

Numerical groundwater modelling in karst^{7.1}

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Abstract: The success of translating a conceptual site model for a karst site into a numerical groundwater model will depend on both the experience of the user and the capabilities and limitations of the selected computer program. Despite its numerous advantages, even MODFLOW – probably the most widely used, tested and verified modelling program currently available – has conceptual limitations that many karst hydrogeologists have to deal with on a routine basis while searching for an equivalent porous medium approach that may work. This includes assigning very high values of hydraulic conductivity to those model cells known, or suspected, to contain highly transmissive conduits, or assigning an unreasonable, very low effective porosity to the model cells with virtual ‘conduits’ to simulate high groundwater velocities. A new version of MODFLOW called MODFLOW-USG (UnStructured Grid) has been developed and released to the public domain. This new version retains full compatibility with previous versions of MODFLOW while taking advantage of unstructured grids and finite volume numerical solutions. It enables hydrogeologists to accurately translate even the most complex conceptual site models in karst into a numerical environment, thus eliminating the need for various surrogate modelling solutions based on an equivalent porous medium approach.

Karst groundwater systems present ongoing challenges for the application of physically based numerical models. The main explanation for these challenges is straightforward: in aquifers with intergranular porosity, the equations of groundwater flow are mostly based on the relatively simple Darcy’s law. In karst aquifers, however, the nature of the porosity requires the application of different sets of flow equations for three distinct types of porous media: (1) the rock matrix; (2) rock discontinuities, such as faults, fractures and bedding planes; and (3) voids enlarged by solution, such as the channels and conduits developed from the initial discontinuities. Any meaningful quantitative integration of various equations describing these distinct flow regimes is further complicated by the uncertainties associated with the field distribution and identification of different porosity types. Unfortunately, the results of the related numerical modelling efforts have generally lagged behind the advances in the hydrogeology of intergranular (non-fractured, non-karstic) aquifers. As a consequence, the majority of modelling approaches in karst aquifers are still based on various applications of time series analyses, as well as general statistical and probabilistic methods developed in surface water hydrology. Such methods have one common thread: the need for a relatively long time series of data on aquifer recharge and spring discharge and the various input–output relationships. This, however, is also the key limiting

factor for many practical engineering projects with short execution times, including some common tasks such as predicting the effects of new pumping activities or artificial aquifer recharge (Kresic 2009).

Because they are easy to design and understand – and require less mathematical involvement – finite difference numerical models have prevailed in hydrogeological practice. Several excellent finite difference modelling programs have been developed by the US Geological Survey and are in the public domain, which ensures their widest possible use. One of these is MODFLOW, which has become the industry standard as a result of its versatility and open structure. Independent subroutines called modules are grouped into packages that simulate specific hydrological features. New modules and packages can be easily added to the program without modifying the existing packages or the main code.

The main advantage of the classic MODFLOW program and the companion fate and transport models, such as MT3D and RT3D, is their broad user base and continuous updates, including the frequent introduction of new modules and numerical solvers. Most modelling concepts currently used across various computer programs are therefore indirectly or directly based on concepts first implemented in MODFLOW, so an experienced MODFLOW user usually has little trouble when transitioning to another program. Groundwater modelling is now more efficient than ever before because modern

computers and computer operating systems do not place limitations on the model size for most practical applications. Models can have hundreds of layers and millions of cells and still be solved relatively quickly using a desktop PC.

Despite its numerous advantages, however, the classic MODFLOW program has conceptual limitations that many karst hydrogeologists have to deal with on a routine basis. Six limitations that immediately come to mind are: (1) the inadequacy of the equivalent porous medium (EPM) approach to quantifying flow through more discrete features such as karst conduits and channels; (2) the inadequacy of Darcy's equation to simulate turbulent flow; (3) the requirement that all model layers have to be continuous throughout the model domain; (4) the instability of the model when trying to simulate large vertical displacements caused by faults or artificial structures; (5) the condition that all the cells in the model must be rectangular, with rows and columns extending from one edge of the model to the other; and (6) the instability of the model when simulating the contacts between porous media with highly contrasting hydraulic conductivities. These limitations seriously affect attempts to simulate the complex three-dimensional geological relationships and discontinuities characteristic of karst, as well as the water fluxes between model cells.

Because of these limitations, hydrogeologists and groundwater modellers either avoid numerical modelling of karst aquifers altogether or are engaged in searching for an EPM approach that may work. This includes assigning very high values of the hydraulic conductivity to those model cell known, or suspected, to contain highly transmissive conduits, or assigning a very low effective porosity to simulate the high groundwater velocities. These solutions are inadequate and cannot then mimic the dynamics of flow and solute migration in karst environments. None of the EPM models can simulate an important hydraulic interaction between the conduits and the surrounding matrix following some rapid recharge episodes – namely, as the hydraulic head quickly rises in the conduits as a result of a recharge event, there may be a significant transfer of water from the conduits into the surrounding matrix (Kresic 2013). An EPM model will always keep the heads in the high hydraulic conductivity virtual conduit cells lower than in the surrounding model cells.

A new version of MODFLOW, called MODFLOW-USG (UnStructured Grid), that addresses these limitations has now been developed and released to the public domain, retaining full compatibility with previous versions of MODFLOW while taking advantage of unstructured grids and finite volume numerical solutions (Panday *et al.* 2013). It enables hydrogeologists to accurately translate even the most complex conceptual site models in

karst into a numerical environment, thus eliminating the need for various surrogate modelling solutions based on an EPM approach. MODFLOW-USG is now part of several commercial graphical user interface (GUI) programs, including Groundwater Vistas.

There are other codes available that can solve for conduit flow coupled with porous medium flow. A popular code is MODFLOW-CFP (Shoemaker *et al.* 2008), which simulates the conduit flow process within the MODFLOW framework. The connected linear network (CLN) package of MODFLOW-USG is fashioned after the CFP package, with further generalizations that include different flow formulations such as the Darcy–Weisbach equation with the Colebrook and White formula for the friction factor (as in MODFLOW-CFP), Manning's equation, the Hazen–Williams equation and a laminar flow formulation (the Hagen–Poiseuille equation). MODFLOW-USG may further benefit from the flexibility in grid design, the adaptability of conduit connectivity with multiple nodes or layers, a greater robustness and efficiency in solution due to a fully coupled solution between groundwater and conduit domains, and a robust methodology of handling the wetting and drying of groundwater cells or conduits.

The MODFLOW-NLFP (Mayaud *et al.* 2015) code does not include conduit flow, but simulates the Darcy–Forchheimer equation in MODFLOW. The Darcy–Forchheimer equation has advantages compared with the equations solved in the CLN package in that it automatically accommodates the transition from laminar to turbulent flow, whereas the CLN package requires the selection of one of the options.

Other proprietary codes are available that solve for flow through both the matrix and fractures, including FEFLOW (DHI 2016) and FRAC3DVS, a precursor to the HydroGeoSphere code (Therrien & Sudicky 1996). These simulators are frequently developed and enhanced, but, because they are privately owned, their current capabilities in simulating conduit flow through karst conduit networks are unclear.

Features of MODFLOW-USG

MODFLOW-USG was developed to support a wide variety of structured and unstructured grid types, including nested grids and grids based on prismatic triangles, rectangles, hexagons and other cell shapes. Unstructured grids provide a high level of flexibility of discretization by implementing differently shaped grid block geometries and by using nested grid structures. The grid may be created as a combination of nested grids and polygons of different geometries. Pinching of layers, sub-layering and vertical displacements along faults may be directly accommodated without excessive discretization. Flexibility in grid

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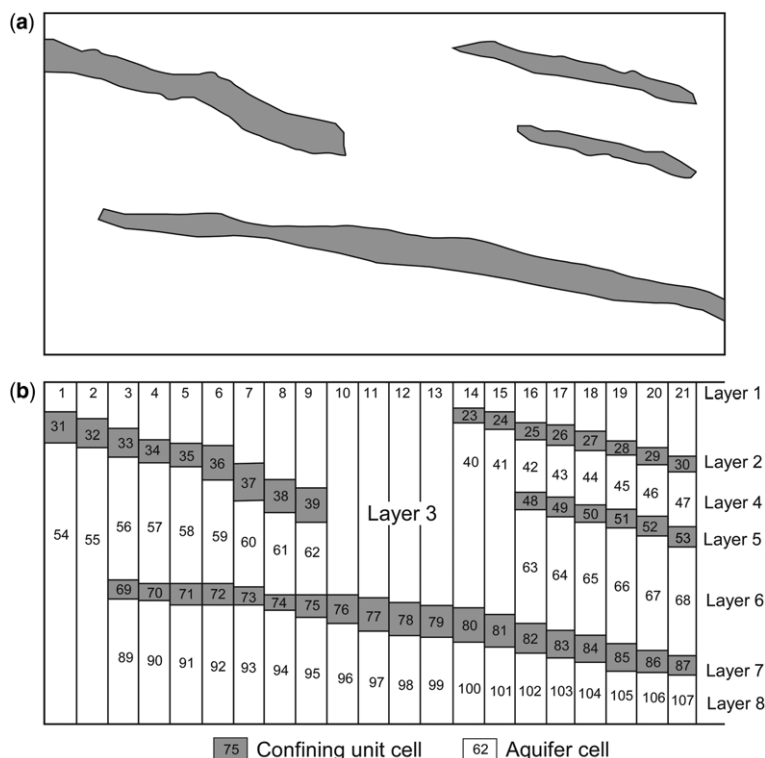


Fig. 1. Cross-sectional diagrams showing (a) pinching hydrostratigraphic layers and (b) an unstructured grid that could be used to represent the hydrostratigraphic layers (Panday *et al.* 2013).

design can be used to focus the resolution along karst conduits, channels, rivers and around wells, for example, or to sub-discretize individual layers to better represent hydrostratigraphic units (Figs 1 & 2).

As described in detail in the published MODFLOW-USG documentation (Panday *et al.* 2013), the program is based on an underlying control volume finite difference formulation in which a cell can be connected to an arbitrary number of adjacent cells. To improve the accuracy of the control volume finite difference formulation for irregular grid cell geometries or nested grids, a generalized ghost node correction package was developed, which uses interpolated heads in the flow calculation between adjacent connected cells.

The program includes a groundwater flow (GWF) process based on the GWF process in MODFLOW-2005, as well as a new CLN process to simulate the effects of karst conduits, multi-node wells and tile drains. The CLN process is tightly coupled with the GWF process in that the equations from both processes are formulated into one matrix equation and solved simultaneously. This robustness results from using an unstructured grid with unstructured matrix storage and solution schemes.

MODFLOW-USG also contains an optional Newton–Raphson formulation, based on the formulation in MODFLOW-NWT, for improving solution convergence and avoiding problems with the drying and rewetting of cells. Because the existing MODFLOW solvers were developed for structured and symmetrical matrices, they were replaced with a new sparse matrix solver package developed specifically for MODFLOW-USG. The sparse matrix solver package provides several methods for resolving non-linearities and multiple symmetrical and asymmetrical linear solution schemes to solve the matrix arising from the flow equations and the Newton–Raphson formulation, respectively (Panday *et al.* 2013).

Connected linear networks in karst

The CLN process was developed for MODFLOW-USG to provide the framework for incorporating one-dimensional connected features into a structured or unstructured three-dimensional GWF process grid. A one-dimensional CLN feature is any hydrogeological or hydrological water conveyance feature

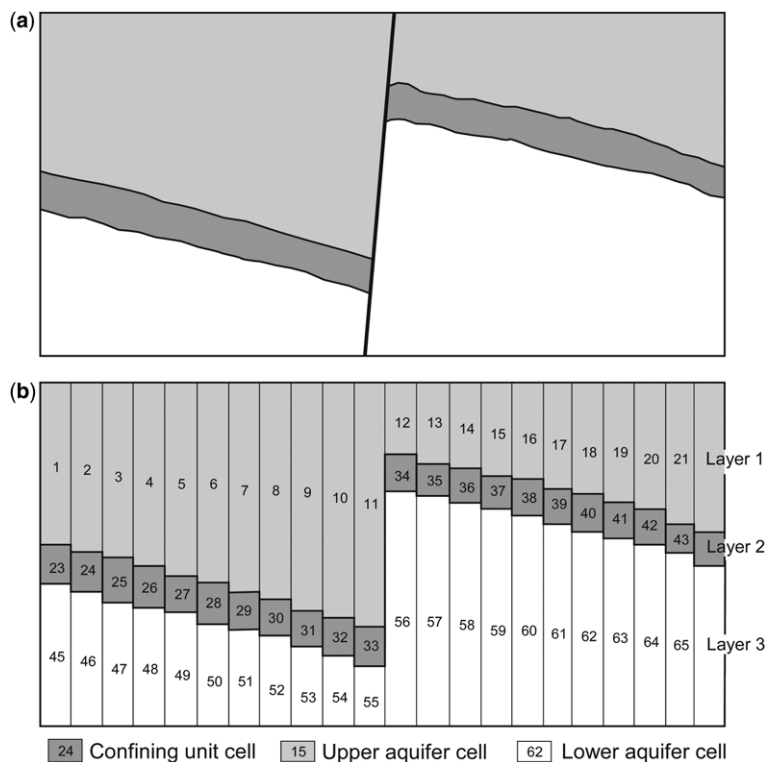


Fig. 2. Cross-sectional diagrams showing (a) the offset of hydrostratigraphic layers from a fault and (b) an unstructured grid that could be used to represent the faulted system (Panday *et al.* 2013).

that has a cross-sectional dimension much smaller than the longitudinal flow dimension and the size of the encompassing GWF cell. Flow is computed in the longitudinal direction of the network of connected one-dimensional features using specified cross-sectional properties; flow between the CLN and GWF cells is computed across the upstream wetted perimeter of the one-dimensional CLN feature. The CLN process thus provides a mechanism for including features with small cross-sectional areas relative to the GWF cell sizes without having to build this level of detail into the grid used for the GWF domain. An example problem is provided to further demonstrate the use of the CLN process.

As described in detail in the published MODFLOW-USG documentation (Panday *et al.* 2013), the CLN flow process is solved simultaneously with the GWF process. This means that the total number of cells in a MODFLOW-USG simulation is equal to the combined total of GWF and CLN cells. The CLN flow process solves for the flow of water within a network of linear features and for the interaction of the features with the porous medium. There are two types of flow calculation that occur with the addition of the CLN domain:

flow within the CLN domain and flow between CLN and GWF cells. The CLN process does not inactivate dry cells as in MODFLOW-2005 for the GWF cells. Instead, a head value is always calculated for active CLN cells as in the upstream weighted formulation. As the saturated thickness approaches zero, the conductance values with connected cells also approach zero and the cell responds as if it were dry.

For flow within the CLN domain, the CLN process implements the solution of one non-linear equation per CLN cell. The CLN cells may represent wells, pipes, fractures, canals, rivers, streams or other linear one-dimensional features within a simulation domain that need to be represented by flow connections that are separate from those of the aquifer. The formulation is general enough that different types of feature can flow into one another. For instance, pipes can flow from or to open channel features. Extension of the code to include other features or geometries is a straightforward exercise in implementing functional forms for cross-sectional areas and volumes as a function of the flow depth at the CLN cells within the appropriate subroutines.

The current version of MODFLOW-USG incorporates cylindrical conduit geometry types. Flow

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within each segment can be laminar or turbulent and the formulations are derived in a general manner. Laminar flow is computed using the Hagen–Poiseuille equation. Three optional formulations are provided to simulate turbulent flow: the Darcy–Weisbach equation, the Hazen–Williams equation and Manning’s equation. The turbulent flow formulations neglect the inertial term in the St Venant equations and therefore solve the diffusion wave equation. The dynamic wave equation for flow in open channels requires a solution to two equations per channel segment (one for continuity and a separate one for momentum) and therefore is not readily accommodated by the present form of the CLN process (Panday *et al.* 2013).

For flow between CLN cells and connected GWF cells, the CLN process implements the solution of one non-linear flow equation for each CLN to GWF connection. Various options are provided to compute the effective leakance between them, including input of the effective leakance value, computation from skin conductance and thickness or the use of a Thiem solution to provide radial influences and efficiency considerations for flow between CLN and GWF cells. The formulation is general enough that extension of the code to include other connection geometries or special considerations is straightforward as long as functional forms for the respective wetted surface areas with flow depths for the CLN to GWF connection can be provided. The CLN to GWF transfer equations are generalized to accommodate unstructured grid cells.

The CLN process uses the concept of a CLN segment, which is one or more CLN cells connected end to end. A CLN segment, of any length, may be used to represent a well, for example, or a karst spring represented by a drain cell. CLN segments can also be connected to one another to form a network (Fig. 3). A CLN network may be manually defined within the GUI by the user and is useful for representing karst conduits, radial collector wells or other connected linear features. Three-dimensional linear networks can also be easily imported from external programs such as geographical information systems (Table 1).

A CLN cell can be vertical, horizontal or tilted. Cell lengths may be dimensioned such that several CLN cells (from the same or different CLN segments) may be connected to one GWF cell, or one CLN cell may be connected to several GWF cells depending on the scale of the conceptualization of flow within the CLN and GWF domains. These connections can also be defined or re-defined after being imported from external geographical information system programs where the karst conduits are first conceptualized. In addition, there is no need for specific upstream to downstream sequential ordering of cells as may be necessary in other packages or codes.

The CLN process, when applied with cylindrical conduits and the Thiem solution for CLN to GWF connection, provides some of the functionalities of the multi-node well (MNW and MNW2) (Halford & Hanson 2002; Konikow *et al.* 2009) packages of MODFLOW-2005. A single cylindrical CLN cell

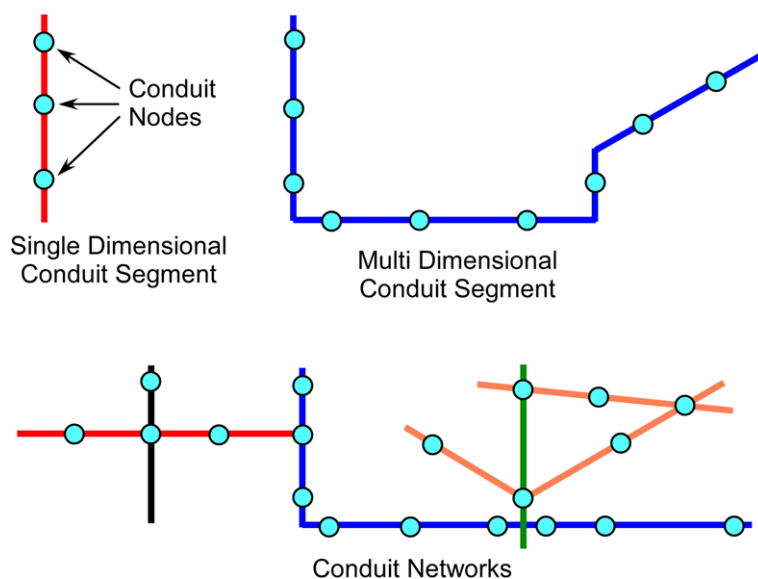


Fig. 3. Examples of conduit domain geometries supported by MODFLOW-USG (Panday *et al.* 2013).

Table 1. Format of a three-dimensional shapefile table of a karst conduit suitable for import to MODFLOW-USG South Conduit in Figures 6 and 7

ID	Xstart	Ystart	Zstart	Xend	Yend	Zend
1	2979.60	353.85	120.00	3025.70	368.15	93.00
2	3025.70	368.15	93.00	3065.45	371.33	90.00
3	3065.45	371.33	90.00	3152.89	369.74	89.00
4	3152.89	369.74	89.00	3284.85	369.75	85.00
5	3284.85	369.75	85.00	3412.03	361.79	80.00
6	3412.03	361.79	80.00	3593.27	363.38	70.00
7	3593.27	363.38	70.00	3729.99	366.56	62.00
8	3729.99	366.56	62.00	3947.80	369.74	57.00
9	3947.80	369.74	57.00	4062.27	368.15	56.00
10	4062.27	368.15	56.00	4345.26	404.72	55.00
11	4345.26	404.72	55.00	4513.78	434.93	54.00
12	4513.78	434.93	54.00	4644.15	477.85	52.00
13	4644.15	477.85	52.00	4760.20	503.29	51.00
14	4760.20	503.29	51.00	4831.74	531.91	45.00

Xstart and Ystart are, respectively, the X and Y coordinates of the beginning of the conduit segment; Xend and Yend are, respectively, the X and Y coordinates of the end of the conduit segment; Zstart and Zend are, respectively, the top and bottom elevations of conduit segment. All units are metres.

connected to multiple GWF cells may be pumped to simulate multi-node well conditions, in which the CLN cell extracts water from the GWF cells connected to it as part of the solution to the coupled CLN and GWF flow equations. A CLN cell can be pumped by use of the well (WEL) package by assigning a source or sink to that CLN cell. If flow through a narrow conduit is important to the production of a multi-layer well (for instance, the well bore resistance governs how much water is produced from each of the multiple aquifers), the well may also be represented by a segment consisting of multiple CLN cells. In this case, a CLN cell can be added to each GWF cell or layer and flow would be simulated within the conduit. This may be especially important when the conduit radius is small and resistance in the well bore affects the flow through the conduit. This approach is also useful for simulating borehole flow within wells that are screened to multiple aquifers.

The continuity equation for flow through a CLN cell is a function of flows from connected CLN cells and flows from connected GWF cells and may be written in difference form as

$$\frac{\Delta V_n}{\Delta t} = \sum_{m \in \eta_n} Q_{nm} + \sum_{p \in \eta_n} \Gamma_{cpn} \quad (1)$$

where ΔV_n is the change in the volume of water in CLN cell n at a given time, Δt is the time step size, Q_{nm} is the volumetric flow between connected CLN cells n and m and Γ_{cpn} is the volumetric flow from connected GWF cells p to CLN cell n .

The left-hand side of equation (1) is the storage term of the CLN cell, the first term on the right-hand side is the flow between cell n and the connected CLN

cells, m , and the second term on the right-hand side is the interaction flow between cell n and all connected GWF cells, p . The summation in the first flow term on the right-hand side is over all m CLN cells connected to CLN cell n , whereas the summation in the second term on the right-hand side (the interaction term) is over all p GWF cells connected to CLN cell n .

Treatment of the term Γ_{cpn} in equation (1) is detailed in Panday *et al.* (2013). A flux coupling is provided between the GWF and CLN domains with three options to couple the domains. The first two options follow the MODFLOW-CFP (Shoemaker *et al.* 2008) formulation and include the user input of leakance or a skin hydraulic conductivity and thickness. The flow then occurs across this skin through the wetted perimeter between the CLN and GWF domains as a result of the hydraulic gradient. A third option uses a modified Thiem equation, which is particularly useful for vertical conduits or wells, to account for a radially logarithmic draw-down between large GWF cells and the comparatively small conduit radius.

Flow within the CLN domain may be computed by three alternative equations. For laminar flow between any two CLN nodes the volumetric flux is expressed by the Hagen–Poiseuille equation, whereas for turbulent flow it may be expressed either by the Darcy–Weisbach equation or the Hazen–Williams equation. Detailed formulations of the flow equations are provided in Panday *et al.* (2013).

Example simulation

Figures 4 and 5 illustrate the MODFLOW-USG model set-up for a hypothetical site with two karst

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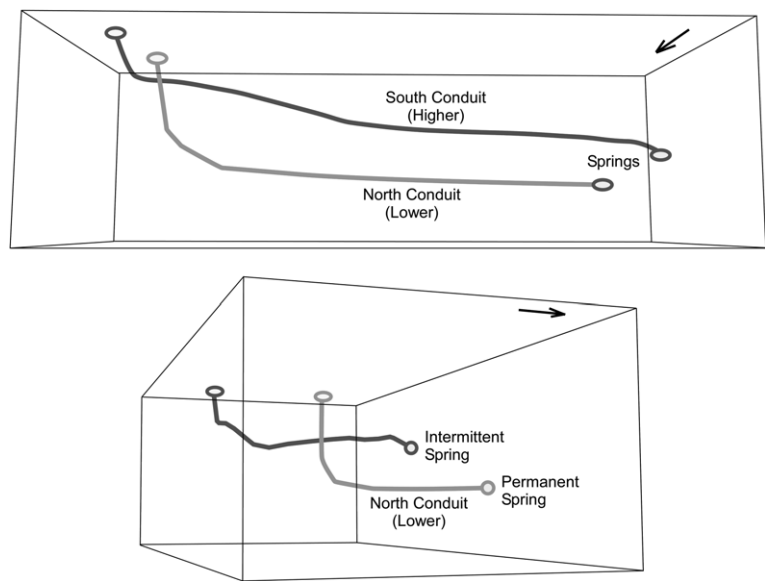


Fig. 4. Two views showing spatial position of the karst conduits at the modelled site.

conduits at different elevations, each connecting a sinking stream and a karst spring. The site is representative of typical karst conditions in the southeastern USA, developed in Mesozoic limestones and dolomites and with a subtropical humid climate. The northern conduit is lower and the flow in it is permanent, as is the flow of the sinking stream and the karst spring connected by the conduit. The

southern conduit has intermittent function, connecting an intermittent sinking stream and an intermittent spring. The model has 12 layers, each 10 m thick, to accommodate the more precise vertical placement of various sections of the two conduits. The model simulates three time periods: the first period is one year long and without recharge from the land surface; the second time period lasts for

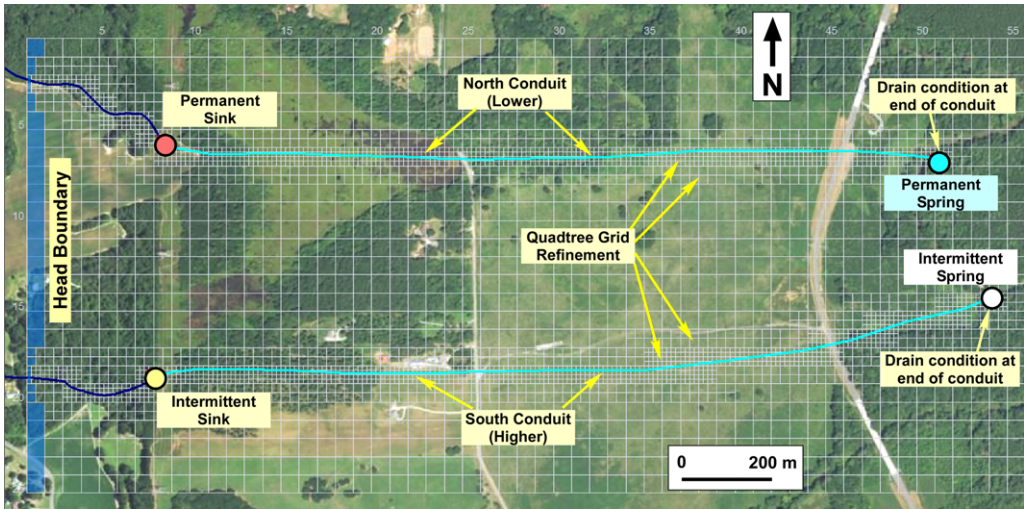


Fig. 5. General model set-up and boundary conditions.

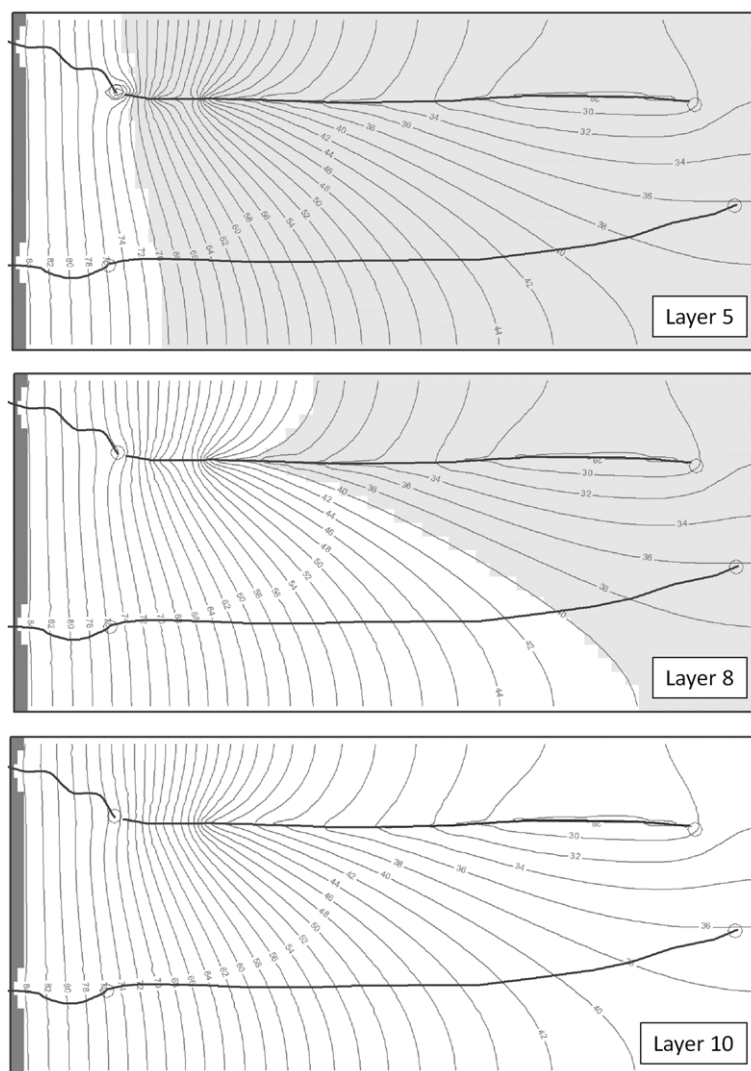


Fig. 6. Simulated potentiometric surface map at the end of time period 1 in layers 5, 8 and 10. The dry cells in a layer are shaded.

two days and simulates an areal recharge event from rainfall (0.15 m day^{-1}); the third period, 30 days long, simulates recession after the recharge event. Figures 6–8 show the modelled potentiometric surface contour lines at the end of the three time periods for select model layers. The simulated hydrographs at the two springs are shown in Figure 9.

Discussion

The CLN process in MODFLOW-USG provides for the physically based simulation of groundwater

flow within preferential flow paths of karst aquifers, such as fully or partially water-filled conduits, which can have both permanent and intermittent flows and a varying three-dimensional geometry of the conduit networks. Conduits can be effortlessly brought into the model from external three-dimensional geographical information system shapefiles via user-friendly input screens, or can be added manually and connected with any of the existing CLNs in all three dimensions as needed. For example, Figure 10 illustrates the effects of adding and connecting one ‘manual’ conduit to the permanent North Conduit imported from a

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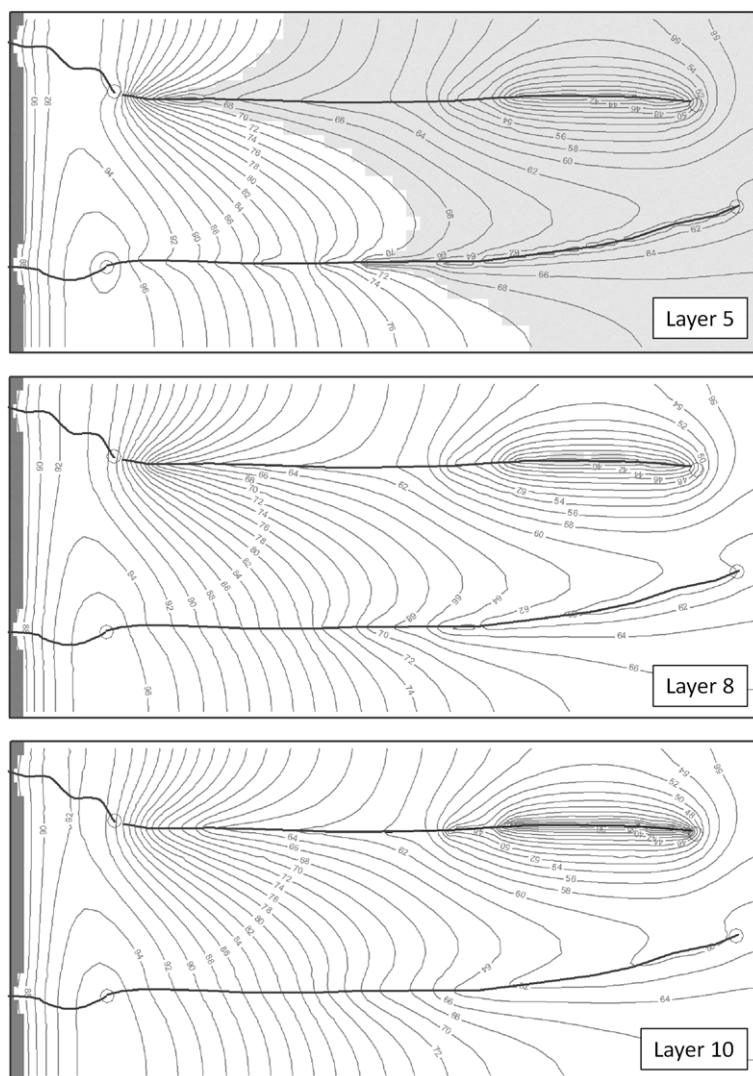


Fig. 7. Simulated potentiometric surface map at the end of time period 2 (end of high recharge episode) in layers 5, 8 and 10. The dry cells in a layer are shaded.

geographical information system file to the example model.

The CLN conduits can extend through both the saturated and unsaturated zones, can have vertical sections and can become fully submerged and/or dewatered depending on the assigned transient boundary conditions. Any section of a conduit can have a different radius from the adjacent sections and the groundwater flow within it can be described with any of the four available equations. In addition, the interaction between any individual conduit section and the surrounding aquifer matrix

can be described with a set of unique parameters. This flexibility allows for a powerful sensitivity analysis of various CLN input parameters and assumptions. Notably, a section of a conduit can act as a linear drain for the surrounding aquifer matrix for a given set of boundary conditions and can also lose water to the matrix for another set of boundary conditions, such as during high recharge episodes, including recharge from distributed precipitation and from the focused sinking of surface water features, such as intermittent/activated sinks (Fig. 11).

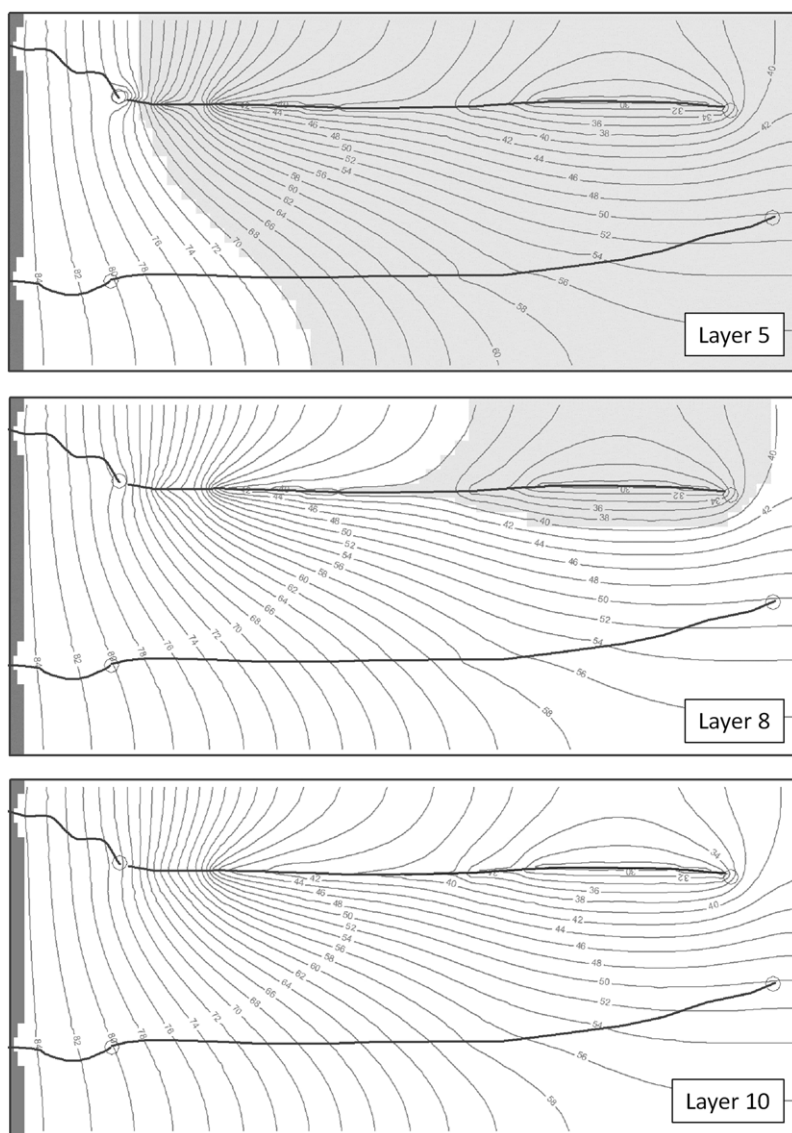


Fig. 8. Simulated potentiometric surface map for time period 3, 15 days after the end of the recharge episode, in layers 5, 8 and 10. The dry cells in a layer are shaded.

MODFLOW-USG includes simulations of the contaminant fate and transport (F&T) in both unsaturated and saturated zones and in both the aquifer matrix (Darcian porous media, i.e. GWF process model cells) and CLNs. Simulation options in the current beta version include linear and Freundlich types of sorption, diffusion, isotropic and anisotropic dispersion, zero- and first-order decay on soil, in water, and on soil and water, and dual domain transport. Contaminants can both enter and leave CLNs following the groundwater flow gradients.

Figure 12 is an example F&T simulation showing the development of a dissolved phase plume from a constant-strength source at the ground surface. The results in layer 10, which is always saturated and contains the longest stretch of the North Conduit, show the contaminant plume entering the conduit and flowing to the spring.

MODFLOW-USG is a powerful new groundwater flow and contaminant F&T numerical modelling program with a number of tools and solutions well suited for the simulation of karst aquifers and their

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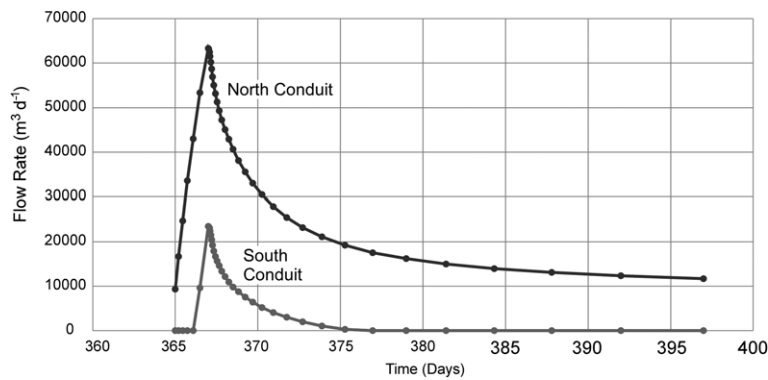


Fig. 9. Simulated flow rate at the two springs (drain cells at the end of conduits).

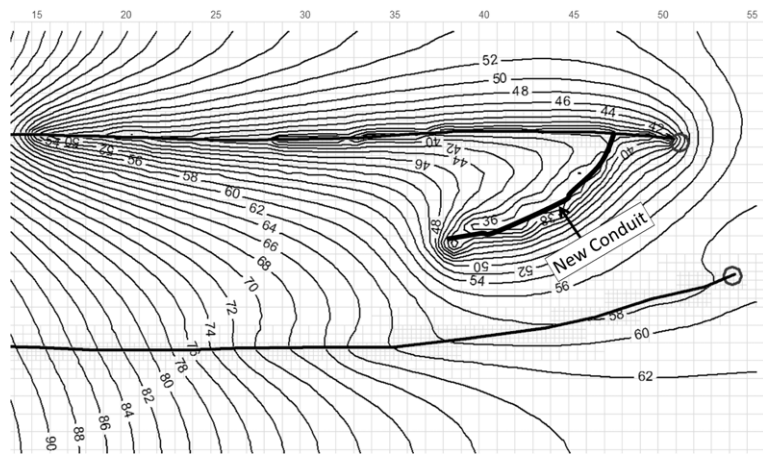


Fig. 10. Effect of an additional conduit in layer 10 on groundwater flow conditions. End of time period 2 (end of recharge episode).

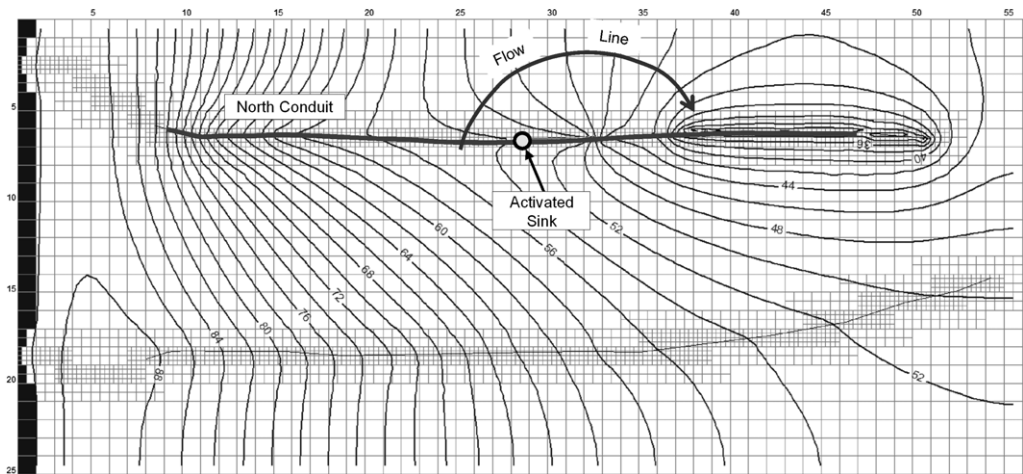


Fig. 11. Effect of a simulated intermittent sink connected to the North Conduit on the groundwater flow conditions. The North Conduit backs up and loses water to the surrounding matrix.

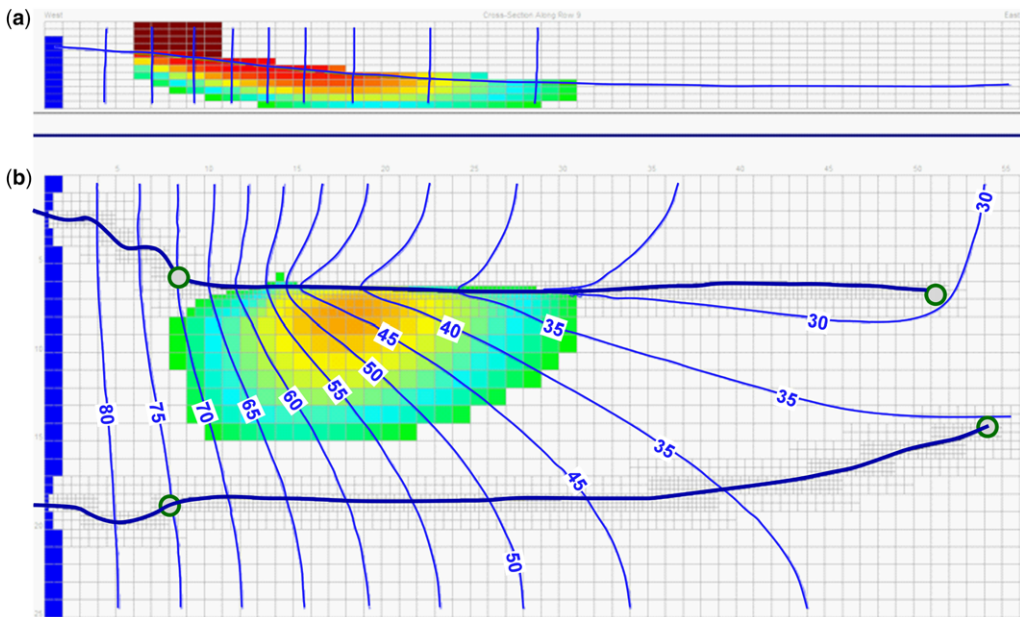


Fig. 12. Example simulation of contaminant fate and transport (F&T) with MODFLOW-USG. (a) Cross-sectional view along row 9. (b) Contaminant distribution in layer 10. The constant-strength source of contamination is at the land surface. The model solves flow and F&T in both unsaturated and saturated zones.

interactions with surface water features. It is in public domain, supported by a number of GUIs, and therefore easily accessible to various users.

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