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Modelling of karst genesis at the catchment scale – influence of spatially variable hydraulic conductivity

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ABSTRACT:

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The aim of this work is to study the genesis of karst aquifers at the catchment scale. Especially the influence of different boundary conditions and geological setting is investigated in several scenarios. A hybrid continuum-discrete flow model is used for the modelling of conduit development. Effects of heterogeneity in hydraulic conductivity and in fracture spacing are examined in four scenarios. For homogeneous conditions a shallow water-table cave develops. If an area of reduced hydraulic conductivity is introduced, the conduit system evolves around this area and a deep phreatic cave is formed. This is true only, if the contrast in hydraulic conductivity is large enough. If an area of higher fracture density is introduced, this area is more intensely karstified, and a local system of deep karstification develops.

Key words: Genesis Modelling, Karst, Hydraulic conductivity.

INTRODUCTION

The permeability of karst aquifers increases during their exposure to circulating water, undersaturated with respect to calcite. The water enlarges the fractures in the soluble rock and leads to the development of karst conduits. The evolution of karst aquifers depends on a variety of processes and geological as well as climatic boundary conditions. The most important of these are summarised schematically in Text-fig. 1. Karst aquifers exhibit a dualistic flow system (KIRALY 1998), consisting of a fissured or matrix system, which represents the mass of permeable fractured limestone, and a conduit system summarising the karst tube network. The latter is characterised by a high hydraulic conductivity and low storage, while the fissured system is characterised by low hydraulic conductivity and high storage. Exchange between the two systems is controlled by differences in hydraulic head. Geological and climatic factors influence the evolution of a karst aquifer, i.e. geometry, fracture density, lithology as well as temperature, recharge and partial pressure of CO_2. Karst aquifer evolution is also influenced by the development of the landscape, i.e. altitude of the river as base level and relief.

A number of numerical models have been developed to study karst aquifer genesis. This became possible after the quantification of calcite dissolution kinetics (PLUMMER & *al.* 1978, BUHMANN & DREYBRODT 1985a, 1985b). Initially single fracture models with simple boundary conditions (DREYBRODT 1990, PALMER 1991) were employed. Subsequently, two-dimensional models, capable of simulating the development of a conduit network, were developed by GROVES & HOWARD 1994a, 1994b; DREYBRODT 1996, CLEMENS & *al.* 1996 and KAUFMANN & BRAUN 1999).

The depth of development of cave systems under the water table has been studied intensively in karst

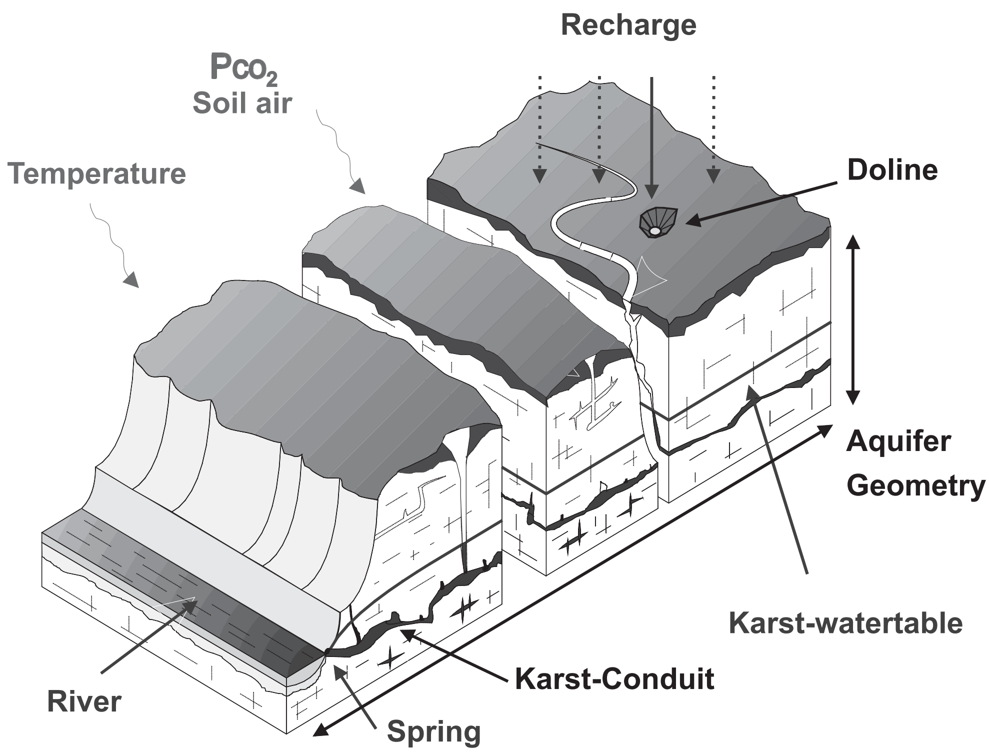

Fig. 1. Major factors influencing the genesis of a karst aquifer (schematically): geological conditions and climatic parameters

literature. In some theories of cave development (MARTEL 1921) it was argued that caves developed in the vadose zone, due to highest solutional capacity of the recharge water there (vadose theory). DAVIES (1930) concluded from field observation, that caves develop at random depth below the water table, and suggested a model, where caves follow the curving stream tubes of a Darcy flow net. SWINNERTON (1932) suggested a water table model of cave development, in which the fastest route determines the position of the cave developing. FORD & EWERS (1978) explained the development of both deep phreatic caves and shallow water table caves in their four-state model. The main factor determining the type of cave developing in their model is fissure frequency. A high fissure frequency leads to a water table cave, while deep phreatic caves develop at low fissure frequencies, when no alternative routes near the water table are present.

This paper uses a numerical karst genesis model to study conditions for deep phreatic karstification. The effect of hydraulic heterogeneity is studied using scenarios with varying fracture density, as motivated by the work of FORD & EWERS (1978), as well as different initial conduit diameters.

MODELLING APPROACH

In order to model the characteristic flow patterns of karst aquifers, the dualistic structure of the flow system has to be considered (Text-fig. 2). Conceptually, the flow system of a karst aquifer consists of a conduit system, which is characterised by low storage and high hydraulic conductivity, and a fissured system with high storage and a much lower conductivity. Karst genesis models also have to consider calcium transport in the conduits, dissolution of calcium from the conduit walls and thus enlargement of the conduits. These processes have been implemented in the model CAVE (CLEMENS & *al.* 1996) by coupling the discrete continuum flow calculation to a carbonate dissolution model.

Groundwater flow in the fissured system is described by a continuum approach using Boussinesq's equation:

$$\vec{\nabla}(K\vec{\nabla}h_M) + R_M + \Gamma = S\frac{\partial h_M}{\partial t} \qquad (1)$$

where K is the tensor of hydraulic conductivity, h_M is the piezometric head in the fissured system, R_M is recharge to the fissured system, Γ is the exchange flux between the fissured system and the conduit system, S is the storage coefficient in the fissured system and t is time (Text-fig. 3).

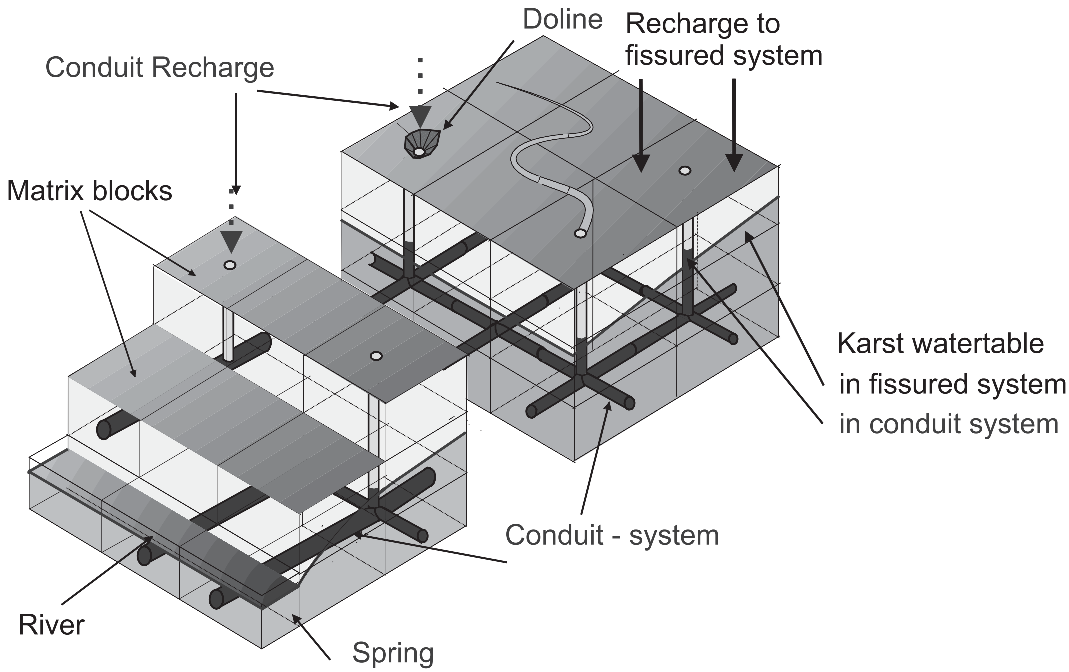

Fig. 2. Schematic representation of the hydraulic aspects of the dualistic model concept of a karst aquifer; a typical spring catchment and its representation in the numerical model CAVE is depicted

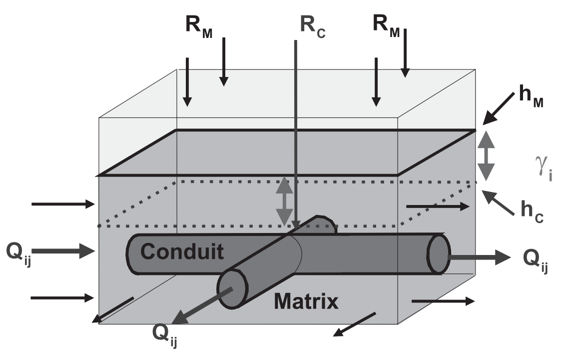

Fig. 3. Hydraulics of CAVE represented at one balance volume containing a conduit node embedded in a block of the fissured system. R_M and R_C are recharge to the fissured and conduit system, h_M and h_C are heads in the fissured and the conduit system, Q_{ij} are the flow rates to the adjacent nodes and γ_i is the exchange flow rate

Flow in the conduit system, which is assumed to be fully phreatic all the time and to be represented by cylindrical tubes intersecting at nodes, is governed by Kirchhoff's rule, stating that total inflow and total outflow balance at each node. For each node i therefore:

$$\Sigma Q_{ij} + R_{C,i} + \gamma_i = 0 \qquad (2)$$

where Q_{ij} is the flow rate between node i and node j, $R_{C,i}$ is recharge to node i of the conduit system and γ_i is the volumetric exchange rate between the conduit system and the fissured system at node i. No storage is assumed for the conduit system. Q_{ij} is calculated according to the flow condition. In case of laminar flow the Hagen-Poiseuille formula is applied, while in the case of turbulent flow the Colebrook-White equation is used.

Exchange of ground water between the fissured and the conduit system is modelled by a linear steady-state exchange term (BARENBLATT & *al.* 1960), i.e. the water flux is assumed to be proportional to the head difference between the flow systems:

$$\gamma_i = \alpha_i(h_{M,i} - h_{C,i}) \qquad (3)$$

The proportionality factor α_i is termed the exchange coefficient, while $h_{M,i}$ and $h_{C,i}$ are the hydraulic heads of the fissured and the conduit system at node i, respectively. Estimates on the parameter α_i can be found in BAUER & *al.* (1999).

Transport of calcium ions in the conduit system is described by the 1D advection equation, with an additional source term accounting for the increase in concentration due to calcium dissolution at the conduit walls (Text-fig. 4):

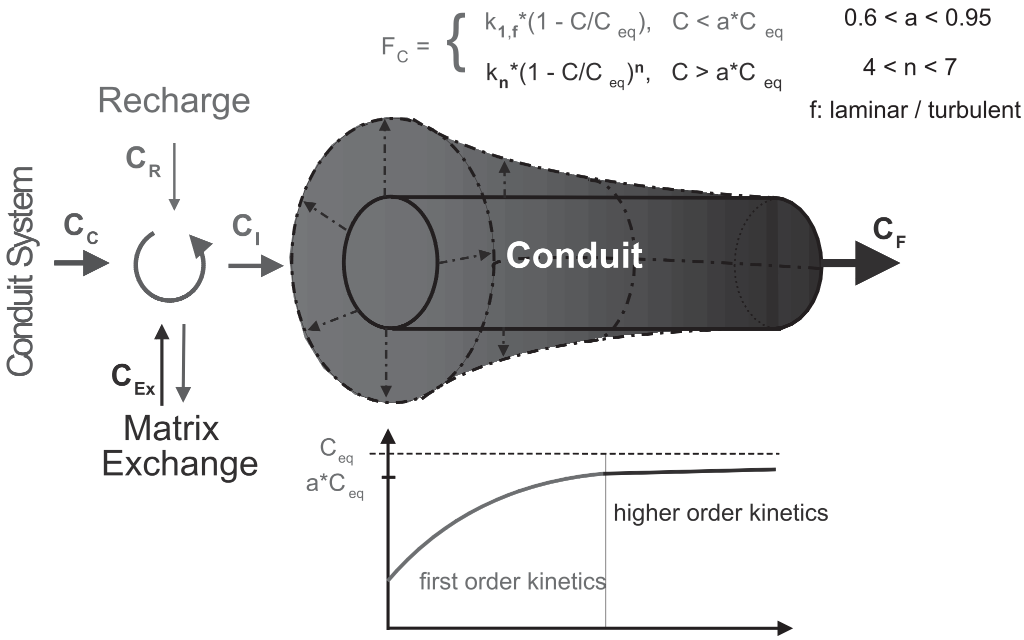

Fig. 4. Chemistry of CAVE demonstrated at one node and tube. Water coming from recharge, the upstream conduit system and the fissured system with the corresponding concentrations C_R, C_C and C_{Ex} is mixed instantaneously and given to a conduit tube with initial concentration C_I. A possible concentration profile along the tube is depicted as well, with $a*C_{eq}$ the switching concentration from first to higher order kinetics

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + F \qquad (4)$$

C is the concentration of Ca^{2+}, u is the flow velocity along a pipe and F is the dissolution rate of calcite. At the nodes of the conduit system additional inflow of calcium ions from the fissured system and from recharge is considered and instantaneous and complete mixing of all inflowing concentrations is assumed.

Modelling of carbonate dissolution is based on experimental findings by BUHMANN & DREYBRODT (1985a,b), which show that dissolution kinetics is fast if the calcium concentration is far from saturation with respect to calcite (first order kinetics) and slow if the concentration is close to saturation (higher order kinetics). The dissolution rate F is given by:

$$F = k_1 (C_{eq} - C), \quad C < C_s$$
$$F = k_n (C_{eq} - C)^n, \quad C \geq C_s \qquad (5)$$

where C_{eq} is the calcium equilibrium concentration, n is the reaction order, k_1 is the rate constant for first-order and k_n for higher-order dissolution. C_s is the switching concentration, at which dissolution rates switch from lower to higher order kinetics. Different values of k_1 apply for laminar and turbulent flow conditions, because the diffusion of species into the solution has to be accounted for in the case of laminar flow. The amount of carbonate mass dissolved from the conduit walls is used to determine the increase of conduit diameter with time. Flow in the fissured system is simulated by central finite differences using MODFLOW (MCDONALD & HARBAUGH 1988). Flow in the conduit system is solved utilising the iterative Newton-Raphson method in order to deal with the non-linearities occurring for turbulent flow conditions. Transport of calcium in the tubes is modelled by employing an upwind-finite difference scheme with integrated reaction kinetics. The model supports a wide variety of boundary conditions, thus enabling a good approximation of natural situations. For more details and model verification see CLEMENS & *al*. (1996).

MODEL DOMAIN AND SCENARIOS

A small catchment was chosen to study the effects of spatially varying hydraulic conductivities on the karstification process. Text-fig. 5a depicts a vertical cross section of this small catchment, with a water divide to the left and a river to the right. In a unit of uniform limestone there is a region of different conductivity, which is not penetrating the full depth of the limestone and is not connected to the river or the water divide. The limestone is assumed to overly a less permeable and insoluble formation, e.g. a clay layer. The region of different

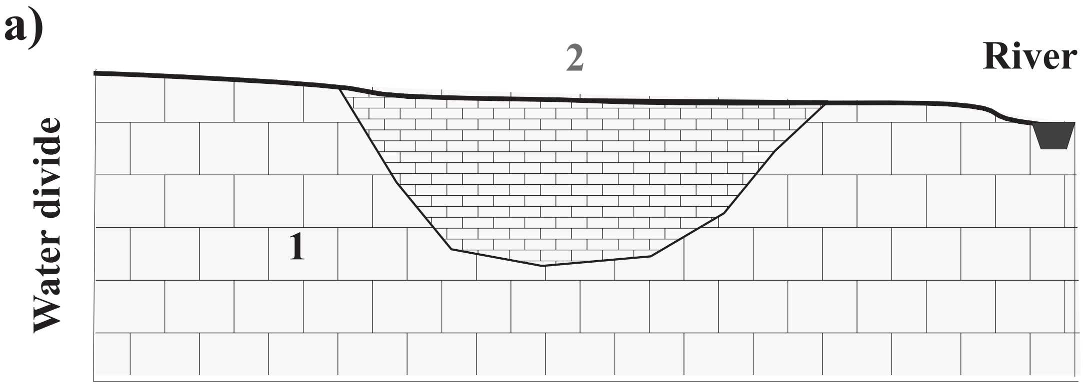

Fig. 5. a – Vertical cross section through a small catchment area; the river is to the right, a water divide to the left and in the middle a region of different hydraulic conductivity, marked as region 2, is embedded in the limestone (region 1); flow direction is from left to right; b – Model scenario used for the simulations with the initial conduit network and the two regions marked as 1 and 2

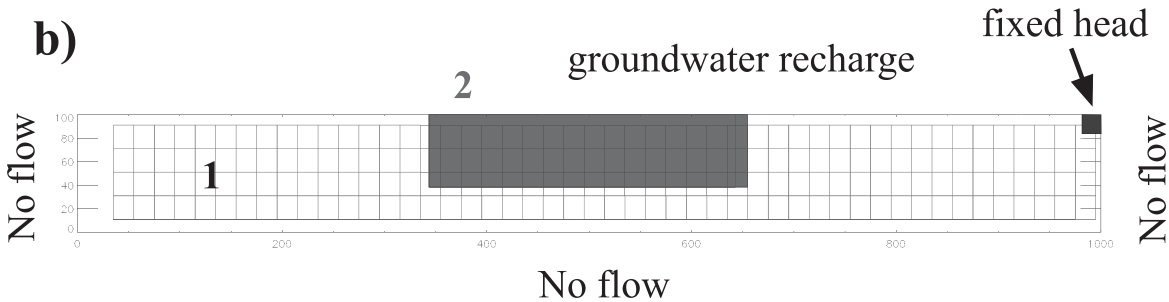

Fig. 5. b – Model scenario used for the simulations with the initial conduit network and the two regions marked as 1 and 2

conductivity is assumed to have different conductivities in the fissured as well as the conduit system compared to the limestone. The chemical composition is assumed to be the same as for the limestone, so that dissolution chemistry is the same in both regions and only differences in the hydraulics are active during the modelling.

The model scenario used for the numerical investigation of the influence of heterogeneity in conductivity is depicted in Text-fig. 5b. Only a vertical cross-section through the three-dimensional model domain is shown, containing one plane of solutionally enlargeable conduits. The model domain is 1000 m long, 1000 m wide and 100 m thick. Boundary conditions are no-flow boundaries (Q=0) at all sides and the bottom of the model domain. The river is represented by a constant head boundary condition on the right and recharge (fixed flow boundary condition) is applied to the top. The conduit system has equal spacing of 20 m between the nodes and is directly connected to the river. The hydraulic conductivity of the fissured system is assumed to be 10^{-6} ms^{-1} and the aquifer is considered as confined. River head is fixed to 100 m. The exchange coefficient is set to 10^{-6} m^2s^{-1}. Groundwater recharge is 0.3 m a^{-1}, of which 1% is entered directly into the conduit system at the uppermost nodes. Initial conduit diameter is $5*10^{-4}$ m.

Calcium equilibrium concentration is 2 mol m^{-3}. Water entering the conduit network by recharge has a calcium concentration of 0 mol m^{-3}, while water entering the conduit system from the fissured system by exchange flow has equilibrium calcium concentration. The fast first order kinetic rate constants for laminar and turbulent flow are $2.5*10^{-7}$ m s^{-1} and $5*10^{-7}$ m s^{-1} respectively. The kinetic rate constant for the higher order dissolution, where a slow fourth order dissolution is assumed and which is active if calcium concentrations are above 90 % of the equilibrium concentration, is $1.3*10^{-23}$ m^{10} mol^{-3} s^{-1} for both laminar and turbulent flow conditions.

The following scenarios are considered:

- Scenario 1 without heterogeneity. Region 2 has the same parameters as region one.
- Scenario 2 with lower hydraulic conductivity in region 2. In region 2 the initial tube diameters are reduced to $1*10^{-4}$ m, groundwater recharge is reduced to 0.03 m a^{-1}, because increased runoff is assumed, the hydraulic conductivity of the fissured system is reduced to 10^{-7} m s^{-1} and the exchange coefficient is reduced to 10^{-7} m^2 s^{-1}.

- Scenario 3 with a third of the fracture density in region 2 as compared to Scenario 1. Initial conduit diameters are set to $5*10^{-4}$ m, all other parameters are the same as in Scenario 2.
- Scenario 4 with half the fracture density in region 1 as compared to Scenario 1, but all other parameters the same as in Scenario 1.

Scenario 1 is the homogeneous case, when no spatially varying hydraulic conductivities are present. In Scenario 2, the lower hydraulic conductivity of the conduit network in region 2 has been implemented by reducing the initial conduit diameters, while in Scenario 3 it has been modeled by reducing the fracture density. This scenario could represent the case of a marl bed, where region 2 represents a bed of less conductive marls in a limestone massive. In contrast to Scenarios 2 and 3, Scenario 4 has a higher hydraulic conductivity in region 2 as compared to region 1, since the fracture density is higher there. Thus there is a region of higher hydraulic conductivity embedded in a less conductive rock. This scenario could represent a riff facies (region 2) which is surrounded by marly limestone. Both scenarios are typical for the Swabian Alb in Southwest Germany.

SIMULATION RESULTS

Text-fig. 6 shows the development of the conduit system with time for Scenario 1 for 1600 a, 3600 a and 20000 a. Widening of the conduit system begins at the river to the right and is propagating back upgradient into the catchment area, because near the river the gradients are highest and thus flow rates are largest. After the conduits near the river have been widened, the location of the largest hydraulic gradient is shifted upgradient from the river and, as a result, highest dissolution is then active there. Only the uppermost layer of the conduit system is widened, because here the highest gradients are observed and, due to the direct recharge to the conduit system, the water is most aggressive there. After 3600 a conduits 800 m upgradient from the river have been widened. Conduits near the river are widened more rapidly, as more water is flowing here, which is added at each node in the uppermost layer by direct recharge. This effect can still be seen after 20000 a, when maximum diameters are about 0.5 m in the conduits near the river.

Text-fig. 7 depicts the development of the conduit system with time for Scenario 2. Conduit development starts at the river and is propagating upgradient into the catchment, until the region of lower hydraulic conductivity is encountered and the back propagation is stopped. After 10000 a, conduits in the left part of the catchment have been widened. Enlargement starts at the recharge locations, where aggressive water is entered into the conduit system, and development is directed towards the river. Since the hydraulic conductivity in region 2 is reduced, the water is flowing around region 2, because this is now the pathway of least flow resistance. Thus, conduits beneath region 2 are widened (15000 a). After 20000 a this pathway evolving under region 2 is joined and drainage of the catchment area is exclusively through this pathway. A deep

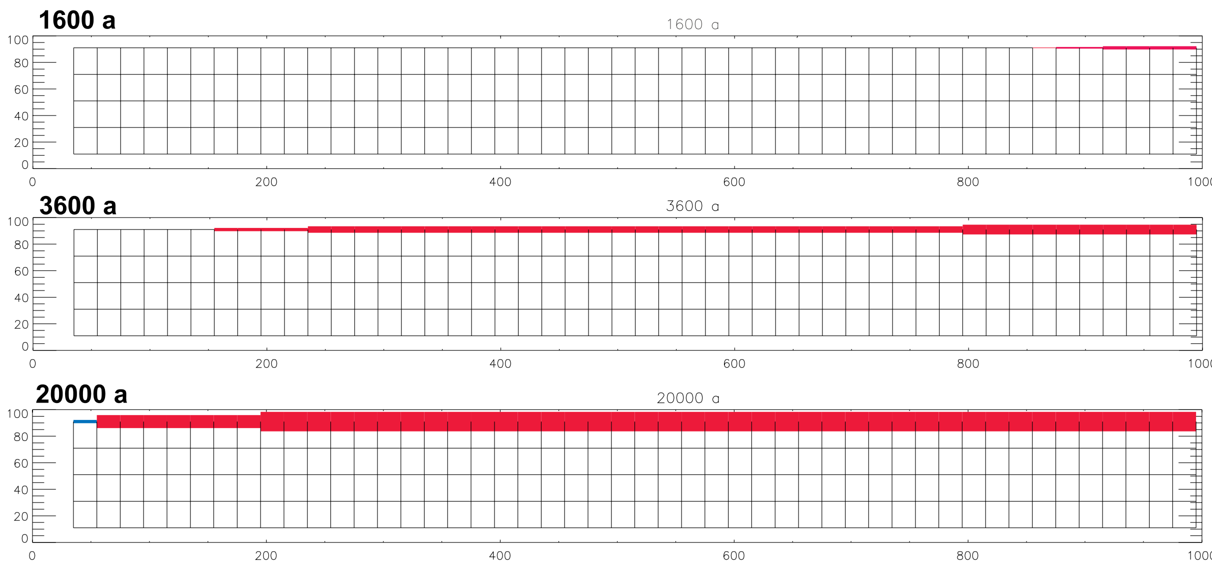

Fig. 6. Model results for Scenario 1, depicting the conduit network after 1600 a, 3600 a and 20000 a, respectively. Line thicknesses represent conduit diameters of >0.0005 m, >0.005 m, >0.01 m, >0.1 m, >0.2 m and >0.3 m, respectively. A shallow watertable cave develops

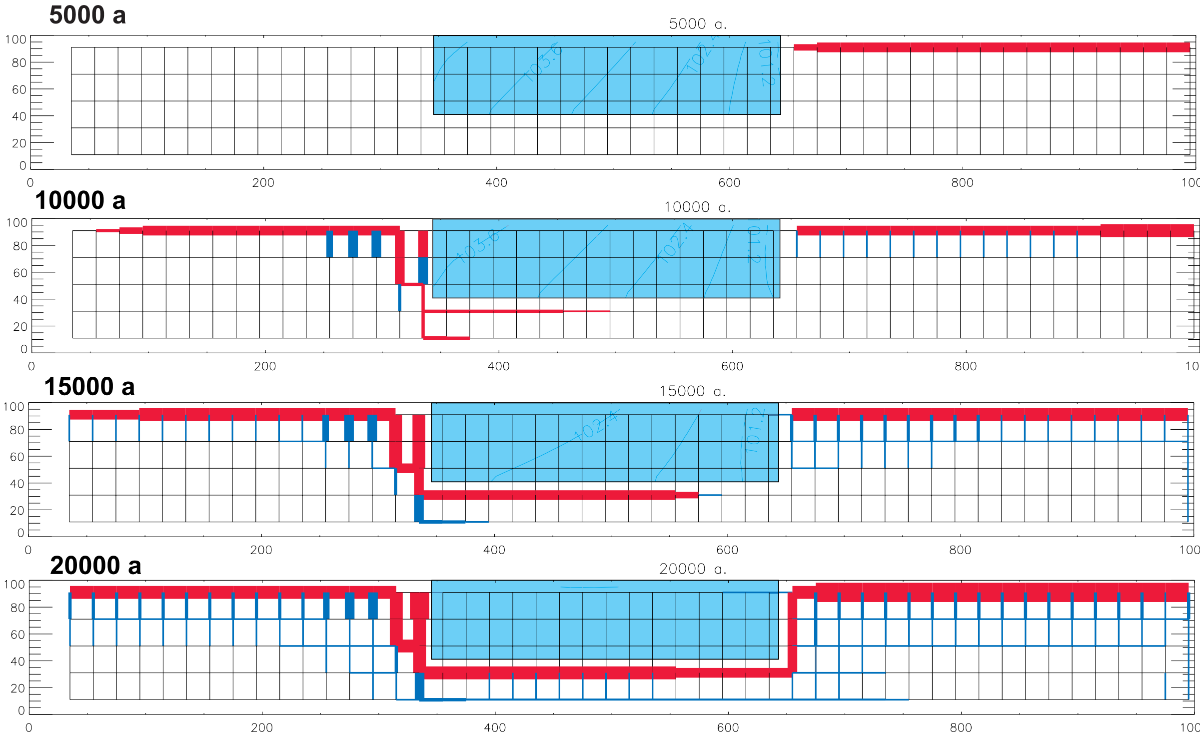

Fig. 7. Model results for Scenario 2. Around the zone of reduced hydraulic conductivity a deep phreatic cave evolves; for legend see Fig. 6

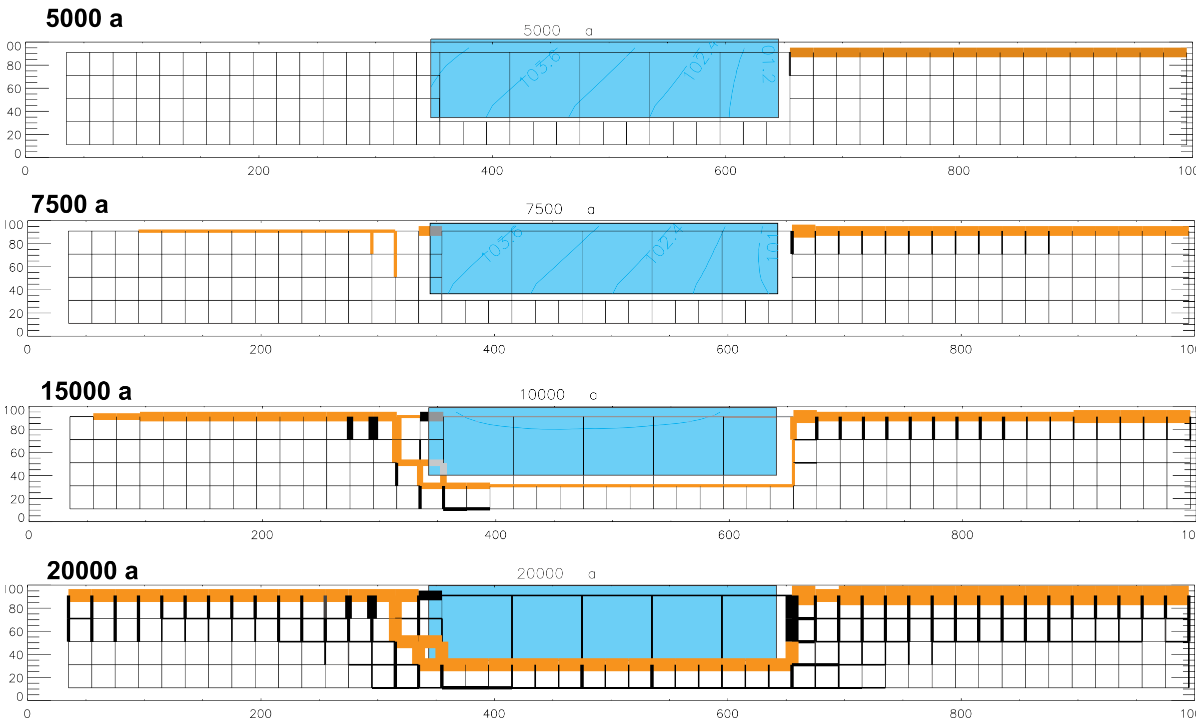

Fig. 8. Model results for Scenario 3. Deep karstification is initiated around the region of lower fracture density and thus hydraulic conductivity; for legend see Fig. 6

phreatic cave has developed. Upgradient of the area of reduced hydraulic conductivity, a number of vertical conduits are widened to some extent. Widening of these conduits stopped, when the passage under region 2 was completed, because then all flow from the upstream part of the catchment was channelled

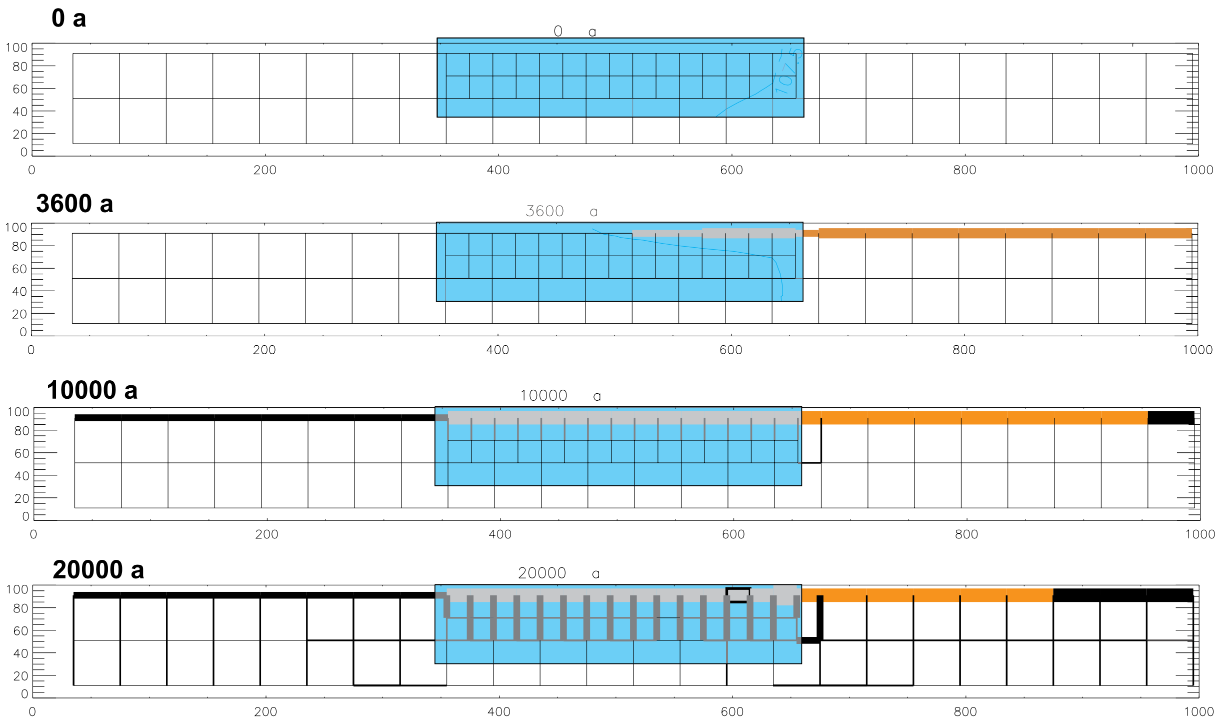

Fig. 9. Model results for Scenario 4. Now region 2 has the higher hydraulic conductivity than region 1; deep karstification is initiated in the region of higher fracture density (region 2); for legend see Fig. 6

through this single pathway and flow in all other conduits decreased. After 20000 a, maximum conduit diameters are 0.33 m near the river, while the conduits in region 2 have been widened to about $2*10^{-3}$ m of diameter only.

Text-fig. 8 shows the conduit development for Scenario 3. Here the lower hydraulic conductivity of the conduit network in region 2 is represented by reducing the density of conduits to a third. Conduit development is very similar to Scenario 2, again a deep phreatic cave develops under region 2. As in Scenario 2, a number of vertical conduits started to develop upgradient of the region of low conductivity. In contrast to Scenario 2, now conduits in the region of reduced hydraulic conductivity are widened noticeably (15000 a), until the passage beneath region 2 is joined and all flow is channelled through this deep phreatic loop. Conduit diameters after 20000 a are 0.33 m near the river, while the conduits in region 2 have diameters of about 0.01 m.

Text-fig. 9 depicts the development of the conduit system with time for Scenario 4. Now region 2 is the region of higher hydraulic conductivity, since fracture density is twice as high as in region 1. Widening of the conduits again begins at the river and propagates upgradient into the catchment area. Region 2 now is not an obstacle to conduit development anymore, and thus a water table cave develops as in Scenario 1. In the region of higher fracture density, all vertical conduits have been widened, and thus deep phreatic karstification is initiated there. Since these conduits are not connected to the river via a high-conductivity flow path other than the one at the water table, no deep phreatic cave is developed close to the river, but rather all loops are completed in the region of higher fracture density. Conduit diameters after 20000 a are again about 0.33 m near the river, while the conduits in region 2 have diameters between 0.001 m and 0.002 m.

DISCUSSION AND CONCLUSIONS

Model results indicate that deep karstification depends on the hydraulic conductivity ratio between a less permeable region (region 2) and a background value (region 1), For instance, if the initial diameters of the conduits in region 2 in Scenario 2 were larger (> $2*10^{-4}$ m), no deep phreatic loop would develop, because of the higher hydraulic conductivity the flow path in the uppermost conduit layer across region 2 would be the preferred route rather than the one below region 2. Thus conduit development would occur near the watertable, like in Scenario 1. If likewise in Scenario 3 the fracture density of region 2 would only be reduced to half the density of region 1, again a shallow watertable cave would develop. In the scenarios presented here, the values of the initial diameter in Scenario 2 and of the fracture density in Scenario 3 where chosen to initiate deep karstification. These values therefore give minimum contrast values of the hydraulic conductivity between region 1 and region 2, at which deep karstification is initiated. These threshold values are of course dependent on the geometry, which affects the hydraulic gradient, and the other parameters, e.g. geochemical properties of the limestone. For the model scenario chosen, it is necessary to reduce either the fracture spacing to one third (Scenario 3) or to reduce the initial diameters to one fifth (Scenario 2), together with reducing the conductivity of the fissured system and recharge by a factor of ten, to initiate deep karstification around the region of lower hydraulic conductivity.

Our model results are in accordance with the findings of FORD & EWERS (1978). If fracture density is reduced sufficiently, as in Scenario 3, a deep phreatic cave develops, as stated by their four-state model. In addition to their work, deep karstification is also possible, if the fracture density is the same everywhere, but if initial diameters of the fractures are sufficiently small to divert water to greater depth. It could thus be shown that not the pure existence of fractures but rather their conductivity determines the type of karstification.

The results of Scenario 4 indicate, that enhanced deep karstification is also possible, if fracture density is locally increased. A region of higher fracture density, which is not connected directly to a river or a spring, can be karstified to greater depth than the surrounding rocks. This is due to the higher initial conductivity, which allows for easier circulation of water to greater depths in this area and thus slowly widens the vertical conduits. As can be seen from Text-fig. 9, widening of these conduits is much slower and less intense than the development of the watertable cave, and begins after about 10000 model years. This seems to contradict the findings of FORD & EWERS (1978), but they only investigated homogeneous rocks in their four-state model, while heterogeneity is included in the scenarios studied here.

Summing up it may be concluded that cave development is strongly determined by fracture density as well as conductivity of the fractures and the spatial variability of the hydraulic conductivity. Different types of caves may evolve according to the specified initial distribution of these hydraulic properties.

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