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Can one identify karst conduit networks geometry and properties from hydraulic and tracer test data?

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A B S T R A C T

Karst aquifers are characterized by extreme heterogeneity due to the presence of karst conduits embedded in a fractured matrix having a much lower hydraulic conductivity. The resulting contrast in the physical properties of the system implies that the system reacts very rapidly to some changes in the boundary conditions and that numerical models are extremely sensitive to small modifications in properties or positions of the conduits. Furthermore, one major issue in all those models is that the location and size of the conduits is generally unknown. For all those reasons, estimating karst network geometry and their properties by solving an inverse problem is a particularly difficult problem.

In this paper, two numerical experiments are described. In the first one, 18,000 flow and transport simulations have been computed and used in a systematic manner to assess statistically if one can retrieve the parameters of a model (geometry and radius of the conduits, hydraulic conductivity of the conduits) from head and tracer data. When two tracer test data sets are available, the solution of the inverse problems indicate with high certainty that there are indeed two conduits and not more. The radius of the conduits are usually well identified but not the properties of the matrix. If more conduits are present in the system, but only two tracer test data sets are available, the inverse problem is still able to identify the true solution as the most probable but it also indicates that the data are insufficient to conclude with high certainty.

In the second experiment, a more complex model (including non linear flow equations in conduits) is considered. In this example, gradient-based optimization techniques are proved to be efficient for estimating the radius of the conduits and the hydraulic conductivity of the matrix in a promising and efficient manner.

These results suggest that, despite the numerical difficulties, inverse methods should be used to constrain numerical models of karstic systems using flow and transport data. They also suggest that a pragmatic approach for these complex systems could be to generate a large set of karst conduit network realizations using a pseudo-genetic approach such as SKS, and for each karst realization, flow and transport parameters could be optimized using a gradient-based search such as the one implemented in PEST.

Introduction

Karst aquifers are extremely heterogeneous and difficult to characterize [2]. Their heterogeneity is induced by the presence of highly permeable preferential flow paths created by the dissolution of the surrounding rock. Those preferential flow paths are often fractures and bedding planes that are enlarged by dissolution, often resulting into karstic conduits which are organized in hierarchical networks.

Annable [1] gives an exhaustive overview of the evolution of the conceptual models of speleogenesis over the last two centuries. The conceptual model that is considered in the present study [[63], e.g.] is the following: the karst aquifer is composed by 2 main hydrofacies: the matrix which represents more than 90% of the volume of the aquifer, and has an important storage role; and the conduits which represent a very small volume, but have a very high importance for flow, since they are considered to be responsible for more or less 90% of the total flow.

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Although karst aquifers have already been studied for more than a century they are still very difficult to model [1]. Over the last 3 decades, several numerical modeling techniques have been developed to provide better understanding of these aquifers, but also to manage water quantity and quality. A review of these techniques is provided by Ghasemizadeh et al. [23]. A striking feature of this review is that only direct approaches, i.e. modeling flow and transport when the geometry and the properties of the conduits are known, are described. Following the same line of thought, Saller et al. [52] show the benefits of coupling conduit flow (pipes) with matrix elements, but points out the uncertainty regarding the location of the conduits (which strongly influences the flow field) and the extreme difficulty of calibrating such models.

More generally, among the approaches used to solve inverse problems [57] in groundwater hydrology, gradient-based methods are frequently used. They consist in modifying iteratively the hydraulic conductivity values either in predefined zones [10] until the error between observed and calculated state variables reaches a minimum or stabilizes at an asymptotic value. This is extremely efficient if zones of constant but unknown hydraulic conductivity values are predefined. If the spatial distribution of the permeability field itself is unknown, it can be inferred as well using techniques such as pilot points, gradual deformation, or probability perturbation methods [9,30,48] which are also using gradient optimization.

In the case of karstic aquifers, the progressive deformation of the conduit structure and especially topology to reach a maximum likelihood or minimal error solution is particularly difficult to achieve. Preliminary tests conducted in this research have shown that the application of methods such as the probability perturbation lead to extremely discontinuous behavior of the objective function, making the use of gradient optimization completely useless. This is explained by the fact that during the progressive deformation of the geometry, disconnection and reconnection of the conduits occur leading to abrupt changes in the hydraulic and transport response.

Such difficulties explain partly why there are so few studies that considered applying inverse methods for karst aquifer distributed parameter models. Notable exceptions areLarocque et al. [40,41] and Panagopoulos [46] who used inverse methods to calibrate karst hydrogeological models. But, both group of authors do not include discrete karst conduits in their models and represent the karst aquifer with a 2D equivalent porous medium. Moreover, in these previous works, transport data have not been considered.

In this perspective and before conducting or developing any inverse methodology, it is important to understand better which parameters (like the hydraulic conductivity and porosity, or the shape and the number of conduits) mainly control the simulation results and therefore the value of the objective function.

Moreover, the ability of a classical optimization technique to effectively (and possibly efficiently) calibrate the physical properties of karst aquifers has also to be tested when simulating complex systems, with Darcy laminar flow in the matrix and turbulent Manning–Strickler flow in discrete pipes.

In this perspective, the present paper investigates whether inverse methods could be used to obtain information about the structure of the karstic network or the distribution of the conduit dimensions.

Two distinct numerical experiments are carried out. The first considers the influence of changing geometry and topology of the karst conduits on the simulation results. 150 different geometries with varying karst conduit radius and matrix hydraulic conductivity are considered. All these models are generated using the pseudo-genetic algorithm previously developed by Borghi et al. [8]. In practice, the test is performed by comparing the results of 18,000 2D flow and transport EPM (Equivalent Porous Medium) finite elements simulations (Sections 3). The second test investigates the ability of an inverse algorithm such as PEST [17] to retrieve optimal physical parameters when using a more complex model, i.e. a 3D model with karst conduits meshed as 1D pipe elements and non linear flow dynamics in the conduits.

1. Literature review

1.1. Flow simulation

Mathematical black-box models consider the whole aquifer as a single reservoir whose global behavior can be described with simple mathematical relations between an input signal and an output response: e.g. global parameter models [e.g. [42]], or neural networks [e.g. [29]]. An exhaustive review of these kind of models can be found in Ghasemizadeh et al. [23]. Unfortunately, as explained by De Marsily [14], these models may be sufficient to predict spring hydrographs, but they do not provide any spatial information about the karstic conduit system.

As opposed to black-box models, distributed parameter models are based on the discretization of the model domain into sub-units. Each sub-unit has homogeneous parameters in the space that it delimits (see Section 2.2). As Ghasemizadeh et al. [23] say, *the challenge of distributed modeling approaches to represent karst groundwater systems is to cope with the high spatial heterogeneity of karst aquifers*. Many authors have already modeled karst aquifers using parameter distributed models. The easiest way is to consider the whole karst aquifer as an equivalent porous medium (EPM), where matrix, fractures and conduits are brought together in an equivalent hydrofacies (e.g. [6,39]). Unfortunately, EPM models have a very low applicability in very kartified fields and may lead to catastrophic situations like the case of Walkerton (Ontario, Canada) where, in May 2000, 7 people died from a bacterial contamination of the municipal water supply because the spring protection zone was based on an EPM model, which gave much larger transit time than what was observed (later) by field tracer tests (Worthington, [64]; Goldscheider, [25]; Kresic and Stevanovic [37]).

To avoid this kind of issues, other authors have developed models, which use the available information about the conduit geometry to add heterogeneity in their model. Worthington [62] models the Mammoth Cave aquifer using MODFLOW, and he defines the mesh elements where karst conduits were explored as cells with higher hydraulic conductivity. He also had to increase the hydraulic conductivity according to the hierarchy of the conduits to be able to simulate realistic head distributions. Király [33], Király et al. [35] modeled the conduits as discrete 1D or 2D features embedded in a 3D matrix using a discrete-continuum approach, flow in conduits being laminar. The discrete–continuum approach is often used to develop speleogenesis models [1,18,22]. These speleogenesis models are useful to understand the complex kinetics of karst aquifers. In addition, as Jeannin [32] pointed out, turbulence is often observed in conduit flow. Nowadays there are computer codes that allows non linear flow equations to be used in discrete conduits, as MODFLOW-CFP [Conduit Flow Process, [38]] or GROUNDWATER [12]. De Rooij [15] developed a model that is able to simulate also unsaturated flow in pipes. Recently, Saller et al. [52] show the benefits of the application of a discrete conduit model for the simulation of the Madison aquifer of Southern Dakota (USA).

1.2. Conduit network modeling

The models of De Rooij [15] and Saller et al. [52] show enhanced results with respect to EPM models, because they solve more complex physics, but their authors agree on the difficulty that is posed by the unknown conduit location. In order to use realistic conduits, one could use the networks resulting from speleogenetic models [1,18,22], but the computation of these models is