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A combined continuum and discrete network reactive transport model for the simulation of karst development

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Abstract A numerical model for the simulation of the development of karst aquifers is presented. In this reactive model, calcite dissolution is coupled to the flow using a two-step approach. The flow module calculates laminar and turbulent groundwater flow in a conduit network coupled by a linear exchange term to a porous continuum representing the fissured system. It is a highly dynamic modelling approach, i.e. the potentials in the system and therefore the flow and consequently the rate of enlargement of the conduits are dependent on the diameters and the rate of groundwater recharge, both of which vary with time. First results of a simple example with one conduit show that the model is able to simulate the development of a karst groundwater catchment. During an initial stage the flow system resembles very much to a fractured aquifer, and changes to the extremely heterogeneous mature karst system. It is shown that the enlargement of the conduits is initiated at the spring and propagates upgradient.

INTRODUCTION

Karstified limestone aquifers are often a very prolific and due to the high flow velocities a very vulnerable source of groundwater. They have therefore been studied in many countries in great detail. In southwest Germany approximately 20% of the area consist of karstified limestones and one-third of the water supply relies on karst groundwater resources. In order to predict groundwater flow and transport in these systems, numerical models have been used (e.g. Teutsch, 1988; Sauter, 1992). Due to the extreme heterogeneity in the hydraulic parameters of carbonate aquifers, flow and transport are difficult to quantify. This heterogeneity and the complexity of the flow system is primarily determined by the degree of karstification (matureness of the karst) and the contrast between a highly permeable, low storage conduit system and a less permeable, high storage fissured system. Depending on lithology, type and time of aquifer exposure to erosion and the prevailing structural features, a more or less mature conduit system might have developed which is mainly responsible for the frequently high fluctuation in spring discharge and the high transport velocities. Due to the infrequent occurrence of these conduits and the often large depth of the aquifer, it is very difficult to obtain detailed information on the geometry, the areal distribution and the hydraulic parameters of the conduit network. One way of characterizing the flow system in karst areas is by

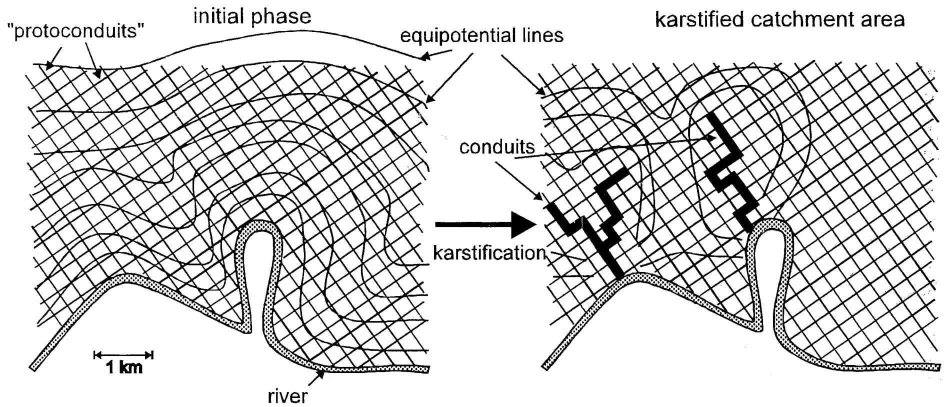

Fig. 1 Conceptual model for the development of karst aquifers. During the initial phase some fractures exist ("protoconduits") that are able to develop into conduits.

obtaining information on the development of the aquifer from geological and geomorphological investigations, such as data on the spatial distribution of intensively karstified zones. A conceptual model of the development of a karst system is shown in Fig. 1.

In the past few decades, the amount of field and laboratory data related to the development of karst areas has increased considerably. More than 20 000 km of cave passages have now been mapped (Courbon & Chabert, 1986) and classified into several end-member patterns (Palmer, 1991). Controlling geological, hydrological and hydrogeochemical processes were summarized by several authors (e.g. Ford & Ewers, 1978; White, 1988; Ford & Williams 1989).

The thermodynamics for the CO_2-H_2O-$CaCO_3$ system was examined by Plummer & Busenberg (1982). The application of equilibrium theory to the prognosis of the development of karst systems could not explain the persisting undersaturation of the infiltrating recharge water close to the groundwater table. One process of explaining this undersaturation is mixing corrosion (Bögli, 1964).

Kinetic effects were first considered by Weyl (1958), who coupled the laminar groundwater flow through a fracture with a diffusion limited rate law for calcite dissolution. He calculated a "penetration length" for water entering initial fractures. This "penetration length" is the distance from the entrance of a fracture, at which water has reached a certain percentage of saturation. This distance appears to be very short compared to the distances between the location of groundwater recharge and the spring in a natural catchment. However, closer examination of the solution process of calcite by several authors (Berner & Morse, 1974; Plummer & Wigley, 1976; Plummer *et al.*, 1978; Buhmann & Dreybrodt, 1985a,b) showed that also other processes apart from diffusion determine the dissolution of carbonate rocks. White (1977) introduced the kinetic trigger concept. From the data of Berner & Morse (1974) he concludes that the dissolution rates drop significantly when the reaction is close to equilibrium. The change in the carbonate dissolution rate can be quantified by a fast first order kinetic rate law far from equilibrium and a much slower fourth order dissolution rate close to equilibrium. Because of the slow fourth order dissolution water can reach the spring without becoming fully saturated. This leads to an enlargement of a conduit also far from the recharge location. The conditions close to equilibrium and the effects of inhibitors on the dissolution surface were further examined by Reddy (1977), Reddy & Wang (1980), Palmer (1991), and Svensson & Dreybrodt (1992).

In the early nineties, one-dimensional flow models were used to determine the sensitivity of parameters, such as rate constants, the conduit length or the hydraulic gradient on karstification processes (Dreybrodt, 1990; Palmer, 1991; Groves & Howard, 1994a). These models use fixed potentials at the inlets and outlets of the conduits. The results of these models show that for large times the width of the fracture narrows down towards the outlet and adopts a conical shape. As the fracture enlarges, the discharge increases and the penetration length of the fast dissolution kinetics far from equilibrium increases accordingly. Finally at the "breakthrough time" (Dreybrodt, 1990), the fast dissolution is active over the entire length of the fracture and the aperture is increased rapidly at more or less constant rate.

Recently, Groves & Howard (1994b) developed a model for the simulation of the early evolution of karst systems in two dimensions. This model uses either fixed potentials at the inlets and outlets or limits the maximum discharge in the tubes. The tube diameters in their model are lognormally distributed. The distribution of the preferential flow paths developed in their model might be predetermined by the initial distribution of tube diameters.

In this paper a numerical model for the simulation of flow and calcite dissolution in karst aquifers is presented. The model calculates laminar and turbulent groundwater flow in a conduit network coupled by a linear exchange term to a continuum model representing the fissured system. It is a highly dynamic modelling approach, i.e. capable of modelling the potentials in the system and therefore the flow and, consequently, the rate of enlargement of the conduit diameters and the rate of groundwater recharge, both of which vary with time.

MODEL STRUCTURE

The model CAVE (Carbonate Aquifer Void Evolution) comprises three components: (a) a porous continuum flow module (b) the discrete pipe network flow and transport module, and (c) a carbonate dissolution module which calculates in a two-step procedure the widening of the conduits (Fig. 2).

User input allows selection of hydraulic conductivities and initial and boundary conditions for the fissured system of the model domain such as no flow boundaries or constant head boundaries and recharge. For the pipe network the initial diameters, the spatial distribution, the exchange coefficients of the tubes as well as the constant head or flux boundaries have to be specified. The chemistry module requires as input the equilibrium concentration for Ca^{2+} in water, the temperature and the kinetic rate constants for the fast first-order and the slow fourth-order kinetics. Furthermore the proportion of the recharge infiltrating directly into the conduits as well as its spatial distribution can be specified.

The program starts with the computation of the hydraulic heads within the fissured system using MODFLOW (McDonald & Harbaugh, 1984). Afterwards, head values for the pipe network are calculated as outlined below. Based on the head differences between the fissured system and the conduits the exchange of water is calculated using

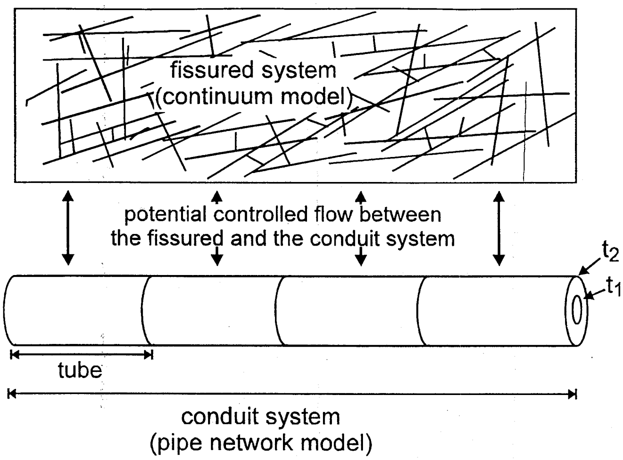

Fig. 2 Conceptual model illustrating the fissured and the conduit system as well as the dissolutional enlargement of the tube diameter for two different times $t_1 < t_2$.

a linear exchange term (Barenblatt *et al.*, 1960; Warren & Root, 1963; Odeh, 1965). The fissured system and the pipe network are coupled iteratively. After convergence, the chemistry module calculates the carbonate dissolution rates within the tubes. The change in conduit diameter is determined according to the mass of carbonate dissolved. This procedure is repeated for each time step within the simulation period.

The theoretical background for the newly developed model components, the pipe network flow module and the carbonate dissolution module, is outlined below.

Pipe network module

This module represents the fast flow system of the karst aquifer. The conduits are assumed to be cylindrical and permanently saturated neglecting the compressibility of the fluid.

In a first step the hydraulic relationships for a single pipe are described. The absolute value of the head loss Δh due to pipe flow is given by the Darcy-Weisbach relationship and may be expressed as

$$\Delta h = \lambda \frac{Lu^2}{d2g} \tag{1}$$

where λ is the friction factor, d is the pipe diameter, u is the average flow velocity, g is the earth's gravitational constant and L is the length of the tube.

The friction factor λ depends on the velocity in the pipe. For small velocities, i.e. laminar flow with a Reynolds number < 2300, so-called Hagen-Poiseuille flow develops. The friction factor is calculated as

$$\lambda = \frac{64\nu}{du} \tag{2}$$

(ν is the kinematic viscosity). This can be substituted into equation (1) and the discharge

Q through a section of the pipe can be calculated

$$Q = \frac{\pi d^4 \Delta h g}{128 L \nu} \tag{3}$$

Experimental observations show that for turbulent flow ($Re > 2300$) the implicit Colebrook-White law is applicable

$$\frac{1}{\sqrt{\lambda}} = -2\log\left[\frac{2.51}{Re\sqrt{\lambda}} + \frac{k}{3.71d}\right] \tag{4}$$

with pipe roughness k and Reynolds number $Re = u\,d/\nu$. For turbulent flow conditions discharge is given by

$$Q = -2Y\log\left[\frac{2.51\pi\nu d}{4Y} + \frac{k}{3.71d}\right] \tag{5}$$

with

$$Y^2 = \frac{\Delta h g d^5 \pi^2}{8L} \tag{6}$$

In a second step, a system of connected pipes with n nodes is considered. According to the Kirchhoff rule, the sum of inflow and outflow at any node i of the network is zero

$$\sum_{j=1}^{n_i} Q_{ij} + R_i = 0 \tag{7}$$

where n_i denotes the number of nodes connected to i. R_i stands for the sources and sinks at the node i, whereby R_i includes the exchange with the fissured system and the recharge infiltrating directly into the conduits. In the general case, tubes with laminar as well as turbulent flow may occur at the same time. Therefore equations (3), (5) and (7) are combined yielding

$$0 = \sum_{j=1}^{n_i^{turb}} (-2Y_{ij}) \log\left[\frac{2.51\pi d_{ij}\nu}{4Y_{ij}} + \frac{k_{ij}}{3.71 d_{ij}}\right] + \sum_{j=1}^{n_i^{lam}} \frac{\pi d^4 ij \Delta h_{ij} g \nu}{128 L_{ij}} + R_i \tag{8}$$

Here n_i^{lam} and n_i^{turb} are the numbers of the tubes with laminar and turbulent flow connected to node i ($n_i^{lam} + n_i^{turb} = n_i$). For every node in the conduit system with unknown head an equation of the form (8) is obtained. Thus, a network with n nodes of unknown head can be expressed as a system of n nonlinear equations with n unknowns. This system is solved by a Newton-Raphson iteration (Press *et al.*, 1986). Starting values are obtained by solving the system (8) for laminar flow conditions in all tubes, i.e. $n_i^{lam} = n_i$ and $n_i^{turb} = 0$.

Carbonate dissolution module

The rates of the calcite dissolution vary as functions of time and position along the conduit. The dissolution rates of $CaCO_3$ by a H_2O-CO_2 solution for closed system conditions with respect to CO_2 have been investigated by Buhmann & Dreybrodt (1985b). For Ca^{2+}-concentrations of $c < 0.9\, c_{eq}$ they calculated the dissolution rate F using

$$F(c) = \alpha(x)\,(c_{eq} - c) \tag{9}$$

where

$$\begin{aligned} \alpha(x) &= \alpha_{lam}\left[1 + \frac{\alpha_{lam} d(x)}{6D}\right]^{-1} && \text{if } Re \leq 2300 \\ \alpha(x) &= \alpha_{turb} && \text{if } Re > 2300 \end{aligned} \tag{10}$$

with c_{eq} the equilibrium concentration of Ca^{2+} and α_{lam} and α_{turb} the kinetic rate constants for laminar and turbulent flow respectively. Values for α_{lam} and α_{turb} are provided by Buhmann & Dreybrodt (1985b). For laminar flow the rate coefficient $\alpha(x)$ considers the influence of mass transport by diffusion for large diameters d depending on the position x within the conduit. D is the coefficient of diffusion for Ca^{2+} in water. For concentrations $c > 0.9\, c_{eq}$ a change in the reaction rate law is observed. Plummer & Wigley (1976) found a fourth-order rate law describing the observed changes in concentrations

$$F(c) = \beta(c_{eq} - c)^4 \tag{11}$$

where β is the kinetic rate constant for the fourth-order reaction. Using equations (9) and (11), it is possible to calculate the flux of Ca^{2+} from the walls of a tube into the water and consequently the increase in diameter of the tube.

SIMULATION RESULTS

In order to study the effects of the enlargement of the tubes with time on the flow in groundwater catchments, a simple rectangular area with a single conduit was selected (Fig. 3). The modelled domain is 1250 by 1250 m, the initial diameter of the conduit, consisting of 25 tubes is 0.4 mm, the hydraulic conductivity of the fissured system is fixed at 1.6×10^{-5} m s^{-1} and a constant recharge of 400 mm year^{-1} is applied. Recharge is distributed uniformly with 1% entering directly the conduit system. The aquifer is assumed to be unconfined and the coefficient for the linear exchange term is equal to 0.0001 m^2 s^{-1}. It is assumed that the water within the fissured system shows a certain degree of undersaturation ($C_{Ca2+} = 0.9\, c_{eq}$). Three sides of the model domain are no flow boundaries and at one side a constant head boundary is specified, representing a river. The recharge data and the hydraulic parameters are derived from a typical karst aquifer system in southwest Germany.

At the beginning of the simulation (Fig. 4(a)) the conduit has no influence on the hydraulics of the fissured system. For the next 1500 years the situation does not change much because the tubes are only enlarged by slow dissolution controlled by fourth-order kinetics (Fig. 4(b)). With the increase in spring discharge due to the growing diameter of the conduit, the penetration length for the fast first-order dissolution propagates farther downgradient in each tube. At the beginning of the simulation the largest hydraulic gradient is observed in tube number 1 next to the constant head boundary, i.e.

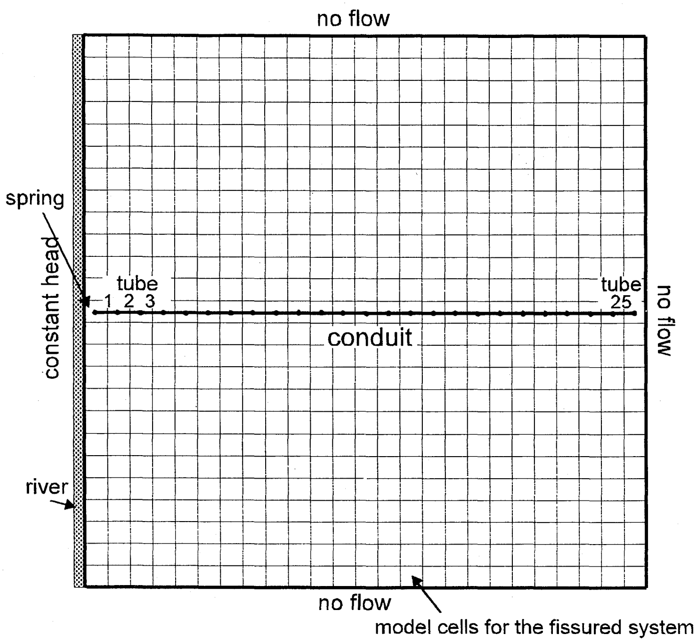

Fig. 3 Model domain and geometry of the conduit.

at the spring. Therefore this tube will be the first one to experience a "breakthrough", i.e. first order dissolution prevails throughout the tube. After this breakthrough the flow increases rapidly and changes from laminar to turbulent flow conditions and consequently dissolution rates are increased considerably which leads to larger conduit diameters. Therefore the hydraulic gradient in tube number 1 decreases. The position of the largest gradient propagates from the spring in an upgradient direction and the conduit is beginning to drain a considerable portion of the catchment (Fig. 4(c) and (d)). The temporal and spatial development of the conduit radius is illustrated in Fig. 5.

DISCUSSION

Our model results generally show that conduit enlargement starts at the spring and propagates upgradient direction. This type of karst development process has been described by Mandel (1966) based on field observations. From the analysis of equipotential maps Rhoades & Sinacori (1941) also concluded that the karstification is initiated at the spring. Theoretical results by Howard (1964) as well as laboratory experiments (Ewers & Quinlan, 1981) show the same effect.

One-dimensional simulations of conduit development by Dreybrodt (1990), Palmer (1991) and Groves & Howard (1994a) use fixed-head boundaries. These models can be applied to model karstification as a result of allogenic recharge (i.e. sinking streams) and to predict the enlargement of conduits below hydraulic structures such as dams. In our model, heads are calculated based on the hydraulic parameters of the growing conduit

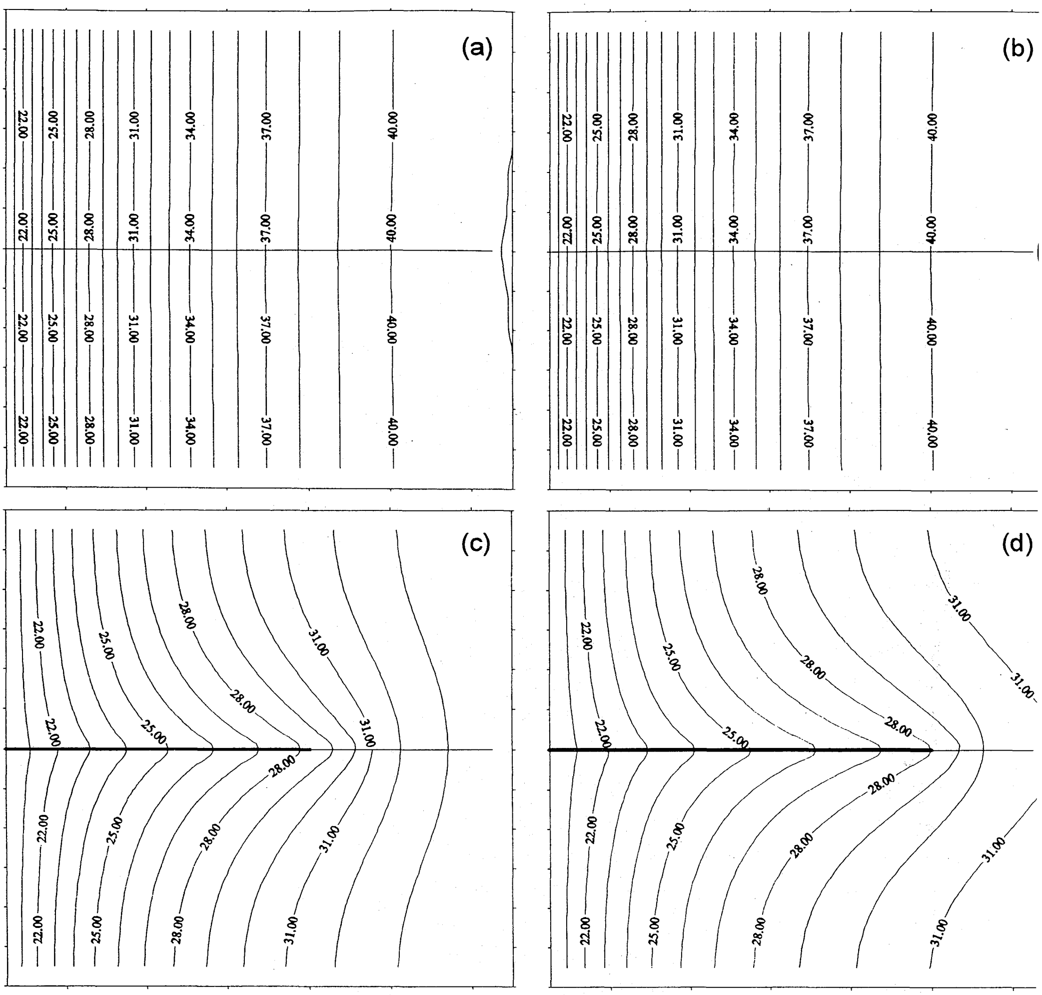

Fig. 4 (a) Model domain and equipotential lines in the fissured system after 500 years; (b) equipotential lines after 2000 years; (c) after 300 years the conduit creates its own catchment area; (d) situation after 4000 years, the conduit has developed farther upgradient.

network, the spatial and temporal variation of groundwater recharge and also on the hydraulic interaction between conduit network and fissured system. This allows more general and more realistic simulations of the flow field in natural karst catchments. Additionally, CAVE takes into account the different effects of direct conduit recharge and water derived from the fissured system on the enlargement of the conduits. While an increase in direct recharge generally leads to an acceleration in the karstification process, the influence of the slightly undersaturated water from the fissured system can be less easily understood. Depending on the fraction of direct conduit recharge, the flow within the conduit and the degree of undersaturation of the conduit water, the water from the fissured system can either lead to an acceleration or a slowing down of conduit enlargement.

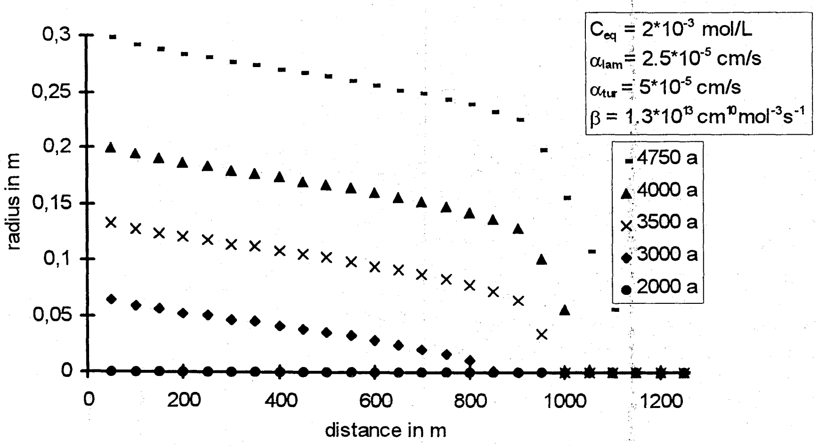

Fig. 5 Development of the radius of the conduit as a function of distance.

Future work will concentrate on sensitivity analyses in order to identify the factors controlling the genesis of karst systems. It is planned to apply the model to natural catchments. In order to gain confidence in our model predictions, the modelled and the natural karst system will be compared based on the characteristics of spring discharge hydrographs.

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