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PAPER

Modeling of groundwater flow and transport in coastal karst aquifers

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Abstract

Numerical modeling of karst water systems is a challenge due to vastly different flow regimes in the solution channels and the porous medium, and because of the complex interactions between them. Recent developments with unstructured grid models have enabled robust simulation of such systems due to full coupling of the system of equations and the interactions, within a flexible gridding framework that allows these domains to be discretized independently of each other. These capabilities have been incorporated into the MODFLOW-USG code, which has been developed and released in the public domain by the United States Geological Survey. Further developments to MODFLOW-USG have continued and have also been released in the public domain. The significant features that enhance simulations in karst environments include various optional turbulent flow formulations, solute transport capability and a density-dependent flow simulation option that can be used to model transport of nonaqueous phase liquids (NAPLs) or freshwater–seawater interactions, for example. A dual-porosity-flow and dual-porosity- 8.1
transport formulation is also included to further expand model scale and flexibility. A physically based representation of flow and transport within the karst conduits (channels) and porous medium eliminates the need for various surrogate modeling approaches in karst, thus enabling solutions to some of the common problems that groundwater professionals face when dealing with groundwater resources management in coastal karst areas. A demonstrative example shows the impact of karst on the saltwater system in a coastal aquifer.

Keywords Numerical modeling · Karst · MODFLOW-USG · Conduit flow · Variable density flow

Introduction

Karst water systems present ongoing challenges for 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. On the other hand, the nature of porosity in karst aquifers requires the application of different sets of equations for distinct porous media: (1) rock matrix, (2) rock discontinuities such as faults, fractures, and bedding planes, and (3) solutionally enlarged voids such as channels and conduits developed from the initial discontinuities. Since almost all widely used numeric groundwater models, until relatively recently, were based on Darcian equations applicable to intergranular aquifers, most groundwater modelers were, and still are, using them to model karst aquifers as well.

In certain situations, karst aquifers may behave as an equivalent porous medium (EPM) at a given scale (Kresic 2013); however, there are analyses for which the EPM approach may not be adequate. Some practicing quantitative karst hydrogeologists not comfortable with the EPM approach are in a continuous search of nonhydrogeologic models as potentially useful surrogates.

General approaches to modeling groundwater flow in karst can be divided into the following main categories:

1 *Time-series models*. These are based on statistical and probabilistic methods mostly developed in surface-water hydrology. They usually require long time series of data for developing model input and output parameters; at the

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same time, they cannot simulate (predict) the effects of common, practical engineering interventions such as new groundwater withdrawals (pumping) or artificial aquifer recharge. Typical examples of stochastic time-series models of input–output processes in karst aquifers include works of Graupe et al. (1976), Salas et al. (1982), Padilla et al. (1996), Kresic (1995, 1997), Margeta and Fistanić (2004), and Labat et al. (2000).

Time-series models in the spectral domain or mixed time-spectral domains are popular in karst hydrologic and hydrogeologic studies. One advantage of using such models is their ability to incorporate multiple cyclic (periodic) input components at different frequencies such as well pumpage and operation of locks and dams on surface streams. Parameter identification performed for spectral-domain models may also reveal superimposed and therefore masked input and/or output components that may or may not be fully known. Papers published on the topic include Mangin (1981), Padilla and Pulido-Bosch (1995) Larocque et al. (1998), Labat et al. (2000), and Rahnemaei et al. (2005)

2 *Numerical models based on the equivalent porous medium (EPM) approach*. Because of their inability to simulate real physical processes in karst such as flow in karst conduits (i.e., network of hydraulically connected solutional features) and exchange of water between the conduits and the surrounding rock matrix, such models rely on various surrogate solutions for many cases of interest. This includes assigning very high values of hydraulic conductivity to those model cells known to contain or suspected to contain highly transmissive conduits or assigning a very low effective porosity to simulate the high conduit velocities. Typical early examples of EPM modeling of karst aquifers are presented by Cooley et al. (1986) and Kiraly (1988). Examples of using classic MODFLOW and the EPM approach include works by Knochenmus and Robinson (1996), Worthington (2003), Lindgren et al. (2004), and Putnam and Long (2009). These solutions may however be inadequate for many situations as they cannot then mimic the dynamics of flow and solute migration in karst environments (Kresic 2013; Kresic and Panday 2017)

3 *Hydraulic models of pipe and/or reservoir networks*. These models either do not simulate the exchange of water between the "pipes" and the bulk of the aquifer porous media, or attempt to do it via a lumped parameter approach that is not based on physical laws of such exchange; therefore, these hydraulic models also cannot predict the future effects of common groundwater management and engineering interventions in karst; typical early example of this concept is presented by Smart (1988). Campbell and Sullivan (2002) describe use of the Stormwater Water Management Model (SWMM), based on rainfall-runoff relationship, as a surrogate for modeling different "segments" of a karst aquifer such as pipes connecting multiple "subcatchments" in the subsurface. SWMM has been developed by the United States Environmental Protection Agency (EPA 2020).

4 *Coupled continuum conduit flow (CCCF) models*. Numerical groundwater flow models that explicitly account for pipe hydraulics by coupling the Darcian porous continuum model with a conduit (pipe) network representing flow in karst conduits and channels are sometimes referred to as coupled continuum conduit flow (CCCF) models. An illustrative overview of the concept's historic development including its mathematical basis is provided by Hu (2009).

One model that simulates groundwater flow and solute transport in the network of karst conduits and the surrounding matrix, in a physically based, spatially distributed manner with advanced capabilities is MODFLOW USG (Panday et al. 2013) Another public domain code that can solve for conduit flow coupled with porous medium flow is MODFLOW-CFP (Shoemaker et al. 2008). However, MODFLOW-CFP has no flexibility of unstructured grids and cannot directly link various MODFLOW packages with the conduits (for example, wells or drains cannot be placed into conduits). MODFLOW-CFP sometimes encountered issues with model instability and long runtimes. Ashok and Sophocleous (2008) tested the CFP with various model setups and found a number of inconsistencies. In one of the analyses, the model was tested by increasing and decreasing the diameter of voids by one order of magnitude, but the results were still the same. The Reynolds' numbers did not seem to have any impact on simulation no matter what the ranges of values between upper and lower Reynolds' numbers were (Ashok and Sophocleous 2008).

Various research-oriented computer programs are also available for simulating dual porosity aquifers but have not been fully documented for wider use (e.g., Clemens et al. 1996; Kiraly 1998; Bauer 2002; Birk 2002). As discussed by Kresic and Panday (2017), there are also several proprietary modeling codes available that solve for coupled flow through fractures and the rock matrix which include FEFLOW (MIKE powered by DHI 2020) and FRAC3DVS, a precursor to the HydroGeoSphere code (Therrien et al. 2010.). The HydroGeoSphere code was recently used to evaluate the impact of one or more fractures aligned in different directions, on the seawater intrusion behavior of the Henry problem (Sebben et al. 2015).

The MODFLOW-USG capabilities for simulating flow in karst aquifers is briefly discussed here. Furthermore, these capabilities have been extended to include additional turbulent flow formulations through conduit networks. Also, solute transport and density-dependent flow capabilities have been added. The additional capabilities are available as an open source, public domain code documented as USG-Transport (Panday 2020). Similar developments are also under way for MODFLOW 6 (Langevin et al. 2017). The extensions that are applicable to karst systems are discussed here and an example problem is presented demonstrating the complex interactions that occur even with the simplest of conceptualizations in coastal karst aquifers.

Formulation for simulating flow and transport in karst aquifers

MODFLOW-USG is based on an underlying control volume finite difference (CVFD) formulation in which a cell can be connected to an arbitrary number of adjacent cells. The program includes a Groundwater Flow (GWF) Process, based on the GWF Process in MODFLOW-2005 (Harbaugh 2005), and MODFLOW-NWT (Niswonger et al. 2011), as well as a connected linear network (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. Fully implicit coupling in this manner is more robust than iterative coupling between the groundwater and conduit domains and results from using an unstructured grid with unstructured matrix storage and solution schemes. Also, use of the Newton-Raphson linearization provides for a robust solution strategy for unconfined flow in the aquifer or for dry and partially filled conduits. Fully implicit coupling of the equations and Newton-Raphson linearization of the flow equations through the karst feature is, to our knowledge, a unique feature of MODFLOW-USG among publicly available codes.

The conduits are represented by the CLN process and the concept of a CLN segment, which is one or more CLN cells connected end to end forming linear sections and networks. Any section of a conduit can have a different radius from adjacent sections enabling simulation of flow constrictions. CLN cells can be vertical, horizontal, or angled. The CLN domain is connected to the groundwater domain via leakance through the wetted circumference of the CLN tube, or via analytical solutions (Thiem solution with modifications for skin resistance and well efficiency) that account for the theoretical water surface elevation shape, as it transitions from the size of the groundwater cell to the radius of the CLN tube. Such analytical solutions help with solution accuracy even with large groundwater grid-block cells. Superposition of the karst cell with the groundwater cell was not used since that approach loses the ability to keep the flows separate between the domains and furthermore requires very fine discretization adjacent to the karst features. Also, this approach of independent domains allows for the CLN domain discretization to be independent of the groundwater domain discretization allowing multiple CLN cells to be present in one groundwater cell or one CLN cell to span multiple groundwater cells. Thus, each domain can be discretized as per the scale of flow within it and is not reliant on discretization of the other domain. This also is a unique feature of the CLN process. A detailed explanation of MODFLOW-USG is provided in the published public-domain documentation by the United States Geological Survey (Panday et al. 2013.)

Additional developments to MODFLOW-USG are of further interest for numerical simulations in karst environments. The CLN flow formulations were expanded to include turbulent flow equations. Laminar flow computed using the Hagen-Poiseuille equation, is supplemented by three optional formulations for turbulent flow—the Hazen-Williams equation, the Manning equation, and the Darcy-Weisbach equation. The Hazen-Williams equation is popular for computation of flow in pipes. The Manning equation is often used for flow in open channels. Both these equations include empirical coefficients that are prescribed for various channel or conduit surface materials. The Darcy-Weisbach equation is a general turbulent flow equation that results from head loss due to pipe friction and viscous dissipation which are represented by a friction factor. The friction factor is represented by the Colebrook-White formula that includes the pipe surface roughness and the flow Reynolds number in an implicit manner. These conduit flow equations are linearized using a Newton-Raphson approach and are solved fully simultaneously with the groundwater flow equations for a robust solution to the flow system. These various turbulent flow options provided in a fully coupled software solved using advanced nonlinear schemes are, to our knowledge, a unique feature of the CLN process.

Solute transport capability was also developed for unstructured grids. Transport mechanisms include advection, hydrodynamic dispersion, first-order and zeroth-order decay, and retardation. The transport solution is fully compatible with the groundwater domain for any shape and size of grid cells, the CLN domain, and interaction between domains due to advection and dispersion. A mass-conserved solution scheme was used to accurately account for solute species mass as it migrates through the subsurface; a reduced transport equation was not implemented as it could cause solutes to numerically appear or disappear which is usually critical to modeling objectives. Spatial discretization used a total variation diminishing (TVD) process to provide solutions that are free from oscillations with minimal numerical dispersion; upstream weighting schemes have excessive numerical dispersion and higher order schemes suffer from numerical oscillations depending on the Courant number of the problem. Implicit time discretization was used to provide unconditionally stable results; explicit schemes suffer from a Peclet number constraint often causing restrictive time-step sizes for lengthy simulations as required by analyses of environmental settings. Solution of fully coupled transport through conduit and groundwater domains on an unstructured grid is, to our knowledge, a unique feature of MODFLOW-USG among publicly available codes.

A density-dependent flow simulation capability was further included which couples flow and transport (of only the first species component). This capability is operational in the groundwater domain as well as in the CLN domain thus allowing for evaluation of coastal karst environments. The hydraulic head formulation for density-dependent flow and transport (Langevin et al. 2020) provides modules to correct any standard flow and transport solution for density effects. This allows for easy implementation of the density correction with advanced numerical methods and non-Darcy (turbulent) flow conditions, both of which are implemented into MODFLOW-USG. The density correction is conducted in a time-lagged manner and therefore often longer simulations are required to equilibrate the flow and solute system for initial conditions to typical investigations. Such simulations are quick and need only be performed once to obtain initial conditions which may be reused for various investigations at a site. Robust solution of density dependent flow and transport in confined/unconfined coastal karst systems is, to our knowledge, a unique feature of MODFLOW-USG among public domain codes.

Other enhancements that are pertinent to karst settings include the ability to simulate dual porosity flow and dual porosity transport. On a regional scale, with high-density solution features, a karst environment may be characterized as a dual porosity system, where the solution features facilitate flow of water and transport of solutes, while the matrix function is more dominant for water storage and may have a significant impact on solutes. Thus, when flow is transient, water may also flow between the matrix and the solution feature within a groundwater grid-block besides interacting with the adjacent cells (groundwater or CLN). Furthermore, for dual porosity transport, the fracture-matrix interaction includes advection in addition to the classical diffusion mass transfer process. Details of formulation, numerical implementation, and application of these capabilities are provided by Panday (2020). Having all these capabilities for simulating complex processes in karst aquifers, in one open source, public domain software is a unique feature of MODFLOW-USG.

Examples of MODFLOW-USG applications to some common groundwater flow problems in karst conduit networks and the surrounding aquifer matrix are provided by Kresic and Panday (2017). This includes simulations of fully saturated and intermittently saturated karst conduits feeding springs, flow to and from the conduits into the surrounding porous matrix, and solute fate and transport. The current set of examples evaluates the behavior of groundwater flow and density-dependent solute transport in coastal karst systems.

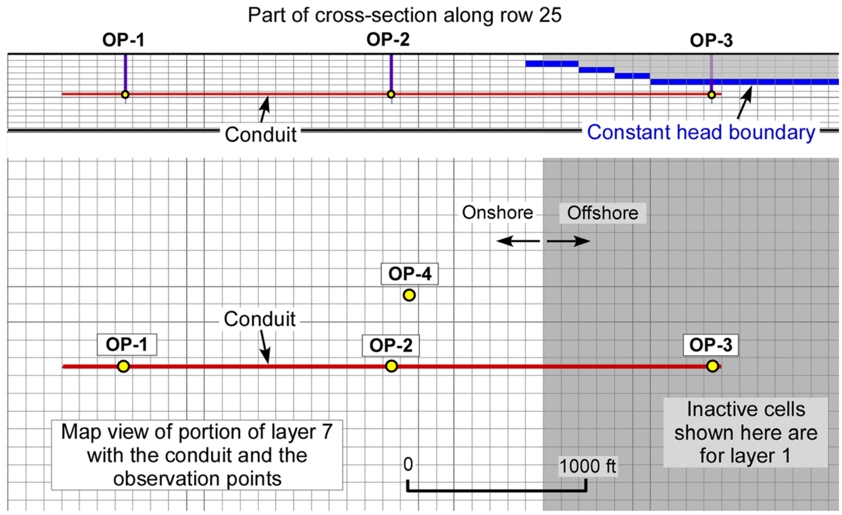
Example of submerged conduit in coastal karst environment

The current example demonstrates the complex interactions between submerged karst conduits and the surrounding rock matrix in coastal areas, with freshwater in the conduits flowing from the upland areas into seawater causing inversion and instability where freshwater discharges beneath saltwater.

A karst aquifer system is simplified in the current example to highlight the impact of conduits and solution channels in coastal settings. Setup of the variable-density groundwater flow model developed in Groundwater Vistas (Graphic User Interface program for the MODFLOW suite of models; ESI 2017–2020) is shown in Fig. 1. The model has 100 columns, 50 rows and 12 layers. The model bottom elevation is −52.5 ft (below sea level). The hydraulic head at the sea boundary is 0.0 and the saltwater concentration is dimensionless 1. The karst conduit of 2-ft radius, placed at elevation of −25 ft. (in layer 7 of the model), extends from onshore to offshore below the sea floor. The conduit was discretized automatically by Groundwater Vistas from a 3D GIS shapefile, with five CLN cells spanning the karst feature, ranging from 600 to 900 ft in length. Flow through the conduit domain was simulated using the laminar flow equation for the simulations. Each groundwater cell that includes the conduit is connected to it by use of a large leakance value such that there is no skin resistance to flow between the GWF and CLN domains. The hydraulic conductivity of the surrounding rock matrix is assumed to be isotropic in all three main directions and fairly high (50 ft/day or 15 m/day, typical of young limestone with high matrix effective porosity such as in Florida (USA) or Yucatan (Mexico), for example). The model was first run in steady-state conditions with and without the conduit, assuming an average long-term annual recharge rate. Figure 2 shows comparison between the two simulations in plan and cross-sectional views along the model row with the conduit. The nonconduit simulation (Fig. 2a, b) shows a classic wedge interface between the fresh groundwater and seawater within the aquifer. The simulation with the conduit (Fig. 2c, d) shows redistribution of the groundwater salinity due to mixing of incoming fresh water in the conduit and the seawater in and around it. The conduit acts as a drain, disturbing the classic wedge shape with mixing of water from above and below it. The front is particularly sharp above and below the conduit because the flow field is downward from above it, and upward from below it, keeping the respective freshwater and saline water domains separate from each other at the conduit location. In plan view at the location of the conduit, the waters are mixed creating a more diffuse interface.

The conduit model was then run to simulate the impact of a recharge episode from rain lasting for 5 days. This recharge episode was preceded and followed by long time periods of average annual recharge rate. A maximum time step size of

Fig. 1 Setup of the conceptual numeric model with locations of the simulated conduit and the observation points



1 day was used with a smaller time-step size of 0.1 days to start each stress period which was ramped up by a factor of 1.5. There were no numerical instabilities with the simulations using these time stepping parameters. The results of this simulations are shown in Figs. 3 and 4 with maps and cross-sections, in Fig. 5 with chemographs and in Fig. 6 with groundwater velocity vectors. Figure 3 shows the concentration distribution of saltwater at the start of the recharge event (Fig. 3a) and at 1 day into the recharge event (Fig. 3b); Fig. 4 shows the distribution of saltwater at the end of the recharge event at 5 days (Fig. 4a) and after equilibration of 100 days with average recharge conditions (Fig. 4b). Figure 5 shows the graphs of relative concentrations vs. time at four observation points located in the conduit and at some distance from it (see Fig. 1 for their locations.) Figure 6 shows the velocity vectors at 1 and 5 days into the recharge event. As can be seen in all the figures, the large inflow of freshwater in the conduit after the simulated rainfall event clearly manifests itself.

The cross-sections in Figs. 3 and 4 illustrate the spatial relationship between the freshwater (blue) discharging from the conduit and the seawater (red). Figure 3b indicates that a day after the rainfall event, freshwater above the conduit has been pushed more seaward and a physical instability is noted where freshwater from the conduit discharges beneath saltwater in the aquifer above.

At 5 days into the rainfall event (cross-section of Fig. 4a), the mixing of fresh and seawater creates a "diluted bubble" underneath the sea; this is followed by the intrusion of the sea water back landward after the recession period. Also, the toe of the saltwater wedge beneath the conduit has moved seaward from the initial steady-state condition by 5 days (cross-section of Fig. 3a). However, this toe has not yet moved back to its original steady-state condition even after 100 days of recession.

The complex dynamic relationship between the seawater and the incoming freshwater during the rain event is best illustrated with the constantly changing directions of velocity vectors in the system. For example, the mixing of freshwater and seawater starts at day one of the rainfall but is limited to a narrow zone around the conduit, and almost exclusively in the upward direction where the high freshwater head in the conduit is able to overcome the dense seawater head (see Figs. 3a and 6a). The strong upward gradient from the conduit results in discharge of this mixed ("brackish") water at the sea floor above, causing activation of a submarine seep/spring. The redistribution of the hydraulic head in the system also causes

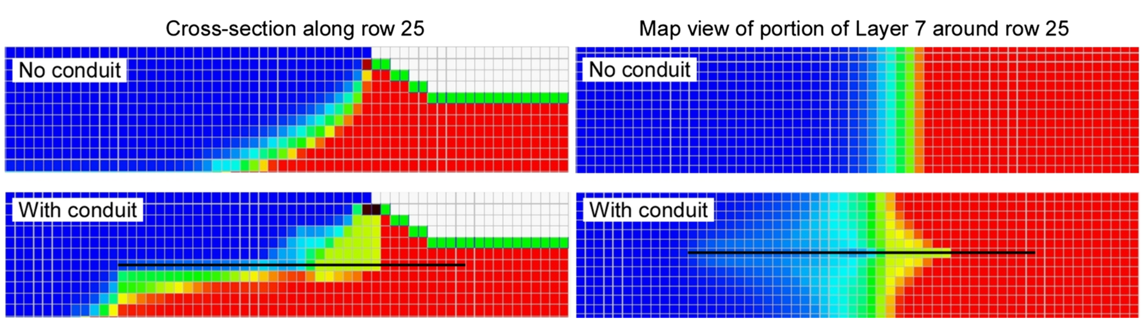


Fig. 2 Results of the variable-density steady-state simulation of the freshwater–seawater interface without (**a**–**b**) and with a conduit extending between onshore and offshore, below sea floor (**c**–**d**). Blue color denotes fresh groundwater, red color denotes seawater within the aquifer. Mixing of the two is denoted with transitional colors

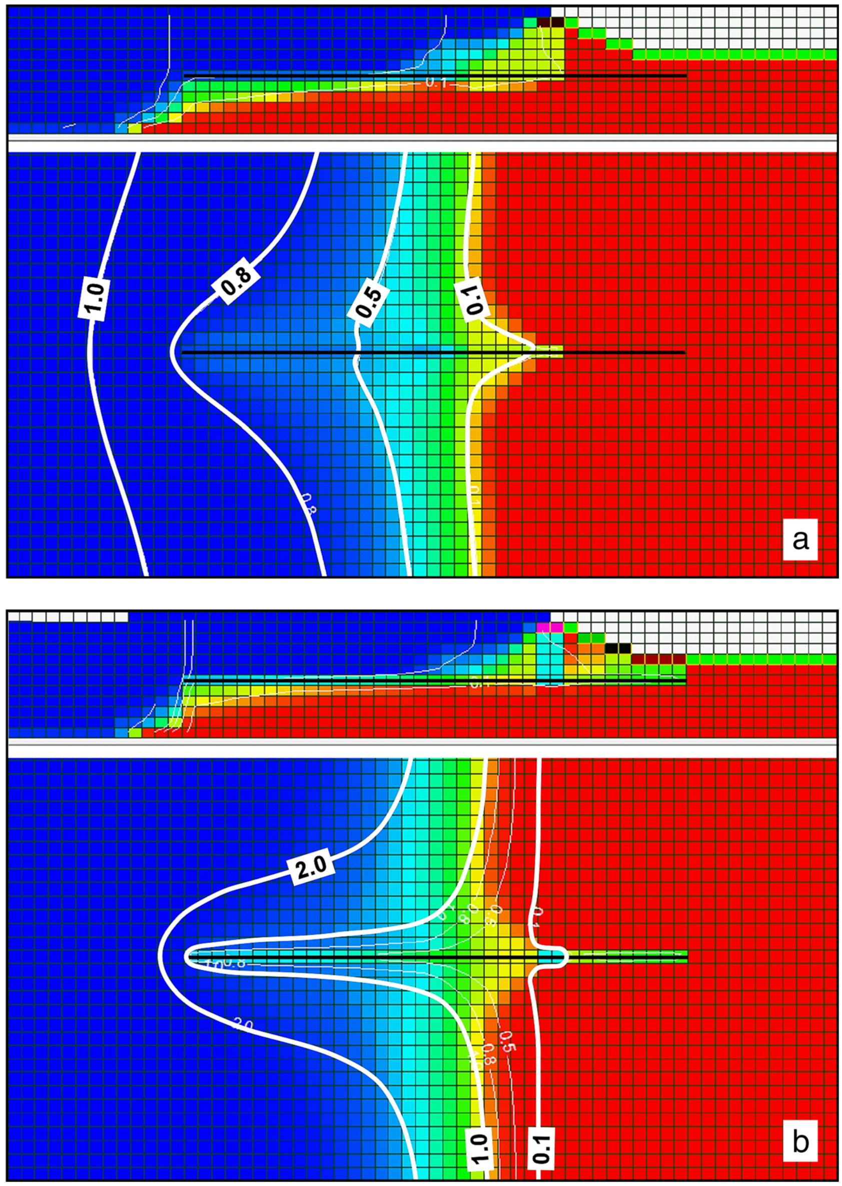


Fig. 3 Comparison of the results of **a** the steady-state model and **b** the transient model for the end of day 1 of the rainfall episode (cross-sectional and map views). The map views show contours of the simulated hydraulic head, in feet above sea level, in layer 7 where the conduit is placed (black line). Blue color denotes fresh groundwater, red color denotes seawater within the aquifer. Mixing of the two is denoted with transitional colors

a physical instability in the conduit itself resulting in formation of several internal hydraulic divides (Fig. 6a).

Figure 5 shows the behavior of saltwater at the various observation locations. At inland locations within the conduit (OP-1 and OP-2), the rainfall event is noted to induce larger dispersion and mixing which dissipates after the event. At OP-3 beneath the sea, the rainfall event causes water to freshen up; it then returns to saltwater concentrations after approximately 100 days of equilibration with average rainfall conditions. At OP-4 away from the conduit, the rainfall event causes a decrease in saltwater concentrations with saltwater intruding again after 100 days of average rainfall conditions. This is in contrast to OP-2 where the conduit caused larger mixing.

The situation at the end of a 5-day rainfall episode is illustrated with Figs. 4a and 6a. The high hydraulic head of the incoming freshwater in the conduit “pushes” freshwater into the denser seawater in all directions, but the mixing is still limited to a narrow zone around the conduit. The discharge of the activated submarine seep/spring at the sea floor at this point has the lowest salinity: approximately one third of the sea water salinity. By 100 days (Fig. 4b), the system has returned to prerainfall conditions similar to Fig. 3a.

Discussion

MODFLOW-USG is a versatile, physically based numeric groundwater flow, and contaminant fate and transport modeling program well suited for simulation of karst aquifers and their interactions with surface water features. It has a number of unique features that enable simulation of complex

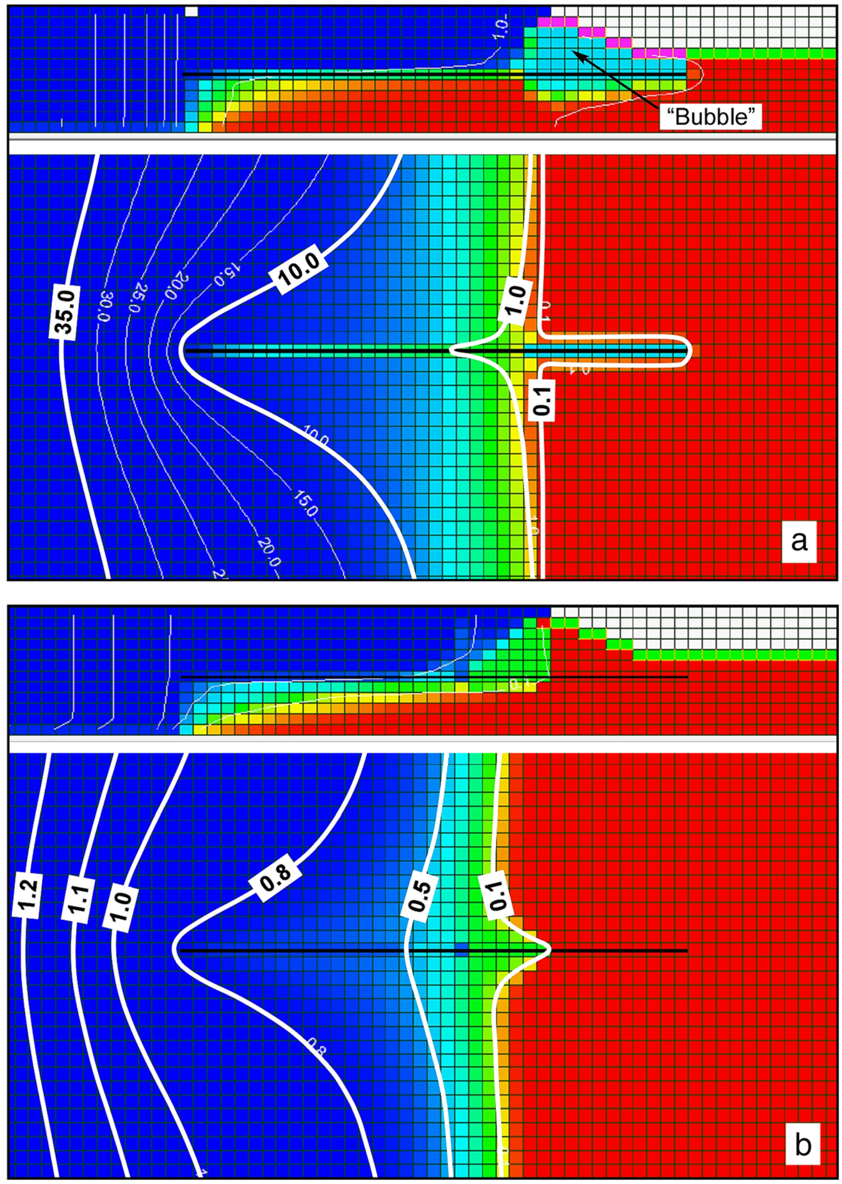


Fig. 4 Results of the transient model for **a** the end of the 5-day rainfall episode and **b** 100 days after. The map views show contours of the simulated hydraulic head, in feet above sea level, in layer 7 where the conduit is placed (black line). Blue color denotes fresh groundwater, red color denotes seawater within the aquifer. Mixing of the two is denoted with transitional colors

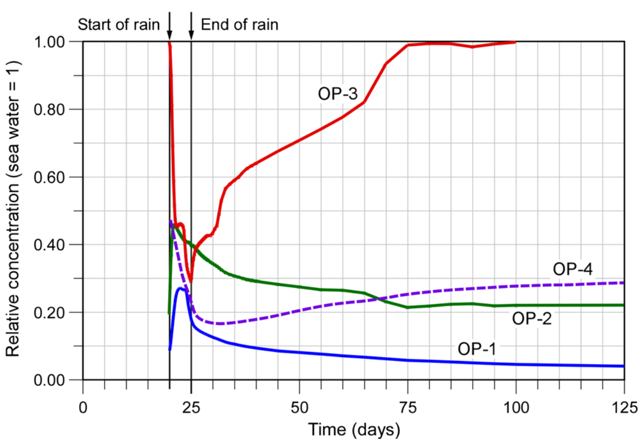


Fig. 5 Graph of calculated relative concentration at the four observation points during and after the simulated 5-day rainfall episode. Locations of the observation points are shown in Fig. 1. Seawater is simulated with dimensionless concentration of 1

subsurface conditions. It includes solutions inherent to equivalent porous media (EMP) modeling approaches as well as hydraulic (nonhydrogeologic) models that conceptualize karst aquifers as networks of pipes; furthermore, it allows for flow interactions between these domains. The CLN process in MODFLOW provides for simulation of groundwater flow through preferential flowpaths of karst aquifers such as fully or partially water-filled conduits. The exchange of flows between the conduits and the surrounding aquifer matrix is simulated with optional analytical solutions to reduce numerical grid size effects. Equations for flow in the CLN domains have been extended to include turbulent flow conditions and conform with the well-established equations describing groundwater flow through these distinctly different types of porous media. The CLN conduits can extend through both the saturated and unsaturated zones, including vertical sections, and

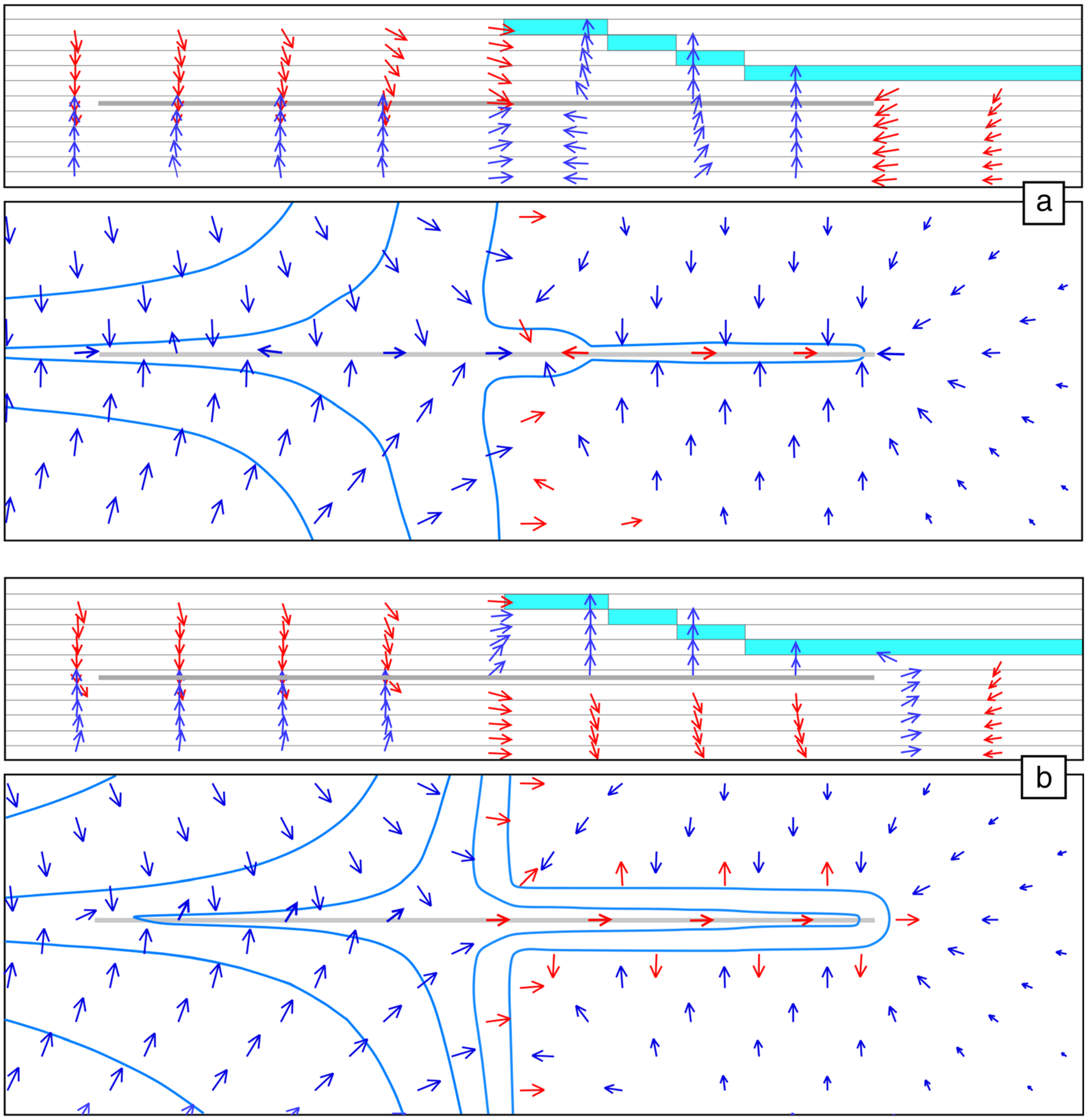


Fig. 6 Calculated velocity vectors in the area around the conduit, in cross-sectional and map views: **a** at the end of day 1 of the rainfall episode; **b** at the end of day 5 of the rainfall episode. Blue vectors have an upward direction, red vectors have a downward direction

can have both permanent and intermittent flows according to transient conditions. Any section of a conduit can have different radius than the adjacent sections and conduits can be effortlessly brought into the model from external 3D GIS shapefiles or can be added manually, in all three dimensions and with any orientation as needed.

MODFLOW USG has been extended to include solution for solute transport of multiple species, including density-dependent flow in coastal karst environments. It is in public domain and is supported by a number of GUIs including Groundwater Vistas which was used for the current examples. It has been continuously updated and supported and provides a robust simulation tool to evaluate complex coastal karst systems.

An example simulation is presented of density-dependent flow in coastal karst aquifers, demonstrating the complexities that can arise from even a single conduit feature. The conduit, as located in the example, acts as a drain feature attracting water from above and below it and causes the saltwater interface to generally intrude further than in locations away from the conduit, as noted in the cross-section figures. Also, the conduit causes mixing of waters with an associated larger diffuse zone than away from it, as noted in the aerial view. A high rainfall event can send a pulse of freshwater through the conduit activating a submarine spring with freshwater exiting below saltwater off the coast. The toe of the interface moved seaward more rapid during the rainfall event than during recovery after the event. All these influences may be of interest to water resources managers and others interested in better understating the complex interactions between freshwater and seawater in karst aquifers.

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