Characterisation of gypsum karst aquifers by heat and mass transport simulations using a pipe flow model

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Abstract A modelling tool is presented, which is designed to support the characterisation of the conduit system of gypsum karst aquifers by simulating short-term fluctuations of gypsum concentrations and temperatures of the spring water. Both parameters depend on the geometric and hydraulic properties of the conduit system. If only one of them is analysed, a unique identification of the structure of the conduit system may not always be obtained. Unsteady-state simulations of both heat and mass transport, however, show that different conduit systems, which are equivalent with respect to spring signals of one parameter, can be distinguished by taking into account the second parameter.

Introduction

The concept of analysing spring data (ASHTON, 1966) has been shown to be useful in the characterisation of flow and transport properties of carbonate aquifers by, e.g., ATKINSON (1977) and SAUTER (1992) who estimated the volumes of conduit water by evaluating the time lag between the increase in flow and the change in hydrochemical parameters at a spring after a flood. In addition, the amplitude of chemical variations at the spring provides information about the conduit system. Based on concentration data and numerical model simulations GRASSO (1998) proposed a relationship between the geometric properties of conduits and the variations of calcium concentrations measured at karst springs. SAUTER (1992) and BENDERITTER et al. (1993) obtained quantitative information about aquifer properties by analysing spring water temperatures. Moreover, numerical simulations of heat transport showed that under unsteady flow conditions temperature signals at a spring can be used to identify conduits of different geometry even if the total conduit volume is identical (HÜCKINGHAUS et al., 1997; LIEDL et al., 1998). It is therefore reasonable to assume that variations of both, hydrochemical parameters and water temperature measured at a spring, can be used to improve the characterisation of karst aquifer properties.

This idea is transferred from carbonate to gypsum aquifers in the paper. A process-based numerical modelling tool was developed to simulate both heat and mass transport in gypsum karst and, as a consequence, to investigate in how far spring water signals can be interpreted in terms of physical parameters and whether this combined approach can reduce the ambiguity in the interpretation. Some first results are presented here, where flow is assumed to be strongly focused to the conduit system.

Modelling approach

The heterogeneity of a karst aquifer can be conceptualised as a dual flow system, i.e. groundwater flow can be divided into diffuse flow in the mass of the fractured rock and localised flow in conduits (ATKINSON 1977). The numerical model presented here is a special case of the karst genesis model CAVE (Carbonate Aquifer Void Evolution). Within CAVE (e.g., CLEMENS et al., 1996) the diffuse flow in the fissured system of the rock is modelled by the continuum flow model MODFLOW-96 (HARBAUGH & M^{C}DONALD, 1996), whereas the localised flow in the conduit system is modelled by a discrete pipe network. In the following, the model is applied to simulate short-term fluctuations of gypsum concentrations and temperatures at gypsum karst springs. As a first approximation, water flow in the fissured system is neglected, thus focusing on the characterisation of the conduit system. For this purpose, CAVE was extended by two transport modules for simulating reactive mass and heat transport.

The reactive mass transport module simulates advective transport of dissolved gypsum in the pipe network. The concentration of the inflow water to each pipe is obtained by assuming an instantaneous mixing of water at the intersections. In order to account for the increase in mass by dissolution of gypsum, the advection equation is expanded by a source term. JAMES & LUPTON (1978) showed experimentally that the dissolution of gypsum obeys a first-order rate law. Since their experiments revealed a dependence of the rate constant on flow velocity, it was concluded that the dissolution process is mainly governed by diffusion of dissociated ions across a boundary layer (Fig. 1).

Heat transfer between the pipe wall and conduit water is analogous to the mass transfer model (BEEK & MUTTZALL, 1975). The equation of heat convection in the pipe is expanded by a source term describing heat transfer across the thermal boundary layer at the pipe wall (Fig. 1). However, in gypsum karst an important difference between mass and heat transfer exists: Gypsum concentration at the rock surface equals the equilibrium solute concentration and thus is constant during the diffusion-controlled dissolution process. Heat transfer between rock and conduit water, however, is

controlled by heat conduction in the rock rather than by heat transfer across the thermal boundary layer (Fig. 1), i.e. the temperature at the rock surface will be successively approach the water temperature. Therefore, the heat transport model has to account for conduction around the conduits to simulate the time-dependent temperature at the rock surface. The temperature of the water entering a pipe is calculated via instantaneous mixing at intersections.

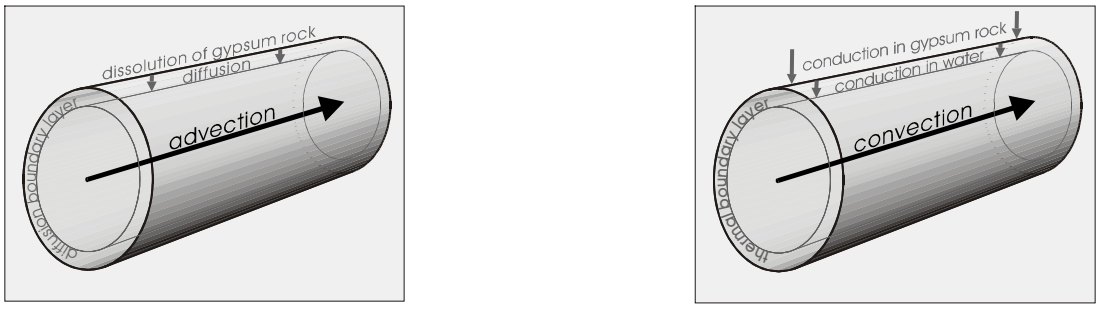

Fig. 1: Mass transfer (left) and heat transport processes (right) in gypsum karst conduits

Model scenarios and results

In a first scenario (scenario 1) temperatures and concentrations of spring water emerging from a single conduit of 1200 m length are compared with spring signals resulting from heat and mass transport in a pipe network (Fig. 2). Both conduit systems consist of 24 pipes with identical diameters (0.2 m) and lengths (50 m). Thus, the volume of the conduit system and the surface area of rock exposed to conduit water is equal in both cases. Moreover, the pipe network is arranged such that the residence time of water is the same in both systems provided the total recharge, which is applied to only one point of the single conduit, is distributed equally on the eight inlets of the pipe network.

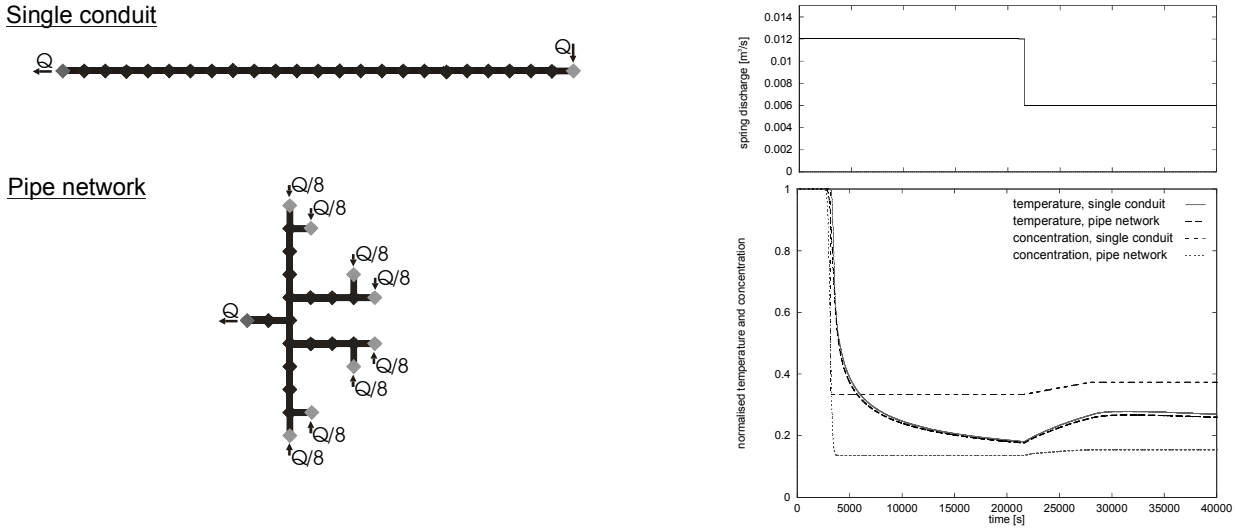

Fig. 2: Conduit systems for scenario 1 (left) and corresponding temperature and concentration BTCs (right)

The total recharge amounts to 0.012 $m^3 s^{-1}$ during the first six hours and 0.006 $m^3 s^{-1}$ after 21600 s, i.e. each inlet of the pipe network is supplied with 0.0015 $m^3 s^{-1}$ and 0.00075 $m^3 s^{-1}$, respectively. As an initial condition, the water in the conduit is assumed to be in hydrochemical and thermal equilibrium with the surrounding rock. Recharge water entering the upstream pipes, however, is less mineralised and colder (see model parameters in Tab. 1).

Fig. 2 shows that the normalised water temperature at the spring is virtually the same for the single conduit and the pipe network. At a flow rate of 0.012 $m^3 s^{-1}$ the water takes about 52 min (3142 s) to flow from the inlet to the spring. After that time the water temperature decreases due to the permanent cooling of the rock as long as the flow rate remains constant. When the flow rate is decreased to 0.006 $m^3 s^{-1}$ the temperature increases during a certain transition period as a result of the enlarged residence time of water in the conduits. The cooling of the rock eventually causes the water temperature to decrease again. LIEDL et al. (1998) showed by model simulations of heat transport in fractures, that

temperature signals in fractures of different geometry can be the same under steady-state flow conditions, but differ during the transition period. These authors concluded that unsteady flow conditions are required for the characterisation of karst conduit geometry by heat transfer analysis. In their simulations the conduit systems consisted of fractures of varying geometry, which were arranged in different sequences. In scenario 1, however, all individual pipes are of identical geometry and the temperature signals of the two conduit systems are nearly identical even during the transition period. Thus, the different conduit structures cannot be distinguished by analysing spring water temperatures only. We will look therefore at the second parameter, i.e. the gypsum concentration of water emerging at the spring.

Tab. 1: Model parameters used in scenarios 1 and 2

Equilibrium concentration of gypsum in water	15 mol m^{-3}	Diffusion coefficient of dissociated gypsum in water	$6 \cdot 10^{-10}$ m^2 s^{-1}
Initial concentration of gypsum in conduit water	15 mol m^{-3}	Concentration of gypsum in recharge water	0 mol m^{-3}
Specific heat of water	4.198 J kg^{-1} K^{-1}	Thermal conductivity of water	0.582 W m^{-1} K^{-1}
Initial temperature of conduit water	281.15 K	Density of water	999.9432 kg m^{-3}
Initial temperature of gypsum rock	281.15 K	Specific heat of gypsum rock	1088 J kg^{-1} K^{-1}
Temperature of recharge water	279.15 K	Thermal conductivity of gypsum rock	1.297 W m^{-1} K^{-1}
Kinematic viscosity of water	$1.472 \cdot 10^{-6}$ m^2 s^{-1}	Density of gypsum rock	2320 kg m^{-3}

Although the gypsum concentration basically exhibits a similar behaviour in either case, the values obtained for the single conduit are higher than for the network (Fig. 2). When recharge water appears at the spring, gypsum concentration drops below saturation and temporarily reaches normalised values of 0.33 and 0.14 at the outlets of the single conduit and the network, resp. The concentration increases during a transition period, which is initiated by the change in flow rates after 6 h (21600 s). Afterwards, the normalised concentration reaches values of 0.37 and 0.15 at the outlets of the single conduit and the network, resp. Thus, the gypsum concentration of the spring water emerging from the single conduit is clearly different from the concentration at the outlet of the network even under steady-state flow conditions, i.e. both conduit systems can be distinguished by analysing spring water concentrations.

This result reflects the different controlling processes of heat and mass transfer in a gypsum aquifer. Heat transfer from the rock is limited by heat conduction in the matrix, which does not depend on the flow conditions in the pipe. Therefore, conduit systems with identical volume, surface area and residence time of water show the same water temperature at the spring. Gypsum dissolution, however, is controlled by the velocity-dependent mass transfer across the diffusion boundary layer between pipe wall and bulk water. Therefore, if the flow conditions are not the same in two conduit systems, which are equal with respect to all other properties, the gypsum concentrations will be different at the outlets of the systems. Within the branches of the pipe network (Fig. 2) the flow rates are obviously smaller than in the pipes of the single conduit. Thus, the diffusion boundary layer is thinner in the single conduit, i.e. diffusion is faster and the gypsum concentration of the spring water is larger as compared to the network.

From the above discussion the question arises, whether a pipe network exists, which shows the same gypsum concentration at the outlet as the single conduit considered before. In fact, a close analysis of mass transfer equations reveals that it is possible to compensate for different flow rates by changing the surface area of rock (scenario 2). However, the total volumes of the two conduit systems still have to be equal. Fig. 3 shows an appropriate pipe network and the corresponding single conduit, which is the same as in scenario 1. As compared to the first scenario the pipe diameter had to be reduced and the pipe length had to be enlarged with increasing distance from the spring.

The resulting gypsum concentrations of the spring water (Fig. 3) are now the same for the two conduit systems. However, the temperatures of water emerging at the outlet of the pipe network are larger than those of the single conduit. In order to make the pipe network equivalent to the single conduit with respect to the gypsum concentration, the area of rock exposed to water had to be increased as compared to the single conduit. Under these conditions heat transfer between rock and flowing water, which is limited by heat conduction in the rock rather than by the velocity-dependent heat transfer across the thermal boundary layer, is faster in the pipe network than in the single conduit, thus accounting for larger temperatures of water emerging from the pipe network.

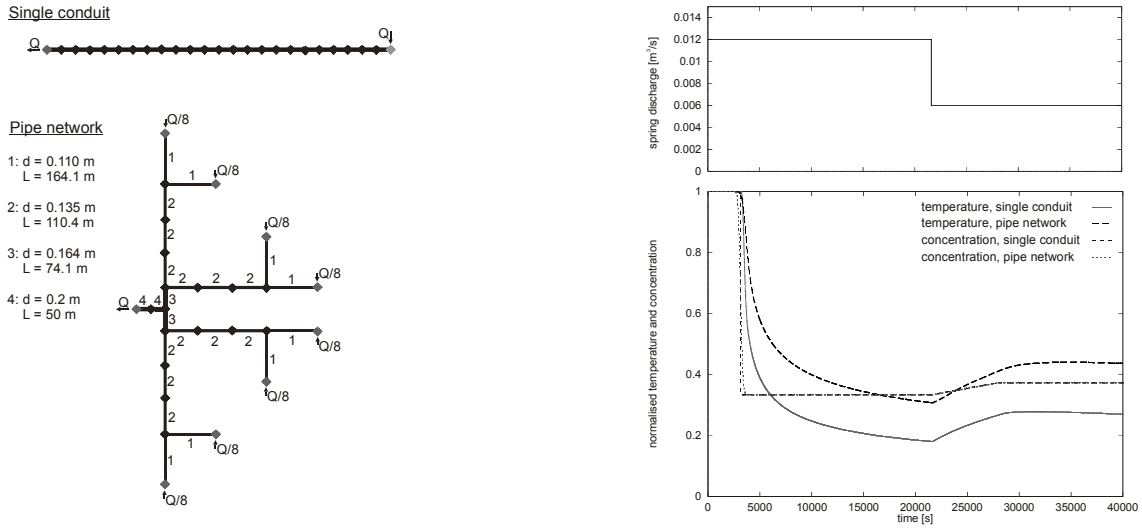

Fig. 3: Conduit systems for scenario 2 (left) and corresponding temperature and concentration BTCs (right)

Conclusions

The model simulations demonstrate that spring water emerging from conduit systems of different geometry can show either the same gypsum concentration or the same temperature. Thus, a unique identification of the structure of the conduit system is not possible by analysing only one of the two parameters. However, conduit structures, which are equivalent with respect to one parameter (e.g. temperature), can be distinguished by taking into account the second parameter (e.g. concentration). Therefore, a combined analysis of concentrations and temperatures at gypsum karst springs reduces the ambiguity contained in the information about the structure of the conduit system. Further investigations will have to address the question of how far heat and mass transport in gypsum aquifers is influenced by the hydraulic interaction between the conduit system and the fissured system and whether the concept of a combined analysis of temperature and concentration data at gypsum karst springs is applicable under field conditions.

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