFLOW-USG, as documented in Panday (2017), an extension of the initial release of MODFLOW-USG that enables vadose zone simulations. The first model was an axisymmetric model, and the second model was a 3D model explicitly representing a circular shaped infiltration basin.

The total vadose zone thickness was assumed 27 m and the confining unit was assumed 0.5 m thick at a depth of 13 m. For both models, the aquifer was vertically discretized into 54 layers with a uniform thickness of 0.5 m. Fifty-one radial coaxial model cells were simulated in each model layer with horizontal spacing varying from 0.5 to 200 m in the radial direction. Grid discretization from the axisymmetric model was mirrored to create the 3D model with 102 rows and 102 columns with the infiltration basin at the center of the model domain. The radius of the circular infiltration basin was assumed to be 20 m. The infiltration basin was represented by the first 40 radial model cells representing the center of the axisymmetric model domain and by a circular footprint of 5008 cells for the 3D model. An infiltration rate of 0.31 m/day was used for the infiltration basin and zero recharge was assumed outside of the basin footprint. Table 1 shows all the vadose zone parameters used in the model. The bottom model layer was assigned a prescribed head boundary of zero representing the water table layer. Vertical lateral model cells were assigned no-flow boundary.

The axisymmetric and the 3D models described above were simulated using the version of MODFLOW-USG documented in Panday (2017). Steady-state saturation profiles comparing the two models are shown in Figure 3. It is clear that results from the two models are in close agreement. As seen in Figure 3, the confining layer restricts the flow from the infiltration basin creating a mound over the confining unit underneath the basin. As a result of the mounding, water spreads over a larger area beyond the infiltration boundary. This model structure was used during the design of a real-world infiltration basin to assess the spatial extent of the impact of infiltration basin and to evaluate the infiltration capacity of the basin to limit the mounding below land surface. The 3D example was prepared for a single simulation to demonstrate applicability of an axisymmetric model, while the axisymmetric model was used in the project.

Table 1
Parameters Used for Vadose Zone Models

Parameter	Aquifer	Confining Layer
Horizontal hydraulic conductivity	35.25 m/day	0.008 m/day
Vertical hydraulic conductivity	3.525 m/day	0.008 m/day
Specific storage	1.0×10^{-4} m^{-1}	
Specific yield	0.27	
van Genuchten α	8.3 m^{-1}	
van Genuchten β	1.35	
Brooks Corey parameter, n	8.8	
Residual saturation	0.013	

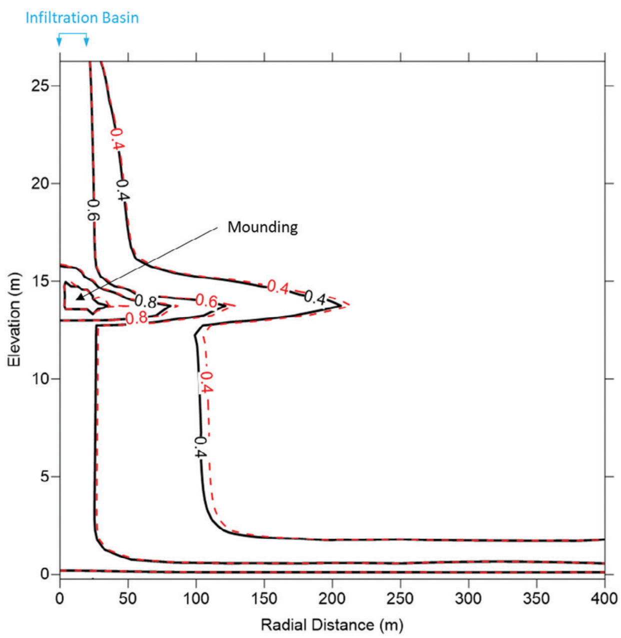

Figure 3. Comparison of steady-state saturation contours for an infiltration basin simulated using an axisymmetric model (black solid lines) and a 3D model (red dashed lines). Both models were simulated using MODFLOW-USG documented in Panday (2017) that enables vadose zone simulations. A 0.5 ft. thick confining unit was simulated within the vadose zone at an elevation of 13.5 m resulting in subsurface mounding underneath the infiltration basin within the vadose zone resulting in perched conditions farther away from the infiltration basin boundary.

Saltwater Intrusion

Saltwater intrusion on a circular island is presented as the third example. An axisymmetric model was developed using MODFLOW-USG to simulate the radially symmetric flow conditions on a circular island surrounded by seawater on all sides with recharge applied on top. Results from the axisymmetric model were compared to an analytical solution provided by Fetter (1972). Axisymmetric model results obtained using MODFLOW-USG were also compared to two SEAWAT models (Langevin et al. 2007): (1) a 3D model spanning the entire circular island; and (2) an axisymmetric version of the SEAWAT model developed by manipulating input parameters as described by Langevin (2008). The 3D SEAWAT model provided run time estimates to assess the efficiency of axisymmetric models and the axisymmetric version of SEAWAT was useful in comparing saltwater intrusion results obtained using the approach described by Langevin (2008), in which surrogate input parameters were used to mimic axisymmetric flow equations, and the approach described in this study.

An island 1 km in diameter was considered for this example with a hydraulic conductivity of 10 m/day. The island aquifer was assumed 35 m thick. A recharge boundary was applied on the island at a recharge rate of 0.635 m/year. Saltwater and freshwater densities were assumed 1025 and 1000 kg/m^3, respectively. Saltwater total dissolved solids (TDS) concentration and freshwater TDS concentration were assumed 35 and 0 g/L, respectively. Given the densities and concentrations used in the model, the rate of change of density with respect to concentration ($\partial\rho/\partial C$) was set to 0.7143. Porosity of 0.1 and longitudinal and vertical dispersivity values of 10^{-4} m were assumed.

The axisymmetric numerical model was developed using the BCT package of MODFLOW-USG documented in Panday (2017) with the approach discussed in the preceding section. The model was discretized vertically into 70 layers with a uniform spacing of 0.5 m, and horizontally into 101 coaxial cylindrical model cells in the radial direction with a uniform spacing of 5 m between adjacent model cells. The horizontal extent of the axisymmetric model represents the 500 m radius of the circular island with the inner-most model cell representing the center of the island and the outer-most model cell representing the saltwater boundary. The saltwater boundary was represented as prescribed hydraulic head and prescribed concentration boundary, with values of 0 m and 35 g/L, respectively. Steady-state saltwater-freshwater interface were compared to the analytical solution presented by Fetter (1972).

A 3D model was created to generate saltwater-freshwater interface for the circular island using SEAWAT. A uniform square grid representing the entire circular island was generated with 202 rows and columns with a uniform spacing of 5 m. A circular prescribed head and concentration boundary was implemented to represent seawater surrounding the circular island and the model cells that fall outside of the circular boundary were deactivated. Steady-state saltwater-freshwater interface generated by the 3D model was compared with the axisymmetric model.

An axisymmetric version of the SEAWAT model was also developed using the same grid structure and dimensions as used by the MODFLOW-USG axisymmetric model. For the SEAWAT axisymmetric model, horizontal and vertical hydraulic conductivity, specific storage, specific yield, and porosity input arrays were manipulated to account for radial flow as detailed by Langevin (2008).

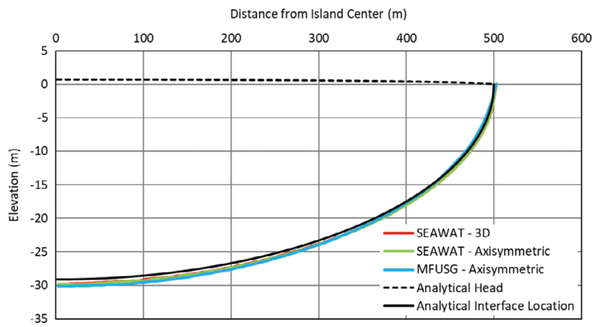

Figure 4. Saltwater-freshwater interface for a circular island with recharge boundary.

In addition to the aquifer parameters, areal recharge was manipulated to simulate axisymmetric conditions within the 3D framework of SEAWAT.

Figure 4 shows the saltwater-freshwater interface obtained by the MODFLOW-USG axisymmetric model and its comparison to the analytical solution and the 3D as well as axisymmetric SEAWAT models. All model results show good agreement. The plotted results for the numerical models show a concentration value of 8.75 g/L (a normalized concentration of 0.25). Note that the analytical solution assumes a sharp interface and therefore, the numerical models were run with the total variation diminishing (TVD) solution scheme. It was noted that SEAWAT uses a third-order TVD scheme which results in lesser dispersion as compared to the second-order TVD scheme used by MODFLOW-USG. A comparison of SEAWAT and MODFLOW-USG results using the upstream-weighted finite difference scheme for the transport equation gave identical results, but with even more numerical dispersion than the TVD schemes. The run times for the fully 3D model was in the order of days while the run time of both the axisymmetric models was in the order of minutes, the difference could be attributed to the difference in the number of model cells.

Summary

This paper presents a natural approach towards unstructured grids of MODFLOW-USG to develop axisymmetric models. The axisymmetric model development in MODFLOW-USG rests on designing the model discretization as coaxial cylindrical model cells. Thus, the framework for creating axisymmetric models is based on providing appropriate area calculations for the cylindrical model grid structure. Changing the source code or manipulating parameter values is not needed for developing axisymmetric models with MODFLOW-USG. Three examples were presented: a pumping well in an unconfined aquifer with delayed yield; infiltration pond impacts within vadose zone containing a confining layer; and, saltwater intrusion on a circular island. The examples presented here demonstrate the use and development of axisymmetric models using MODFLOW-USG for a variety of practical applications.

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