NUMERICAL MODELLING OF SATURATED GROUNDWATER FLOW AND POLLUTANT TRANSPORT IN KARST REGIONS

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ABSTRACT

In karst regions, groundwater flow and pollutant transport occur in two modes: fast-response flow in cave passages and slow-response flow in the aquifer-matrix. This paper presents, computationally efficient numerical model that simulates the behavior of the two flow and transport modes. First, the fast-response flow in a network of cave passages is mathematically modelled by means of a full unsteady hydrodynamic equation and solved numerically using the Preissmann method. The slow-response flow in the aquifer-matrix is modelled by an unsteady Darcy equation and solved numerically using a fractional-step approach. These two equations are iteratively coupled through an exchange term reflecting the water exchange between cave passages and the aquifer-matrix. Next, the pollutant transport equations in the network of cave passages is solved using a characteristic method and in the aquifer-matrix using a fractional-step approach. These two pollutant transport equations are solved iteratively through an exchange term reflecting the pollutant exchange between cave passages and the aquifer-matrix.

INTRODUCTION

Background

Karst aquifers, in contrast to aquifers in homogeneous media, are extremely complex because of their inhomogeneous permeability. As shown in Figure 1, the relation of structures in rock, such as fracture systems and the orientation of cave passages, establishes secondary permeability. These fractures or cave passages represent less resistance to water flow than does neighboring rock. In contrast to aquifers in homogeneous media, karst aquifers, due to their inhomogeneous distribution of permeability, are extremely complex.

Groundwater flow occurs in two modes: fast-response flow in cave passages and slow-response flow in the aquifer-matrix. These two components of groundwater flow are extremely different in the effectivity of groundwater transmission and groundwater storage. These flow characteristics therefore greatly influence pollutant transport in such a region.

Although unsaturated cases are common in the real world, understanding the behavior of saturated groundwater flow is a very important step toward understanding unsaturated cases. Insight from saturated cases can be applied to the study of unsaturated cases. Study of the physical behavior of saturated cases is, therefore, the beginning of on-going research in groundwater flow in karst regions.

Objective

The objective of the present study is to model the behavior of saturated groundwater flow and pollutant transport in karst regions. A new approach is introduced in which the "full" hydrodynamic equation in a cave passage network is solved directly. The pollutant assumed here is a nonreactive, conservative one, meaning that during transport, its quantity does not increase or decrease. As in any study of groundwater flow, little data are available. This is understandable due to the difficulties in measuring soil parameters, initial and boundary conditions, as well as the high cost involved in obtaining the data. For the purpose of the present study, no new field measurements have been performed. The study uses data obtained from competent published sources.

It is very important to mention that the present study is part of a larger research objective; i.e., the present study serves as the deterministic part of a Monte Carlo simulation of water resources in a karst region. Since available observations are limited, system parameters (aquifer properties, system geometry, initial and boundary conditions) must be generated by statistical techniques. Each realization of the data generated becomes the input data for the "deterministic engine" which processes the data to produce one realization of output. In a Monte Carlo simulation, hundreds or thousands of realizations

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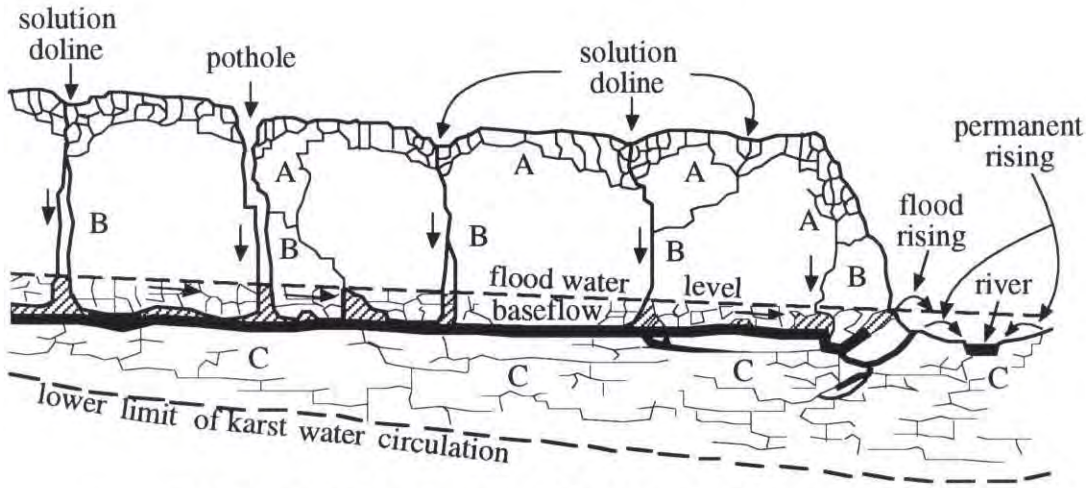
of input may be generated, each of which produces its corresponding output. These in turn must be interpreted by statistical means. In karst regions, the "deterministic engine" will be a model that simulates numerically the behavior of groundwater water and pollutant transport for unsaturated cases. Since the present study is only capable of handling saturated cases, it must be extended to unsaturated cases in order to become the complete "deterministic engine" for the Monte Carlo simulation.

The topology of cave passages and the boundary of the groundwater flow region are inferred from data obtained for karst formations in the Big Spring Basin, a 103 square mile groundwater basin located in Clayton County, northeastern Iowa (Hallberg et al., 1989), see Figure 3. The topography of the region under study is extracted from the USGS (United States Geologic Survey) contour map. Soil parameters, i.e., hydraulic conductivity, specific storage, exchange coefficient, dispersion coefficient, and effective porosity are based on appropriate published literature.



A solution opened joints and bedding planes with seepage water

B potholes and joints with seepage and stream flow

cave with free surface stream, filling in floods

permanently water-filled caves

C solution opened joints and bedding planes permanently water-filled or temporarily flooded

Figure 1. A Karst Hydrologic System Based on the Concept of Independent Conduits, after Cavaille (1962)

MODEL DEVELOPMENT

Introduction

The present study presents a model to simulate a complex, real-life situation. The domain of the model is based on the geometry and topography of the Big Spring Basin, depicted in Figure 4. The domain is three-dimensional, and certain topological conventions are required to handle it. To this end, a so-called "soil-topology" convention has been developed which makes it possible to describe any kind of three-dimensional boundary. All numerical approximations of the governing equations are applied within this topology. In the present study, the finite-difference method is used to approximate the governing equations, and the solution grid is generated to conform as closely as possible to the aquifer topography.

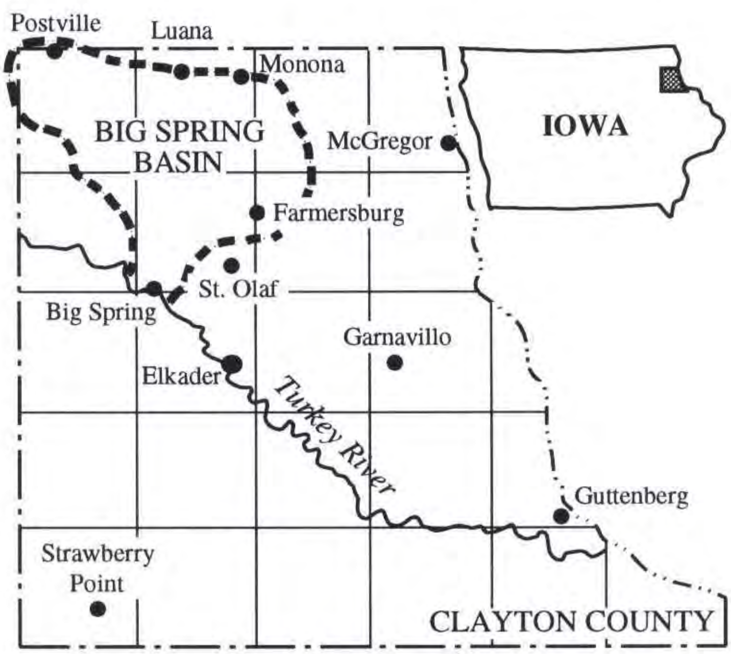


Figure 3. The Big Spring Basin in Clayton County, northeast Iowa, after Hallberg et al. (1989)

Governing Equations

This section describes all the governing equations used in the present study: hydrodynamic equations, equations of pollutant transport, and mass exchange equations for both the aquifer-matrix and megapore network.

Hydrodynamic Equation for Aquifer-Matrix

The governing equation of flow in porous media is derived from the mass conservation law applied to a control volume.

$$\Delta x \frac{\partial}{\partial x}\left(A_x K_x \frac{\partial h}{dx} \right) + \Delta y \frac{\partial}{\partial y}\left(A_y K_y \frac{\partial h}{dy} \right) + \Delta z \frac{\partial}{\partial z}\left(A_z K_z \frac{\partial h}{dz} \right) - W = S\, \upsilon \frac{\partial h}{dt} \tag{1}$$

where K is hydraulic conductivity (LT^{-1}); h is piezometric head (L); W is volumetric source flux (L^3T^{-1}); S is specific storage (L^{-1}); A is cross sectional area of aquifer in each direction, in a finite-difference block (L^2); Δ is the length of control volume in each direction (L); and

$$W = w\, \upsilon \tag{2}$$

In Eq. (2) w is the source term, volumetric flux per unit volume (T^{-1}); and υ is the volume of the aquifer in a finite-difference block (L^3). Volumetric flux, W, is the source exchange term between the aquifer-matrix and megapores.

Pollutant Transport Equation for Aquifer-Matrix

The governing equation of pollutant transport in porous media is also derived from the mass conservation law applied to a control volume. For a nonhomogeneous, anisotropic porous medium, the governing equation can be written in terms of concentration (C) as

$$\Delta x \frac{\partial}{\partial x}\left(A_x D_x \frac{\partial C}{\partial x}\right) + \Delta y \frac{\partial}{\partial y}\left(A_y D_y \frac{\partial C}{\partial y}\right) + \Delta z \frac{\partial}{\partial z}\left(A_z D_z \frac{\partial C}{\partial z}\right) - \\ \Delta x \frac{\partial}{\partial x}(A_x U_x C) - \Delta y \frac{\partial}{\partial y}(A_y U_y C) - \Delta z \frac{\partial}{\partial z}(A_z U_z C) - C_s W = \upsilon \frac{\partial C}{\partial t} \tag{3}$$

where $U_x = \frac{-K_x}{e}\frac{\partial h}{\partial x} \quad U_y = \frac{-K_y}{e}\frac{\partial h}{\partial y} \quad U_z = \frac{-K_z}{e}\frac{\partial h}{\partial z}$ (4)

In Eq. (3) C is solute concentration (ML^{-3}); D is the dispersion coefficient (L^2T^{-1}); U is seepage or average pore water velocity (LT^{-1}); C_s is solute concentration in the sources or sinks (ML^{-3}); e is effective porosity; and U_x, U_y, U_z and W are known quantities from the hydrodynamic computation.

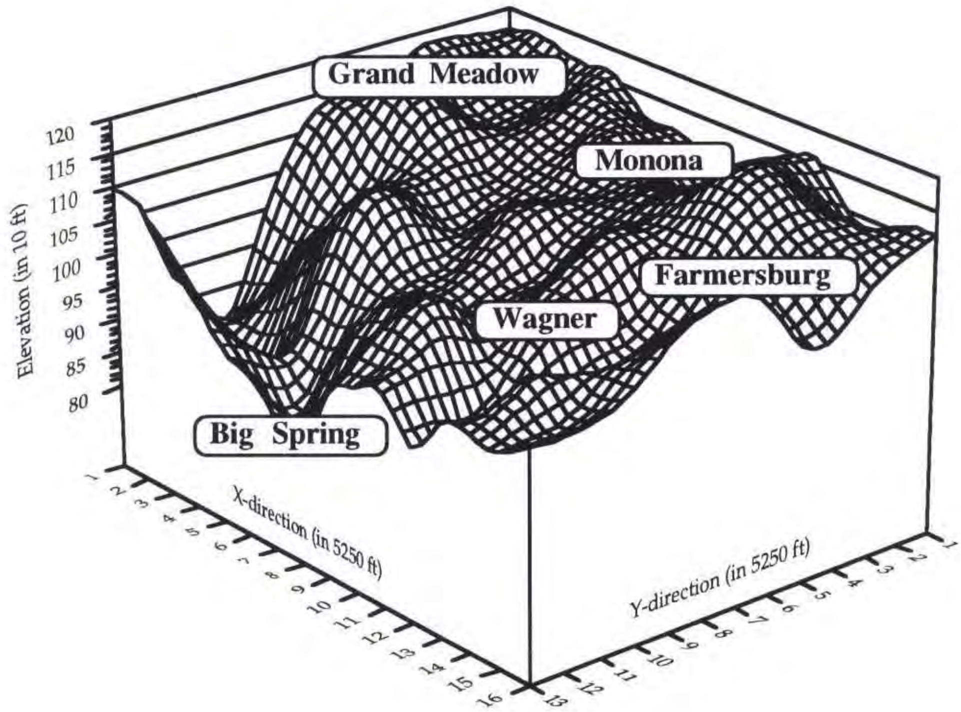


Figure 4. Southeast View of the Big Spring Basin (Iowa, USA)

Hydrodynamic Equation for Megapores

In the present study, the flow is restricted to one-dimensional, incompressible, full-megapore flow, the principal implication of which is that the discharge in a single megapore must at any instant be constant along its length. Of course the discharge may vary from one megapore to another along a series of megapores in a network due to external or aquifer-matrix inflow. From the law of conservation of momentum, the governing equation in any single megapore can be written as

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial s}\left(\frac{Q^2}{A}\right) + gA\left(\frac{\partial h}{\partial s} + S_f\right) = 0 \tag{5}$$

Since $Q \neq Q(s)$ along a megapore, Eq. (5) can be rewritten as

$$\frac{\partial Q}{\partial t} - \left(\frac{Q}{A}\right)^2 \frac{\partial A}{\partial s} + gA\left(\frac{\partial h}{\partial s} + \frac{Q\,|Q|}{K^2}\right) = 0 \tag{6}$$

where t is time; s is the longitudinal megapore coordinate; Q(t) is megapore discharge; A(s) is megapore cross-sectional area; h(s,t) is the megapore piezometric head; S_f(s,t) is megapore energy slope ($= \frac{Q\,|Q|}{K^2}$); K(s) is full-megapore conveyance; and g is gravitational acceleration. In Eq. (6), the four terms are associated with local acceleration, advective acceleration, net normal pressure force, and boundary shear force, respectively.

Pollutant Transport Equation for Megapores

The governing equation for pollutant transport can be derived from the law of mass conservation, with the same assumptions as those used to derive hydrodynamic equation. Following the derivation given by Fischer et al. (1979), the pollutant transport equation can be generalized as

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(AU\,C)}{\partial s} = \frac{\partial(A\,\varepsilon\,\frac{\partial C}{\partial s})}{\partial s} \tag{7}$$

Differentiating the left hand side of Eq. (7) and recognizing that $\frac{\partial A}{\partial t} + \frac{\partial(AU)}{\partial s} = 0$ from conservation of mass, Eq. (7) can be rewritten as

$$A\frac{\partial C}{\partial t} + AU\,\frac{\partial C}{\partial s} = \frac{\partial(A\,\varepsilon\,\frac{\partial C}{\partial s})}{\partial s} \tag{8}$$

where U(s,t) is velocity of megapore flow, and e(s) is the megapore dispersion coefficient.

Mass Exchange Between Aquifer-Matrix and Megapores

The mass exchange between aquifer and megapores consists of two constituents, water discharge and pollutant flux. The water discharge exchange uses the same principle used in computing leakage through a semipermeable layer from an overlying (or underlying) aquifer into another aquifer with a different piezometric head (see Bear, 1979, page 36). Therefore, the amount of mass exchange can be computed as a linear function of the difference between the piezometric head inside the megapore and that of the aquifer-matrix surrounding the megapore. The equation of water discharge exchange can be written as

$$w = \alpha\,(h_s - h_p) \tag{9}$$

where a is the coefficient of exchange ($L^{-1}T^{-1}$); h_s is the piezometric head of the aquifer-matrix (L); and h_p is the piezometric head of the megapore (L).

For the pollutant flux exchange term the assumption is that the advective exchange term is dominant compared to that of the diffusive one. The equation for the pollutant exchange term thus becomes simply the concentration of pollutant in water multiplied by its water discharge:

$$w_s = C_s\,w \tag{10}$$

where w is as defined in Eq. (9).

Topological Structure of the Aquifer

The aquifer is represented by a three-dimensional block of computational grid points, referred to herein as aquifer-matrix grid points. The three-dimensional equations for aquifer-matrix water and pollutant movement are solved numerically on this computational grid.

Preferential flow paths, such as root-zone macropores or karst megapores, are represented as an interconnected network of so-called pipes, within which water and pollutant transport are represented as equivalent to flow in full pipes.

Exchange of water and pollutant between the aquifer-matrix and megapore passages is taken to occur only at aquifer-matrix grid points through which the pipe network passes; these intersections are called nodes. Thus, it is presumed that however the pipe network is generated (e.g., manually, through stochastic simulation, etc.), it is constrained to pass frequently through aquifer-matrix grid points; i.e., that nodes occur as densely as possible.

Figure 5 is a schematic depiction of a possible simple topological structure. The aquifer-matrix grid point coordinates of nodes are shown in parentheses. Nodes 1, 6, 12, 20, and 33 (shown as inverted triangles) represent intersections of the megapore structure with the ground surface; i.e., sinkholes. Nodes 5, 8, 16, and 23 are junctions of multiple pipe-network flow paths. Nodes 11, 19, 32, and many others not shown, represent aquifer-matrix grid points through which pass a single pipe-flow path.

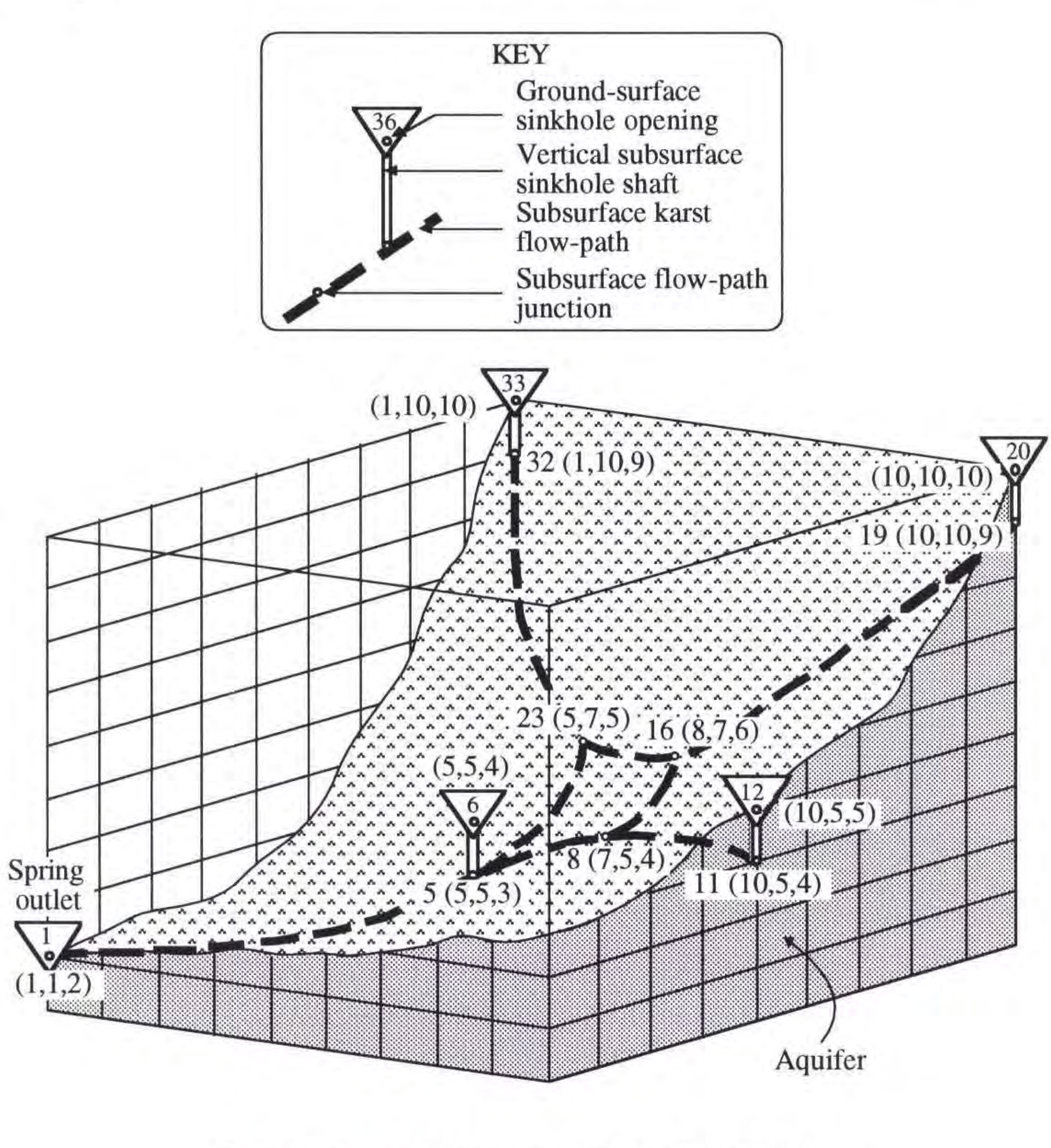


Figure 5. Schematic Representation of the Karst Aquifer

General Computational Strategy

Water and pollutant transport in the aquifer-matrix are essentially diffusive phenomena, governed by diffusion mass conservation equations whose dependent variables are heads and concentrations, respectively. Water and pollutant transport in the pipe network are essentially advective phenomena, governed by energy or momentum and mass conservation equations whose dependent variables are water discharges, heads and concentrations. The water and pollutant exchange between the aquifer-matrix and pipe network is governed essentially by the differences in head and concentration between the two systems at any node. Recall that a node is defined as an aquifer-matrix grid point through which the pipe network passes. The heads and concentrations of both systems are coupled through the water and pollutant exchange. In principle, the entire system of equations — aquifer-matrix diffusion and pipe-network energy or momentum and mass conservation — must be solved simultaneously.

This simultaneous solution poses no fundamental conceptual problems. However, its practical execution would be extremely demanding of computer resources, especially for large and/or complex systems. Therefore, a fractional-step computational strategy is adopted whereby, for each of several iterations in a computational time interval, the aquifer-matrix and pipe-network equations are solved separately, their exchange-term coupling being represented only approximately in each iteration. The details of this procedure are developed in following three main sections. The first section describes the numerical solution of the governing equation for the aquifer-matrix. The second section explains the numerical solution of the governing equation for the pipe network. The last section elaborates the numerical procedure for approximating the exchange terms between aquifer-matrix and pipe network.

TEST AND APPLICATION

This chapter presents tests and applications of the model to the Big Spring Basin. Sensitivity analyses of important system parameters of this basin (megapore diameter, roughness coefficient, hydraulic conductivity of the aquifer, and classes of megapore diameter) are conducted to identify interaction between the parameters and model components. Simulation of dye trace experiments conducted in the basin is performed to demonstrate the capability of the model.

If the present model is to serve as the basis for a broader range of research, it must be shown to be able to simulate field conditions. To do this, the model was run to simulate two of the dye trace experiments conducted by Hallberg et al. (1983). The purpose of these experiments was to establish direct connections between sinkhole recharge points and discharging springs. In the Big Spring Basin, several dye trace experiments were conducted by the Iowa Conservation Commission (ICC) and Iowa Geological Survey (IGS). Figure 6 shows the sinkholes used as dye input points (Hallberg et al. 1983).

From the results of the sensitivity analysis performed in previous sections, the parameters and megapore features affecting the Big Spring Basin can be ranked in order of importance, as presented in Table 1.

Table 1. Parameters and Features Affecting the Big Spring Basin

Parameter/Features	Degree of Importance
Megapore diameter	Very important
Diameter class	Very important
Hydraulic conductivity	Important
Megapore roughness	Important
Dispersion coefficient	Not important

It is important to mention that the above results are based on a fixed megapore topology. Presumably, megapore topology plays a more important role than megapore diameter. Moreover, the above results are based on following ranges of parameters: megapore diameter, D, from 3 ft to 30 ft; hydraulic conductivity, K, from 7.6 x 10–6 fps to 7.6 x 10–5 fps; megapore roughness, ks, from 10 to 35; and Taylor dispersion coefficient, C_t, from 5.05 to 20.2, values which are 50% to 200% of the suggested value of C_t (10.1).

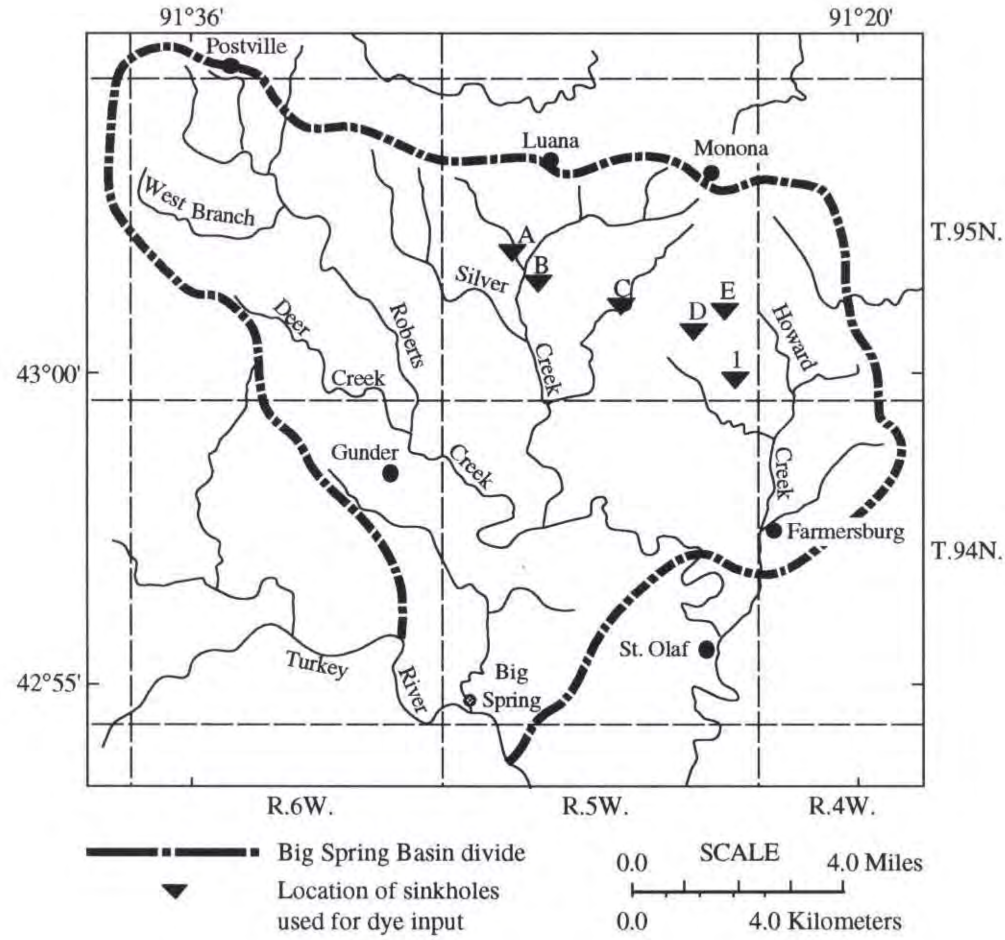


Figure 6. Location of Sinkholes Used for Dye Trace Experiments, after Hallberg et al. (1983)

The results of sensitivity are summarized in the following paragraphs:

(1) The size of the equivalent megapore dictates whether the overall system is responsive or diffusive. Generally, the smaller the diameter, the less responsive the system to a storm hydrograph entering sinkholes. Moreover, for a given megapore diameter, there is a threshold input hydrograph that the megapore can pass directly.

(2) Megapore diameter classes are particularly important for pollutant transport while this feature does not significantly affect discharge response. The same discharge response at Big Spring may be obtained by replacing several megapore diameter classes by one uniform diameter, but it is difficult to get the same pollutant response using this procedure.

(3) After megapore diameters and their classes, hydraulic conductivity of the aquifer-matrix is the third most important parameter. The importance of hydraulic conductivity is due to its contribution to the baseflow of the system. Generally, in any storm event, if there is pollutant in the water, the storm acts only as a carrier to bring the pollutant from outside into the system (i.e., aquifer-matrix and megapore network). Inside the system itself, the pollutant is usually carried by the baseflow, except for the case of small megapore diameters in which small amounts of the pollutant are also carried by the storm, resulting in a flashy downstream pollutant flux.

(4) Megapore roughness is a mildly important parameter. Generally, this parameter only slightly affects the peak discharge of water and pollutant, as well as the time to peak. The overall behavior of responses at Big Spring is not affected by this parameter.

(5) The dispersion coefficient also does not play an important role in the present study since the advective phenomenon is dominant compared to the diffusive one. Variation of the value of the dispersion coefficient, Ct, from 50% to 200% of the suggested value does not give significant differences in pollutant transport at Big Spring.

Figure 7 shows that discharge response at Big Spring for a 20 ft megapore diameter, D, represents a conduit response in which most water flows through megapores, while D equal to 7 ft represents a diffuse response in which most water flows through the aquifer-matrix. This result agrees with the conceptualization of Hallberg et al. (1983), Figure 8, which shows the difference between conduit-flow and diffuse-flow in a carbonate aquifer.

The simulation of the dye trace experiments, shows that travel times of the dye traces are very sensitive to megapore diameter, confirming that megapore diameter is the most important parameter affecting the system. The range in magnitude of diameter that produces the actual travel time is within 1.5 ft of the representative diameter. Even though the representative diameters chosen in the previous section are not necessarily the actual ones, the range of deviation from the representative diameter is an important finding. This narrow deviation shows that megapore diameter significantly affects pollutant transport. These results confirm the conclusion of the sensitivity analysis on megapore diameter.

The simulation results show that the maximum outflow at Big Spring usually coincides with a point in the inflow hydrograph. It should be possible, therefore, to predict the flow at Big Spring using a reservoir-type formulation, which avoids the complexity of a detailed mathematical formulation that considers all the water pathways (megapore network). For pollutant transport, however, the pathways are important and the reservoir formulation is not adequate to determine the concentration of pollutants in the Big Spring flow. Thus, the discharge response at Big Spring can be written as:

$$\frac{dO}{dt} = I(t) - O(t) \tag{11}$$

where I(t) is known storm hydrographs entering sinkholes and O(t) is discharge response at Big Spring. When O(t) reaches maximum value, i.e., $\frac{dO}{dt} = 0$, the discharge response at Big Spring is $O(t = t1) = I(t = t1)$. As the system becomes a diffusive one, i.e., the megapore diameters decrease, Eq. (11) will no longer apply.

CONCLUSIONS

This section summarizes all results obtained from the present study. First, from sensitivity analysis, important parameters and features of the karst region have been identified. The most important parameter is the equivalent megapore diameter, and its distribution throughout the megapore network is the most important feature of the megapores. Other parameters affecting the Big Spring Basin ranked in order of importance are hydraulic conductivity of the aquifer-matrix, megapore roughness and dispersion coefficient. The megapore dispersion coefficient does not affect the basin, since the pollutant transport is dominated by advection rather than dispersion phenomenon.

Second, the main objective of the present study has been achieved by the computer code Labyrinth. The Labyrinth code is capable of simulating the behavior of saturated groundwater flow and pollutant transport in karst regions. The two modes of the flow; fast-response flow in cave passages and slow-response flow in the aquifer-matrix, have been correctly reproduced by the Labyrinth code.

Third, the results of the dye trace simulation, viewed in a Monte Carlo simulation framework, succeed in producing realizations for dye trace A and 1 experiments. Thus, the Labyrinth code has shown the capability to serve as a "deterministic engine."

FINAL REMARKS

As a part of a larger research objective — to serve as the deterministic engine of a Monte Carlo simulation of water resources in a karst region — the Labyrinth code has a promising future. At present, however, due to limited availability of data and time, the Labyrinth code can only produce the qualitative behavior of saturated groundwater flow and pollutant transport. If more field data and resources become available in the future, more thorough tests can be performed on the Labyrinth code to completely understand its behavior and to calibrate parameters, thus enabling the present code to completely understand its behavior and to calibrate parameters, thus enabling the present code to predict future conditions of the Big Spring Basin during wet seasons. Moreover, the extension of the Labyrinth code to handle unsaturated cases and its inclusion in a Monte Carlo simulation will make the code a powerful tool to analyze water resources in karst regions.

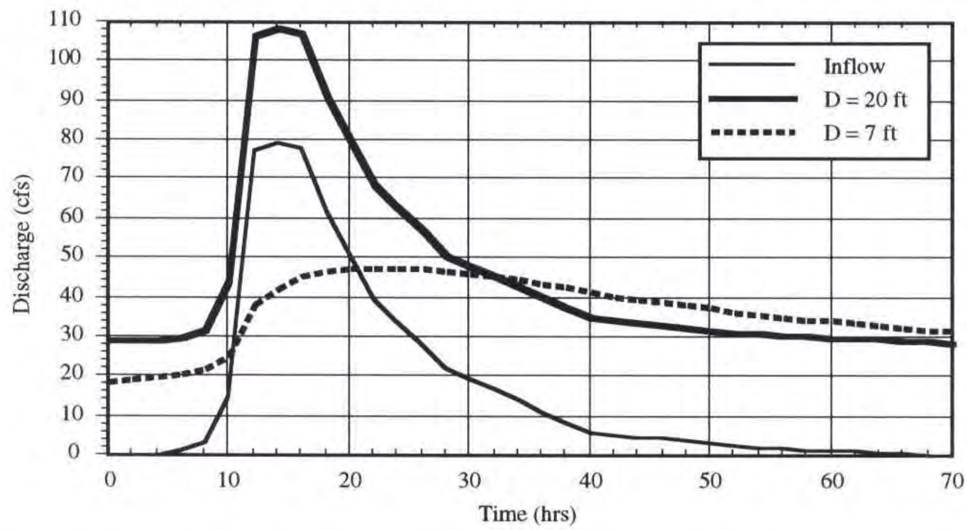


Figure 7. Discharge Hydrographs at Big Spring for Megapore Diameters, D, 7 ft and 20 ft.

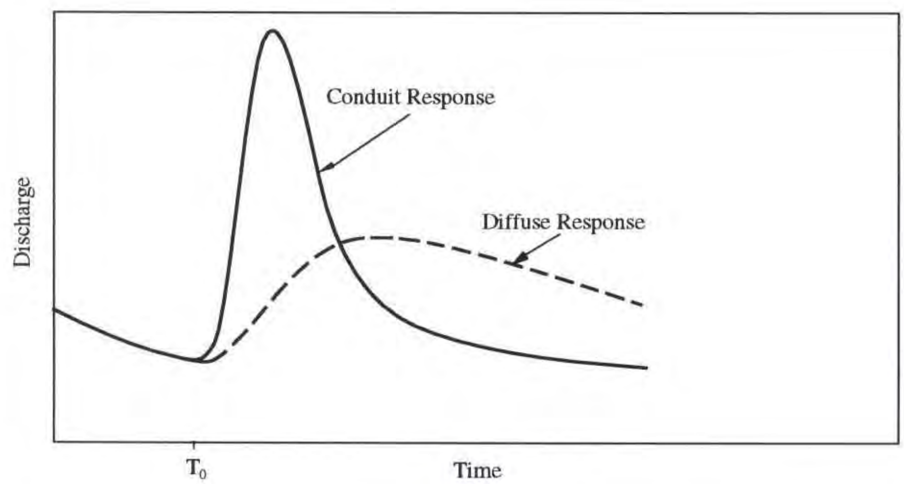


Figure 8. Schematic Hydrographs Showing the Difference between Conduit-Flow and Diffuse-Flow Discharge in a Carbonate Aquifer (e.g., at a spring) over Time, in Response to a Recharge Event at Time, T_0, after Hallberg et al. (1983).

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