Characterization of spatial heterogeneity in groundwater applications

PhD Thesis

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February 2009

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Chapter 1

Introduction

The intrinsic heterogeneity of every natural subsurface formation has been the reason of the blossoming of stochastic hydrogeology. In the last three decades, this subdiscipline of hydrogeology has devoted many efforts to account for the effects of variability and to quantify the uncertainty of the predictions. Since the mid-1980s the stochastic approaches have been gaining in popularity within the research word. Nevertheless as highlighted by *Rubin* [79], the concrete impact of stochastic methods on the standard practice is still limited. This statement is confirmed by the fact that hydraulic and tracer tests are routinely interpreted by practitioners using methodologies based on the assumption of homogeneity.

Since the publication of the Thiem solution [92] and the Theis transient solution [91], pumping tests are used worldwide to infer the hydraulic properties of the pumped aquifer, namely transmissivity, T, and storage coefficient, S. Drawdown data are usually interpreted with a number of analytical solutions that account for different boundary conditions within the aquifer and at the well [90, 49, 95, 7, 44, 43, 73, 39]. As already stated, all these methodologies assume that the medium is homogeneous implicitly lumping the heterogeneity in the parameter estimates. Although a number of modern techniques exist that allow acounting for heterogeneity during the estimation process (e.g. geostatistical inversion), the widespread use of homogeneous models gives to stochastic hydrogeology the challenging task to answer to the following questions:

- What is the physical meaning of those hydraulic parameters estimated using a homogeneous model?
- Is it possible to use these estimates to infer quantitative information of the underlying heterogeneous structure?

Until now the progresses in addressing the second question have been limited. A number of methodologies [66, 16, 67] and frameworks [17] have been developed to infer the spatial structure of the heterogeneous field (variance, covariance function). These approaches give reliable results when a large number of observation points and/or pumping tests are available. Nonetheless, when the number of observation points is limited their results are strongly conditioned by the prior knowledge of the field.

While the task of defining optimum methodologies to infer quantitative information of the heterogeneity is still under development, a number of papers have tried to provide practitioners with a qualitative idea of the physical meaning of their estimates. *Meier et al.* [62] analyzed numerically the meaning of the parameters obtained when interpreting a pumping test by the Cooper-Jacob method [15] in heterogeneous confined aquifers. For low to moderate degrees of heterogeneity, they found that the estimated transmissivity, T_{est}, was close to the geometric mean of the transmissivity field, while the estimated storage, S_{est}, could significantly vary with the observation location, being indicative of the hydraulic connectivity between the observation location and the pumping well. These results were confirmed analytically by *Sanchez-Vila et al.* [83] who obtained an approximate analytical expression for S_{est} by truncation of an infinite series solution. *Knudby and Carrera* [52] analyzed the use of apparent diffusivity, D_r (estimated transmissivity divided by estimated storage coefficient), as a measure of connectivity. They found that D_r has a certain degree of correlation with indicators of both transport and flow global connectivity.

The influence of heterogeneity on the interpretation of tracer tests was assessed by *Guimera and Carrera* [41] that found that the effective hydraulic conductivity, estimated as the ratio of water flux to head gradient, to be highly correlated with the apparent porosity (ratio of water velocity to water flux) based on the first arrival time. The authors concluded that first arrival is controlled by the same flow paths as hydraulic conductivity. *Fernandez-Garcia et al.* [29] analyzed a suite of convergent flow tracer tests performed in a reconstructed anisotropic heterogeneous medium. They found that the arrival time (or the estimated porosity) of tracer breakthrough curves was primarily controlled by the preferential flow paths occurring between the pumping well and the injection location, providing little information on the global properties of the transmissivity field, i.e., T_{eff}. Thus, their results gave an explanation for the observed discrepancy between porosity estimates obtained from field tracer tests and their representative values. This explanation had already been hinted by *Sanchez-Vila and Carrera* [80] in their analysis of a tracer test performed in a highly heterogeneous strongly anisotropic medium.

Additional degree of heterogeneity is observable in unsaturated flow conditions related to $K(\theta)$ where the water content, θ, is heterogeneously distributed in space and time. Flow and tracer tests can also be used in this context (e.g. waste rock piles) to infer the mean residence time of the water within the medium. Nevertheless, in most natural soils irregular paths exist where water and solutes move faster bypassing most of the porous matrix. A better characterization of these mechanisms are of great importance in mining related problems since the chemical composition of mine water release depends on the residence time of the water within the medium. In the last decades several works have documented the existence of preferential flow through the assessment of field evidence. *Roth et al.* [78] analyzed horizontal averaged concentration profiles of chloride that developed after solute was applied at the surface. They observed that the initial pulse of solute split into a main pulse, moving slowly, and a second deeper front (moving quickly). The development of preferential flow mechanisms in a medium having a water repellent topsoil was studied by *Ritsema et al.* [76] who argued that, in these media, water and tracers are horizontally redistributed before finding a preferential flow path. *Flury et al.* [31] studied the flow pathways of water in 14 different soils through the use of dye-tracers. They found that the maximum penetration of water was deeper in structured than in nonstructured soils. Their results also showed that the flowpaths were dependent on the initial soil water content ('wet' or 'dry') although a common model was not found. Observations of the vertical distribution of environmental isotopes (tritium, oxygen 18 and deuterium) demonstrated the existence of preferential flow in the vadose zone of the Negev desert (Israel) [65]. Water discharge and tracer arrival time at different lysimeters located at the bottom of a waste rock pile were studied by *Nichol et al.* [70] to assess the existence of preferential flow. The results of the tracer experiments showed a great spatial variability with some lysimeters having a fast response to the perturbation generated at the surface and others where flow and transport where mainly driven by the matrix.

In summary this thesis aims at giving a perhaps small but indeed significant contribution in filling the gap between stochastic hydrogeology and practitioners. A series of frameworks/guidelines are developed starting from observations of hydraulic and tracer tests in both saturated and unsaturated media. The development of analytical solutions and the application of stochastic techniques is used to give insight into the processes governing the system's response.

1.0.1 Thesis outline

This thesis consists of five chapters after the introductory one. Those chapters are based on papers that have been published or are being submitted to international journals.

Chapter 2 consists of an analytical study of the processes involved in flow and transport point-to-point connectivity. In this chapter we develop an approximated analytical solution that expresses the mean travel time of a solute as a weighted line integral along the particle trajectory involving two parameters: the transmissivity point values, T, and the estimated values of S_{est} along the particle path. The solution has been validated using a sinthetic example and a laboratory tracer test. The results show that the mean arrival time is mainly controlled by the first term of the integral (transmissivity point values along the path line) although the incorporation of the second term improves the delineation of the low connectivity patterns.

In chapter 3 we provide a general framework, based on the analytical solution of chapter 2, that allows delineating connectivity patterns using a limited and sparse number of measurements. The lack of complete knowledge of the variables involved in the problem is overcome by treating them as spatial random functions. The methodology allows conditioning the results to three types of data measured over different scales, namely travel times of convergent tracer tests, estimates of the storage coefficient from pumping tests interpreted using the Cooper-Jacob method and measurements of transmissivity point values, T. The ability of the methodology to properly delineate capture zones is assessed through estimations (i.e. ordinary cokriging) and sequential gaussian simulations based on different sets of measurements.

In chapter 4 we develop a new methodology for the interpretation of pumping tests in leaky aquifers, referred to as the Double Inflection Point (DIP) method. The method is based on the leaky aquifer system defined by *Hantush and Jacob* [44] and makes use of the existence of two inflection points in the drawdown derivative curve. When applied to homogeneous media, the DIP method yields the exact parameters of the aquifer and aquitard (T, S and B); as is the case with other methods such as the Hantush Inflection point method and Walton type-curve method. The primary benefit of the DIP method is when applied to heterogeneous media where each method provides different and valuable indirect information about the heterogeneous distribution of the local transmissivity values.

Chapter 5 examines the impact of heterogeneity of leaky aquifer systems on the flow parameters estimated with three different methods, two of them commonly used in real applications: the inflection-point [42], the curve fitting [99] methods, plus the double inflection-point method presented in chapter 5. This numerical exercise provides a framework to understand the implications of the assumption of homogeneity in the estimates obtained with the different methods commonly used in the interpretation of pumping tests in aquifer-aquitard systems. Since each method give different emphasis to different portions of the drawdown curve and, consequently to different volumes of the aquifer-aquitard system, we argue that using all analysis methods jointly may provide additional information (specifically, about contrasts in the local value of the transmissivty at the pumping well) than using each method independently.

In chapter 6 we model unsaturated water flow through a highly heterogeneous unsaturated medium using a simple linear representation. Such a model cannot accurately describe the complexity of the medium at the local scale but is useful to obtain a first-order identification of the averaged processes occurring within it. The main advantage of this methodology lies in its simplicity that allows inferring information about the characteristic time of the hydraulic response of the matrix and the degree of preferential flow occurring within each section of the pile by looking at the spectral signature of the input and the output.