Three Dimensional Stochastic Modeling of Conductivity Fields in a Fractured Rock Medium

Capilla, J.E. (1), Rodrigo, J. (1), Gómez-Hernández, J.J. (1), Llopis, C (1).

(1) School of Civil Engineering, Technical University of Valencia.

José E. Capilla, School of Civil Engineering, Technical University of Valencia, Camino de Vera s/n, E-46071 Valencia, Spain, jcapilla@fis.upv.es

1. Abstract
Modeling flow and transport in a fractured rock formation requires in many instances an explicit representation of fractures. In such cases discrete fracture models do not always work properly because of the difficulty to be calibrated and the lack of flexibility to be adapted, in an automated calibration process, when the description of fracture locations is not accurate enough. In this case a pseudo porous media approach, in which fractures are represented by high hydraulic conductivity zones, is an alternative model that has already been successfully proven in real case studies. Fractures use to be the most relevant feature to describe when dealing with contaminants migration. In these 2D structures, hydraulic conductivity (K) is usually the most relevant parameter for mass transport modeling. K usually exhibits a high degree of spatial variability and direct measurements of it are very scarce, when available. Thus, in the same way found for a continuous medium, stochastic simulation techniques can be the most suitable tool to model K in fractures. Besides, the goal of obtaining more realistic predictions, while reducing uncertainty in model results, calls for conditioning K fields to the available pressure measurements.

Based on a 3D real case study of flow and transport in a fractured crystalline rock, the paper addresses the way to model K in fractures, and the rock matrix, conditional to pressure data. It is assumed that K in fractures may not be multiGaussian. The simulation of these K fields is achieved by means of a method based on non-parametric statistics that yields K fields in which zones of extreme values of K may appear highly interconnected. The method can support the assumption of independent stochastic processes corresponding to different fracture families. This is achieved using a multi-parameterization approach implemented in the inversion technique known as Conditional Probabilities method.

The paper shows how different can be mass transport predictions when Gaussian and non-Gaussian models are assumed for K fields in fractures. The conclusion is that, in view of available data, models alternative to the common Gaussian assumption should always be considered.

2. Introduction
Modeling flow and transport in fracture rocks has been frequently addressed using discrete fractures approaches, see for instance WEN & CVETKOVIC (1995). The drawback of these models is the difficulty to be calibrated to experimental measurements. This is due to the need of an accurate knowledge of fracture geometries and of the bidimensional distribution of hydrodynamic parameters on them. The problem is that these models tend to be too rigid in the sense that they are not able to re-adapt themselves correcting deficiencies or errors in the fracture geometry definition. A well-known case in which the calibration of these models failed is the set of experiments carried out in Sellafield, U.K. (NIREX 1995).

An alternative approach is assuming a pseudo-continuum media approach in which fractures are consider through the introduction of discretization blocks of very high hydraulic conductivity (K). In this model, blocks intersected by fractures have very high K. However there are still some problems that could lead a model like this to failure. These are (1) poor knowledge of fracture geometries, (2) selection of too large block size (relatively to the domain and fractures geometry), (3) numerical problems due to very different values of K, (4)
lack of connectivity between contiguous blocks (possible in a Finite Differences scheme) and
(5) a bad definition of high K blocks and matrix blocks. Anyway, keeping the above
considerations in mind, it is possible to build a model, based on the pseudo-continuum
approach that successfully accounts for the preferential flow and transport paths defined by
fractures. Sellafield and Åspö are two cases where this approach works very satisfactorily.

This paper presents the application of this type of model to a real 3D case study, where
different models and inversion techniques are being tested. We stress the fact that a proper
modelization of K in fractures is crucial and that assuming a multiGaussian model for the K
field in fractures may lead to unsafe model predictions. The Conditional Probabilities (CP)
method, see CAPILLA ET AL. (1999), is adapted to deal with zones in which different
stochastic properties may apply. The fact that stochastic properties of K are very different in
the rock matrix and in fractures, and that there can also be different families of fractures
responding to alternative stochastic structures, leads to a special formulation of the CP
method. It is based on a multi-parameterization of the process followed to identify K that
allows obtaining K fields made up by zones corresponding to independent stochastic
processes.

3. Model and data description

The block of crystalline rock being modeled has a size of 286 m (deep) × 226 m × 246 m. The
flow and transport equations are solved using the finite differences method. The volume of
rock is discretized in a grid block of 43 × 34 × 37 (54094 blocks). This high number of
blocks, together with the need to solve the inverse problem, has lead to develop very
sophisticated computer codes able to minimize the amount of computer memory needings,
CPU time and numerical errors. The huge matrices generated when solving the flow and
transport equations are stored using the SLAP column format, and the vector equations are
solved using routines from the Sparse Linear Algebra Package (SLAP), see SEAGER (1998).
The programs can be run in a PC although we are using a Silicon Graphics IP27 with 8 CPU
that allows obtaining more accurate results with lower CPU time.

The boundary conditions are prescribed heads in every side of the model block and are taken
from a regional flow model. They have been locally modified to account for the effects of the
underground facilities. These create very local drainage conditions on two of the block sides.
Several pumping and tracer tests have been conducted in the block. They provide a wealth of
information on the hydrodynamic behavior throughout the whole block. The problem is how
to build a model and formulate inverse algorithms able to integrate all these data.

Our research focus on the identification of hydraulic conductivity fields, at a scale of meters
that realistically reproduce natural formation heterogeneity, all the available K measurements
as well as steady state pressure measurements, and flow and mass transport field tests. The
final goal is the identification of K fields that yield realistic mass transport predictions. The
steps followed consider the following stages: (1) model K fields conditioned to K
measurements, (2) include steady state pressure measurements as conditioning data, (3)
include pumping test data and (4) include tracer test data. At present our team has reached the
stages (2) and (3) and is working on an adapted formulation of inverse techniques to deal with
tracer test data (4).

The number of K measurement available is 270 in the rock matrix and 24 distributed in the
identified fractures. However, the number of identified fractures is 20 and, in general, these
constitute structures where K is much higher than in the matrix. Average log K in the rock
matrix is -9.5 log m/s and in fractures is -6.7 log m/s. Figure 2 shows the histogram of log K
data in matrix, slightly asymmetric, and in fractures. The last one does not contribute
information enough to decide on the stochastic model. The variography of log K in matrix
shows more continuity for high values of K. This feature might deserve more attention
because could favour fast migration of mass through the rock matrix. K in fractures is much
higher and its variography cannot be studied with the available data. Connectivity of high
values is a feature to be modelled.
4. Stochastic modeling of hydraulic conductivity

In view of the different data sets characteristics and accounting for the fact that $K$ in fractures usually exhibits a high degree of spatial variability, it was decided to proceed obtaining independent stochastic simulations of log $K$ in both matrix and fractures, and combining them to obtain log $K$ fields for the entire model block. Two different hypotheses are considered. In both of them log $K$ in the rock matrix is assumed as multiGaussian, being the difference the treatment given to log $K$ in fractures. In the first hypothesis (MG) log$K$ is modeled as multiGaussian with the same variogram in every fracture, and with average and standard deviation in agreement with available data. In the second hypothesis (NMG) a non multiGaussian model is assumed, common for all fractures, with a range value as in the rock matrix (40 m) and a mosaic model (same variogram for different cutoffs). Figure 2 shows the difference for the log $K$ field in one of the fractures. The first case (MG) leads to a lower effective conductivity and a typical Gaussian pattern of spatial variability while in the second (NMG), there is a higher effective conductivity with more connectivity for high values of $K$. In both figures darker colours mean higher log$K$ values.

5. Hydraulic conductivity fields conditioned to pressure data

In order to obtain log $K$ fields conditioned to pressure data we are developing a new version of the Conditional Probabilities (CP) method where we introduce a multi-parameterization technique. The CP method was presented by CAPILLA ET AL. (1999) and has the great advantage of being able to reproduce a non multiGaussian model defined by the local
Conditional Cumulative Density Functions (ccdf) at every discretization block and by the spatial structure of the associated probabilities.

Consider the aquifer domain discretized in a grid of N \((i=1,\ldots,N)\) blocks. The CP method is based on perturbing stochastic log \(K\) fields \((Y)\), previously generated and called seed fields, that reproduce \(K\) measurements and the geostatistical structure of probability fields associated to \(Y\) through the ccdf's. Being \(Y^0\) a seed field, a perturbation \(\delta Y\) is determined with the condition that the log \(K\) field given by \(Y^0 + \delta Y\) honors pressure data. The perturbation field, \(\delta Y\), is parameterized by means of the expression given by Eqn. (1), that defines the perturbation \(\delta Y_j\) at every block as a function of perturbations at a limited number of blocks \((m << N)\) called master blocks, \(\delta Y_j\) \((j=1,\ldots,m)\).

\[
\delta Y_j = \left(\frac{df_i}{dY}\right)^{-} \left| \sum_{j=1,\ldots,m} \left(\frac{df_j}{dY}\right)_{Y^0} \right| \lambda_i \delta Y_j
\]

In Eqn. (1), \(F_i(Y)\) is the local ccdf for block \(i\), and \(\lambda_i\) are the kriging weights obtained to estimate the probability value at every block \(i\) \((i=1,\ldots,N)\), \(F_i(Y)\), given the probabilities \(F_j(Y)\) \((j=1,\ldots,m)\) at master blocks.

The computation of \(\delta Y_j\) at master blocks is performed minimizing a penalty function that penalizes the deviations among pressure data and the pressure computed for the perturbed \(K\) field. In order to build it, the flow equation is linearized on \(\delta Y_j\) \((j=1,\ldots,m)\), thus leading to a quadratic programming problem. Due to the linearization it is necessary to perform a few iterations. After every iteration the field \(Y^0\) is updated by solving the flow equation. Then a new perturbation is performed to improve the reproduction of pressure data.

The CP method presents numerous advantages compared to other approaches. It preserves the local ccdf defined for every discretization block. This is of paramount importance because the process to obtain this local density functions may incorporate not only \(K\) measurements but also soft and secondary information, as that coming from expert judgment or from geophysical exploration. This means that if there are zones with ccdf's belonging to independent stochastic processes they are still preserved. However, the parameterization is common to every zone and this may lead to an improper consideration of the spatial continuity of \(K\). Although we believe, and have got some practical evidence, that an adequate number of master blocks and iterations might make this a minor problem, we have develop an extension of the CP method introducing multi-parameterization in Eqn. (1). It is based in the same approach used by HENDRICKS ET AL. (1999) to extend the application of the Self-Calibrated method. The basic idea is to compute sets of interpolation coefficients, \(\lambda_i\), which are independent for zones belonging to independent stochastic processes. In our case, we have independent parameterizations for the rock matrix and for every fracture.

6 Results and discussion

The final goal of the research described in this paper is obtaining log \(K\) fields that yield realistic mass transport predictions. Thus the way to compare realizations for the different hypotheses considered, MG and NMG, is comparing mass transport results. We are currently analyzing results for the convective transport releasing particles in upstream areas that define the origin of pathlines spanning between different sides of the block model. Figure 4 (a) shows iso-surfaces of the piezometric head field corresponding to the first simulation of log \(K\) field, in case MG. The figure shows how piezometric head decreases from NW to SE, and the disposition of the iso-surfaces concentric around the existing underground tunnels. In fact, these tunnels are working as
drains capturing the flow across the rock block. Thus, tracers injected in most parts of the block are found in water drained to these tunnels. In the finite differences model, these tunnels are represented by a prescribed head boundary condition that equals the depth of the tunnel. The piezometric head fields obtained for different hypotheses, conditioned or not to pressure data, are not clearly different and do not provide information on mass transport behavior.

The analysis of results for convective transport yields interesting conclusions that were, somehow, expected. So far we have processed just a few log K realizations and, due to this reason, conclusions on the reduction of uncertainty provided by conditioning to pressure data cannot be yet established. However, the different behavior of the MG and NMG hypotheses can be clearly interpreted.

Figure 4: (a) Isosurfaces of the piezometric head field obtained for the first multiGaussian log K field simulated, and (b) convective transport results for the first simulated log K field in the multiGaussian (MG) and non multiGaussian (NMG) hypotheses.

Figure 4 (b) shows how different are the trajectories obtained for cases MG and NMG. In this figure results of convective transport for the first simulated field are presented. Log K in the rock matrix is exactly the same for the MG and NMG fields. Only log K in fracture differs. Note how prominent is the change in trajectories and the channeling effect in the NMG case. These "fast channels" take place in the fractures and can be observed in different log K realizations and for many different particle releasing locations. Although the analysis of results requires to consider (1) the log K field stochastic structure, (2) boundary conditions, (3) particle releasing locations and (4) location of fractures with respect to the flow field and pathlines, some general conclusions can be established,

· Flow clearly tends to concentrate in fractures as expected.
· The connectivity of high hydraulic conductivity values found in many fractures, when assuming non Gaussianity, promotes very markedly the channeling effect in fractures.
· Particle travel times through the block are not always increased because the connectivity of low K values is incremented too. Some realizations and pathline origins may lead to longer and slower pathlines.
· The non Gaussian assumption for log K in fractures may lead to both lower and higher travel times. This can make wider, although more realistic, the uncertainty associated to mass transport predictions. The application of MonteCarlo techniques to multiple log K fields conditioned to as much information as possible should be the way to reduce this uncertainty.
· The stochastic model adopted for log K has a great influence in transport and the multiGaussian hypothesis may lead to wrong predictions.
7. Further research
The CP method is currently being extended to simulate K fields honoring pumping test as well as tracer tests. Conditioning to concentration data is a much more mathematically and computationally difficult problem. The formulation that we apply in this case for the penalty function is that given by CAPILLA ET AL. (2000) and shown by Eqn (2),

\[ F = \int\left( (p-p^*)^T W_p (p-p^*) + \Theta_p (c-c^*)^T W_c (c-c^*) + \Theta_\eta (\eta-\eta^*)^T W_\eta (\eta-\eta^*) \right) dt \]  \hspace{1cm} (2)

where the vectors \( p, c \) and \( \eta \) correspond to pressure, concentration and other parameters, computed at measurement locations. Measurements are in vectors \( p^*, c^* \) and \( \eta^* \); \( W_p, W_c \) and \( W_\eta \) are weighting matrices, and \( \Theta_p \) and \( \Theta_\eta \) are trade-off coefficients. The integration in time extends over a period that includes the available measurements.

The particular characteristics of the problem at this site have lead to develop a special formulation of the inverse stochastic approach to condition to concentration data. Our knowledge from (1) failures in applying other inversion algorithms, (2) the configuration of our finite differences model, with blocks intending to simulate fractured zones, (3) the assumption that fracture locations are reasonably well known, and (4) the characteristics and limited extension of the tracer tests, lead us to design a new approach. It consists of a mixed Lagrangian-Eulerian scheme that minimizes numerical dispersion, accounts for the fact that mass transport takes place in limited zones of the model, and assumes that in the perturbation process carried out by the CP method, flow velocities are mainly changed in magnitude and not in direction.

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9. References


