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Gradual conditioning of non-Gaussian transmissivity fields to flow and mass transport data: 2. Demonstration on a synthetic aquifer

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S U M M A R Y

In the first paper of this series a methodology for the generation of non-Gaussian transmissivity fields conditional to flow, mass transport and secondary data was presented. This methodology, referred to as the gradual conditioning (GC) method, constitutes a new and advanced powerful approach in the field of stochastic inverse modelling. It is based on gradually changing an initial transmissivity (T) field, conditioned only to T and secondary data, to honour flow and transport measured data. The process is based on combining the initial T field with other seed T fields in successive iterations maintaining the stochastic structure of T, previously inferred from data. The iterative procedure involves the minimization of a penalty function which depends on one parameter, and is made up by the weighted summation of the square deviations among flow and/or transport variables, and the corresponding known measurements. The GC method leads gradually to a final simulated field, uniformly converging to a better reproduction of conditioning data as more iterations are performed. The methodology is now demonstrated on a synthetic aquifer in a non-multi-Gaussian stochastic framework. First, an initial T field is simulated, and retained as reference T field. With prescribed head boundary conditions, transient flow created by an abstraction well and a mass solute plume migrating through the formation, a long-term and large scale hypothetical tracer experiment is run in this reference synthetic aquifer. Then T, piezometric head (h), solute concentration (c) and travel time (τ) are sampled at a limited number of points, and for different time steps where applicable. Using this limited amount of information the GC method is applied, conditioning to different sets of these sampled data and model results are compared to those from the reference synthetic aquifer. Results demonstrate the ability and robustness of the GC method to include different types of data without adopting any Gaussian assumptions, and its high potential to be used together with the Monte Carlo method for uncertainty analysis of flow and mass transport model results. Moreover, the simplicity of the formulation of the method, based on forward flow and mass transport solvers, the flexibility of the stochastic random definition required, and the simple form of the minimization problems solved during the iterative procedure, make this a very valuable tool and robust alternative to other methods for real applications.

Introduction

The gradual conditioning (GC) method for the stochastic simulation of transmissivity (T) fields conditional to flow, mass transport and secondary data was presented in the first paper of this series (Capilla and Llopis-Albert, 2009). The method has been developed in parallel to its application in real formations that have provided very demanding test cases (Llopis-Albert, 2008; Llopis-Albert and Capilla, 2008). In this paper, a detailed verification and analysis of the potential and robustness of the method has been developed through the demonstration of its capabilities on a set of controlled numerical experiments carried out on a synthetic aquifer. The objective of these experiments is to show how efficiently the technique works and to explore its robustness under different situations. This synthetic case, and the experimental scenarios considered, have been designed to verify most of the basic potential of the method. Other implemented features of the method as its ability to deal with variable density flow, three dimensional or dual-domain conditions are not considered in this paper although are being analyzed in applications to real cases, Llopis-Albert (2008).

The synthetic aquifer considered includes a non-Gaussian reference T field within a rectangular flow domain with prescribed head boundary conditions and a transient flow field driven by the activation of a pumping well during a given stress period. Within these flow conditions, a long-term tracer test is performed. The stochastic structure of the simulated T fields is assumed to be exactly as that used to generate the reference field; thus we simplify our analysis avoiding the uncertainty on the stochastic structure and

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expecting a quite adjusted posterior reproduction of this a priori model, with ergodic fluctuations with respect to the reference T structure.

In order to design the different conditioning scenarios we have sampled T measurements from the reference T field, and transient piezometric head, solute concentrations and travel time data from the flow and concentration fields obtained by solving the flow and mass transport problems for the reference T field. Then, the GC method is applied to simulate T fields that are conditioned to different sets of these sampled data, comparing results with those from the reference field. At the same time, the general features and convergence behaviour of the penalty function are analyzed.

Synthetic aquifer and simulation scenarios

Geometry, parameters and boundary conditions

The two-dimensional synthetic case is based on T data of natural origin. It has been taken from a real case study at Äspö Hard Rock Laboratory, Sweden (see Capilla et al., 2002). This real case corresponds to a 3D fractured granite block, from which we have taken a 2D slice. Thus, the flow domain has a size of 226.44 × 246.42 m and is discretized in 37 × 34 square blocks of size 6.6 m.

Prescribed head boundary conditions are assumed, as shown in Fig. 1, originating a general flow from Southwest to Northeast and, in order to create transient flow conditions, a pumping well is located at 16.65 m from the West boundary and 209.72 m from the South boundary. The pumping rate is of 1.8 l s^{-1} and is activated 31.7 years after the initial simulation time, ceasing abstraction at time 761 years. The initial piezometric head table is taken as the steady state flow solution, i.e., without pumping. Porosity is taken as 0.35 and the specific storage as 2.5×10^{-4} l m^{-1}.

To conduct the tracer injection a conservative solute has been considered, injecting a total mass of 4.9×10^{-6} m.u. m^{-3} at the initial time of simulation $t = 0$. The solute injection is uniformly distributed in a square situated between 6.66 m and 33.33 m from the West and from the South boundaries, as shown in Fig. 1. The GC method is implemented, as described in the accompanying paper, to solve the mass transport equation by means of a Lagrangian approach, called random walk particle tracking (RWPT), that treats the transport of a solute mass via a large number of particles. In this synthetic case, a total of 4900 particles have been released simultaneously, assigning a mass of 1000 m.u. m^{-3} to each particle.

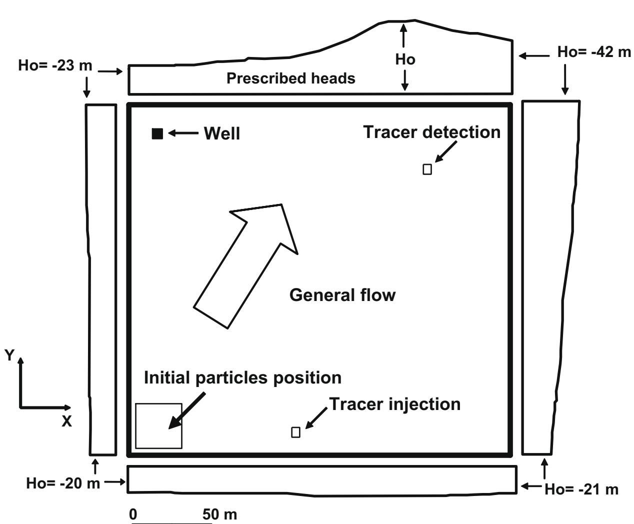

Fig. 1. Synthetic aquifer: definition of geometry, boundary conditions and location of mass releasing area, pumping well, and tracer injection and detection points.

Table 1
A priori conditional cumulative density function of $z = \log_{10}T$ field [log m/s]: marginal cumulative probabilities, $F(z_k)$, and log T thresholds, z_k ($k = 1, \ldots, 9$).

$F(z_k)$	0.001	0.002	0.003	0.004	0.005	0.1	0.4	0.6	0.8
Z_k	−10.5	−10.0	−9.5	−9.0	−8.5	−8.0	−7.5	−7.0	−6.5

Longitudinal dispersivity is taken as $\alpha_L = 0.3$ m and transverse dispersivity as $\alpha_T = 0.03$ m.

The stochastic structure of T has been defined using the marginal cumulative probabilities for nine thresholds, the histogram deciles, as shown in Table 1, and by the corresponding indicator variograms for which a common variogram definition is taken: spherical, range of 40 m, 0.04 of nugget effect, and sill of 0.22. The a priori conditional cumulative density function (ccdf) given in Table 1 shows a highly asymmetrical distribution with a long lower tail. This ccdf might have been obtained using T measurements as well as other types of information from expert judgement or from geophysical surveys. The T reference field is then obtained by means of sequential indicator simulation using the computer code ISIM3D (Gómez-Hernández and Srivastava, 1990). Graphs (a) and (b) in Fig. 2 show the log$T$ reference field, histogram and univariate statistics. Note the non-Gaussian features displayed on the log$T$ map representation as well as in the histogram graph. Graphs (c) and (d) in the same figure show the ensemble of multiple trajectories followed by mass particles released from the square close to the left lower domain corner (c), as well as the travel times histogram, for the 4900 released particles, to reach the boundary domain or the abstraction well (d). Note also that some particles following pathlines towards the well during the pumping time period do not reach it before the ceasing abstraction time, therefore suffering an important change in trajectories and an increased travel time to the boundary domain limit. A fraction less than 1% of injected mass is extracted at the pumping location for the reference field.

Piezometric head and solute concentrations obtained for the reference log$T$ field are represented in Fig. 3. This figure shows the head fields for time steps corresponding to the start of pumping (31.7 years), abstraction cease (761 years), and a more distant selected time (2378,27 years), that define the three stress periods of the flow simulation. The third stress period length allows reaching a piezometric table very close to the initial head conditions. Fig. 3 also presents the solute concentration plume for three snapshots taken at times $t_{c1} = 412.22$ years, $t_{c2} = 792.74$ years and $t_{c3} = 1902.58$ years. Note the slow development of the solute plume, its deviation towards the pumping well at the second snapshot, and the third snapshot plume extension, long after the abstraction cease. At this time, its extension over the aquifer domain clearly follows the general flow direction after having been delayed and deviated during the pumping period. The combination of the abstraction well action and the flow direction driven by the prescribed head boundary conditions introduce transient flow conditions that increase mass solute dispersion creating a more difficult test case but closer to real situations.

Conditioning data and simulation scenarios

In order to define the set of numerical experiments to perform with the GC method we have defined five different conditioning data scenarios based on the following sets of data, sampled as shown in Fig. 4. These data sets are:

- Sixteen regularly spaced T measurements.
- Forty-eight regularly spaced piezometric head measurements on a 4 × 4 grid, at the end of the three stress periods considered of 31.7, 761 and 2378.27 years.