
147: Characterization of Porous and Fractured Media

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The characterization of porous or fractured media is a site, scale, and project-specific process aiming at a quantitative description of the geometry and properties of the geological structures controlling groundwater flow and solute transport. The characterization process involves four main steps (i) the definition of the domain and the goals of the characterization; (ii) the collection and analysis of field observations allowing the construction of a geometrical model; (iii) the collection and analysis of field measurements allowing to construct a property model; and (iv) the collection and analysis of field data relative to the state of the system and their integration within the geometrical and property models (inverse problem). When data are sufficient and structures are relatively well known, deterministic techniques of interpolation can be successfully applied to construct the geometric or the parameter models. However, because of the lack of sufficient data, stochastic models are often employed to characterize the heterogeneity that usually exists; such models also facilitate the quantification of the uncertainty in model predictions. Without describing the details of every technique, this article provides an overview of the tools most often used for the characterization of porous or fractured aquifers.

INTRODUCTION

Aquifer characterization can be defined as the process of data acquisition, analysis, and integration leading to a description of aquifer geometry and properties. This process may be relatively straightforward and limited to mapping the extent of an aquifer, its thickness, and estimating average properties such as transmissivity and storativity. It may as well be a much more complex task, integrating data obtained from various field investigations and involving intensive numerical modeling. The level of complexity of the characterization process is related to the goals of the study, the geological conditions, and the level of confidence required by the stakeholders. For example, evaluating the safety of a deep underground nuclear waste repository requires higher characterization efforts than estimating the amount of groundwater exploitable in a small shallow aquifer. Furthermore, the characterization efforts are oriented toward

specific aquifer properties and objectives depending on the project. In the nuclear waste repository project, it may be important to have an accurate description of the diffusion properties of the geological materials, while this aspect may be irrelevant for the water resource project. Similarly, the thermal properties of the underground will have to be characterized in the framework of a geothermal project, but are not relevant in the case of groundwater protection.

The above examples demonstrate that characterization is a site, scale, and project-specific activity, the aim of which is not to describe all the properties of the system, but to focus on the major structures and properties relevant to the processes of interest. This requires the collection of specific field observations, their analysis, and their quantitative integration into a synthetic descriptive model of the reality.

Most of the difficulties associated with subsurface characterization stem from the high spatial variability of the

subsurface environment. This heterogeneity is an intrinsic property of geological formations and results from the complexity of the geological processes (sedimentation, diagenesis, rock deformation, etc.). Additionally, only sparse information is available from outcrops, boreholes, or geophysics. The lack of information combined with the intrinsic heterogeneity is the source of uncertainty that makes the characterization of subsurface hydrogeological systems challenging.

The aim of this article is to present an overview of the usual steps and techniques used for the characterization of porous and fractured media. Subsequent articles within the encyclopedia cover technical aspects of data acquisition and modeling techniques used for data integration. Some specific technical points such as interpolation methods are covered in more detail, as they are not treated elsewhere within the encyclopedia.

The article encompasses six sections. The first section introduces the main steps involved in the characterization and highlights some key features and difficulties. Subsequent sections discuss deterministic, stochastic, and genetic techniques. The final section is devoted to inverse modeling.

CHARACTERIZATION PROCEDURE

The Typical Steps of Characterization

The goal of characterization is to build a model in which the parameters involved in the processes under consideration are specified everywhere within the domain of interest. The four major steps of the characterization procedure are illustrated in Figure 1.

The first step is the definition of the project goals, domain of investigation, and the selection of the relevant processes and variables. Then, characterization consists of collection, interpretation, and analysis of measurements from various data sources. It is useful to distinguish between static (time invariant) and dynamic (time dependent) properties. This definition is not strict: some static properties in a given context (e.g. the aquifer geometry) may be considered as dynamic in another context (e.g. aquifer geometry during land subsidence; see **Chapter 158, Anthropogenic Land Subsidence, Volume 4**). Another useful distinction is the separation between measurable quantities (state variables) and physical parameters that cannot be directly measured but that parameterize physical laws (e.g. hydraulic conductivity).

The second step is the definition of the geometry of the structures controlling groundwater flow and transport. It relies on local geological observations, general geological knowledge related to the type of environment encountered, and geophysical investigations (see **Chapter 148, Aquifer Characterization by Geophysical Methods, Volume 4**).

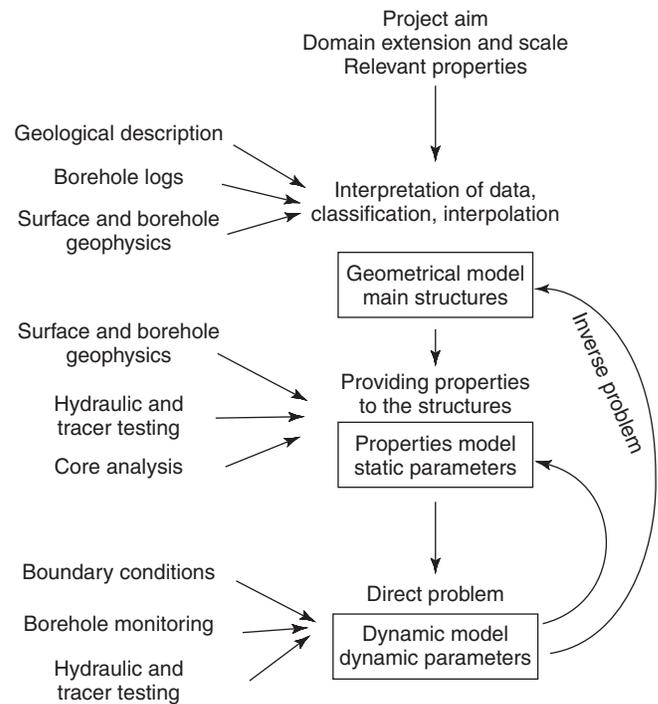


Figure 1 A schematic diagram of the characterization process

The end product is a geometric model that encompasses all relevant features: including aquifer, aquitard, channels, faults, lenses, and so on.

In the third step, field experiments such as hydraulic testing (see **Chapter 151, Hydraulics of Wells and Well Testing, Volume 4**) laboratory experiments, geochemical sampling, and tracer testing allow determination of the physical properties (static and dynamic) of the main structures. Of course, the separation between geometric modeling and defining properties is not straightforward in practice, as the knowledge of the properties is often required to decide whether a geological object is a relevant structure, and whether it is necessary to define its geometry.

The final step is the integration of the dynamic observations (state variables such as hydraulic head) with the static properties. The ultimate goal is that the geometric model and the property model must be in agreement with the dynamic observations. The main objective is therefore to link the geometry, the physical parameters, and the state variables through a system of partial differential equations that can be solved analytically or numerically (see **Chapter 152, Modeling Solute Transport Phenomena, Volume 4; Chapter 155, Numerical Models of Groundwater Flow and Transport, Volume 4; Chapter 150, Unsaturated Zone Flow Processes, Volume 4; and Chapter 157, Sea Water Intrusion Into Coastal Aquifers, Volume 4**). The model is then used in an

inverse procedure (*see Chapter 156, Inverse Methods for Parameter Estimations, Volume 4*) in order to improve the property model and/or the geometric model so that the calculated state variables match the observed ones under certain criteria.

Typical Goals of the Characterization

Depending on the type of aquifer, and on the project goals, different properties may be relevant, but in most cases the basic goal is to characterize the water conductive features. This means that for a porous media the most relevant property is the hydraulic conductivity. For fractured media, the relevant properties are the intensity of fractures, their extension, their connectivity, their apertures, and the hydraulic conductivity of the matrix. Table 1 provides a summary of the typical goals for subsurface characterization.

Deterministic versus Stochastic Methods

The geometric model, the property model, and the dynamic model can be defined within a deterministic or stochastic framework. In the deterministic framework, a unique geometry and property map are considered. On the other hand, in the stochastic framework (*see Chapter 154, Stochastic Modeling of Flow and Transport in Porous*

and Fractured Media, Volume 4), the unique estimate is replaced by an ensemble of equally probable realizations, generally characterized by a statistical model. The main advantage of the stochastic approach is that it provides a formal means to quantify uncertainty. In practice, however, stochastic and deterministic approaches are often complementary: some parts of the characterization process are described deterministically while others are described statistically.

The Scale Issue

One important difficulty that arises during the characterization process is the integration of observations and measurements that have been collected at different scales. It is important to distinguish four main scales of interest (Haldorsen and Lake, 1982; Dagan, 1989): the microscale, the macro or laboratory scale, the mega or local scale, and the giga or regional scale (Figure 2).

Scale issues arise because a physical law that describes a process at one scale may differ when it is averaged or upscaled over a large volume. Furthermore, when the form of the equation remains identical between different scales, values of the physical parameters have to be averaged in a way that is physically consistent. Most often the relevant parameters are not additive and cannot be simply averaged by a standard mean.

Table 1 Typical goals for the characterization of fractured or porous media

All cases	Porous media	Fractured media	Project-specific
Geological and hydrogeological boundaries	Hydraulic conductivity	Frequency of fracture occurrence / density	Thermal properties
Head/ pressures	Specific storage	Orientation – extension	Diffusion properties
Fluxes	Porosity	Aperture	Geochemistry
	Dispersivity	Transmissivity	Stress/deformation
		Connectivity	Salinity
		Matrix properties	

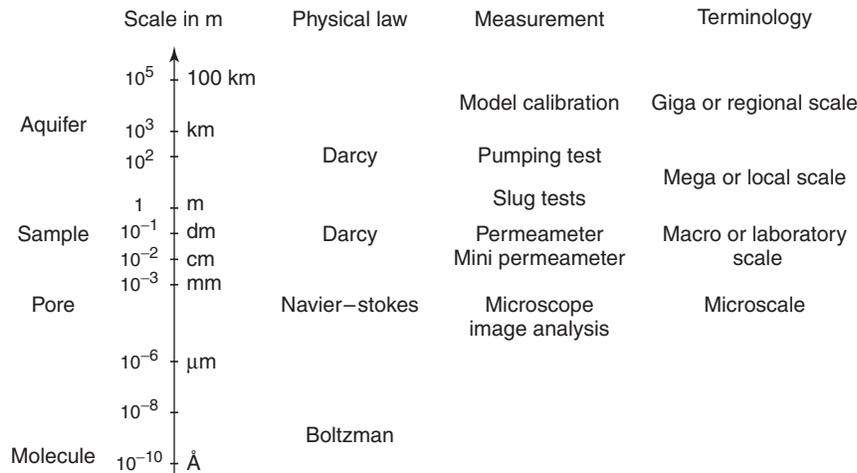


Figure 2 Definition of the characterization scales

To further illustrate these principles, at the microscopic scale the governing equations for groundwater flow are the Navier–Stokes equations (Figure 2). These are parameterized using the fluid viscosity and density, which are the relevant properties at the pore scale. Characterization techniques at this scale include microscopy, X-ray tomography, 3D pore space reconstruction, and so on. Moving to the macroscopic scale, it is possible to demonstrate theoretically that under low Reynolds number, the flux of groundwater through a porous medium obeys Darcy’s law (Matheron, 1967; Mei and Auriault, 1989). The relevant physical parameters that remain are the fluid viscosity and density, but the geometry of the microscopic pore network is now characterized by two macroscopic properties, namely, the permeability and the porosity. Again, moving to a larger scale (mega or gigascopic) it is still possible to prove that the new governing equation is identical in form to Darcy’s law (Matheron, 1967; Sáez *et al.*, 1989), but the permeability represents now an average of the small-scale permeabilities that account for their spatial distribution in

the aquifer, and becomes a tensorial quantity in most cases, even when it is a scalar at the smaller scale. Many upscaling tools exist depending on the type of permeability distribution, but the most accurate techniques require a detailed knowledge of the spatial distribution of the permeability (Renard and de Marsily, 1997).

One of the best examples of a detailed study of scale dependence of the permeability is provided by Tidwell and Wilson (1999). They used an automated mini air permeameter in order to map the permeability of the face of a tuff sample. They measured the permeability with different injection devices (seals) having different radii. In this way, they characterized the permeability field of a sample face at different scales. Figure 3(b) and 3(c) present two permeability maps obtained using different seal sizes. It is apparent from the figures that when the seal size increases, heterogeneities are smoothed out. The statistical description of the permeability field is a function of the scale of observation. The mean slightly decreases with increasing scale (Figure 3e), the variance significantly

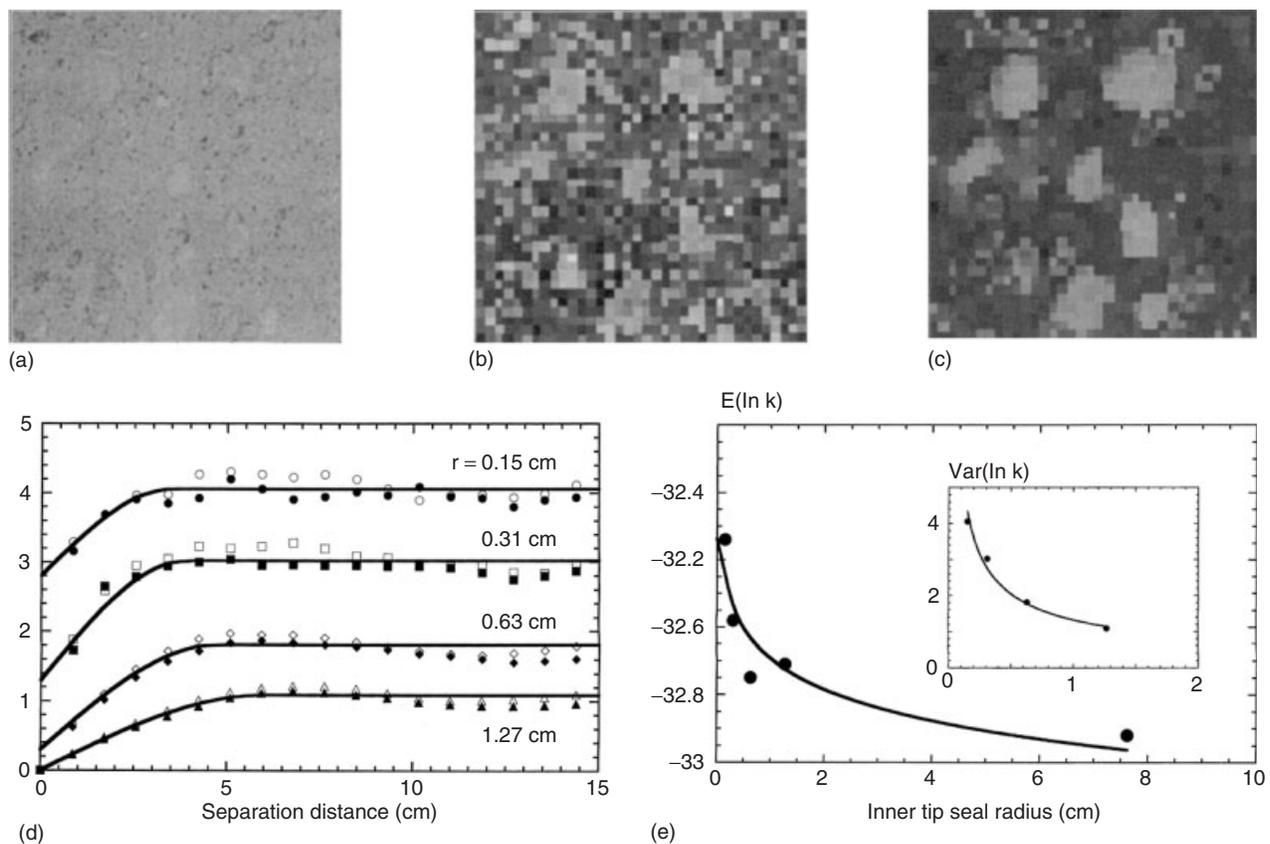


Figure 3 Characterization of the permeability field of a tuff sample at several successive scales. (a) Photograph of the sample face (30 cm times 30 cm); (b) and (c) permeability maps, measured with an injection device having an inner tip seal radius of 0.15 cm and 0.63 cm respectively, showing the smoothing of the permeability contrast with increasing size of measurement device; (d) semi-variograms of the permeability fields as a function of the tip seal radius, r ; (e) expectation and variance of the permeability as a function of the tip seal radius (Reproduced from Tidwell and Wilson, 1999 by permission of American Geophysical Union)

decreases (Figure 3e), and the correlation length increases (Figure 3d).

On a much broader range of scales, several authors (Clauser, 1992; Sánchez-Vila *et al.*, 1996; Schulze-Makuch and Cherkauer, 1998) indicate that the average hydraulic conductivity of a formation increases with scale (Figure 4). These observations contradict the results of Tidwell and Wilson (1999). However, the apparent increase must be analyzed with caution because many experimental data at the laboratory scale are biased towards low values (Zlotnik *et al.*, 2000).

The dependence of hydraulic conductivity with scale is not the exception; the characterization of most parameters strongly depends on the scale of observation. Last but not the least, the elements on which the static and dynamic models have been discretized will, in general, be larger than the support on which measurements have been taken. Therefore, the values assigned to the model elements will always represent some type of averaged, or upscaled value of the underlying hydraulic conductivity distribution. This implies that larger the elements, the smoother their spatial distribution. Large elements should be sampled from probability distributions with smaller variance and larger continuity than small elements. When all elements in the model are of the same size and shape, the only decision to make is the choice of a random function model; however, when the model has been discretized with elements of different sizes, care should be taken to ensure the proper spatial variability for each element size. The rigorous method of defining the parameter values is to establish an upscaling rule to allow the transfer of the statistical characterization that can be inferred from the measurements, at the measurement support, up to the simulation support. Unfortunately, in most cases this extrapolation is never made, and the statistical characterization of the measurement values

is transferred into the simulation support without any correction, incurring in what some authors have termed “not accounting for the missing scale” (Durlafsky, 1992).

DETERMINISTIC CHARACTERIZATION

In this section, we review a few deterministic tools used to define the geometry of a hydrogeological system and to describe the distribution of properties within the geological formations.

Zonation

The whole domain is splitted volume into subvolumes corresponding to different geological objects that can represent hydrostratigraphic units or subunits.

Recently, automatic algorithms have been developed to construct the zonation in three dimensions using geological observations along outcrops, borehole logs, and interpretative vertical sections (Courrioux *et al.*, 2001). Every point that identifies an interface between two zones is represented in three dimensions by a pair of points located on each side of the interface and labeled with a number corresponding to the identifier of the zone. An initial partition of the three-dimensional space is constructed with the help of a Voronoï diagram and interfaces are subsequently smoothed. An example of the application of this method is provided in Figure 5.

Interpolation

Often data are available at points. The data must be interpolated in order to reconstruct either a geometric surface or the spatial distribution of a parameter. The interpolation problem is widely encountered in many fields of

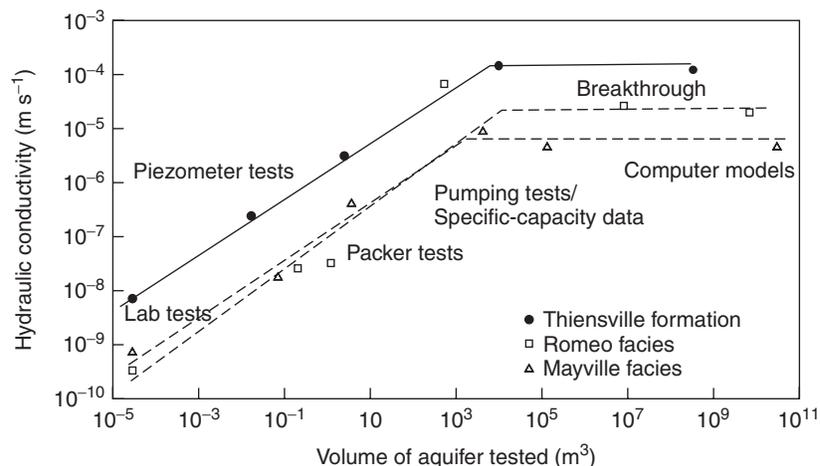


Figure 4 Apparent scale effect in hydraulic conductivity (Reproduced from Schulze-Makuch and Cherkauer, 1998 by permission of Springer-Verlag GmbH)

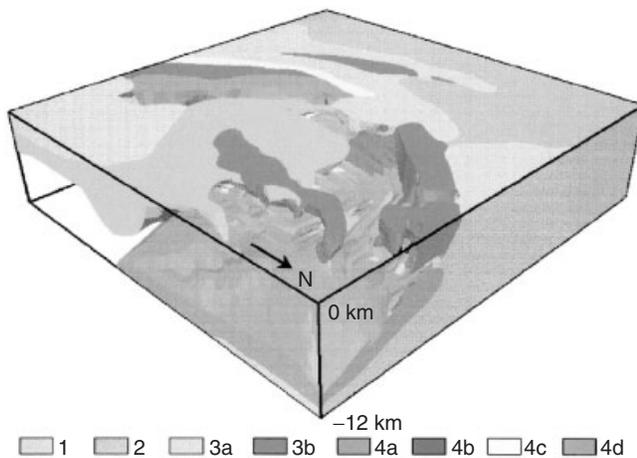


Figure 5 Geometric model of the Cadomian belt constructed automatically using Voronoi diagrams. Every grey level corresponds to a different geological unit ($50 \times 60 \times 12 \text{ km}^3$) (Reprinted from Courrioux *et al.*, 2001. © 2001, with permission from Elsevier) A color version of this image is available at <http://www.mrw.interscience.wiley.com/ehs>

sciences. Consequently, a wide variety of techniques are available. Among the techniques most often used are linear piecewise interpolation, inverse distance weighting, polynomial interpolation, splines, natural neighbor, kriging, and radial basis functions. These techniques are implemented in numerous software packages such as Surfer (<http://www.goldensoftware.com>), ArcGis (<http://www.esri.com>), Idrisi (<http://www.clarklabs.org>), GMS (<http://chl.erd.c.usace.army.mil>), Earth Vision (<http://www.dgi.com>), and FeFlow (<http://www.wasy.de>)

The relative efficiency of interpolation techniques has been investigated in many articles, one of the most recent is the article by Jones *et al.* (2003) who compared the application of inverse distance weighting, natural neighbor, and kriging for the characterization of four different contaminant plumes in three dimensions (Figure 6). This study illustrated that at three sites the kriging technique gave the lowest error; the inverse distance weighting gave the lowest error at one site and performed well otherwise. The natural neighbor method was the least accurate. Note that kriging is considered here as a deterministic method, since only the interpolated values are used but not the estimated uncertainty. The conclusions of Jones *et al.* are not really surprising since kriging (as will be discussed more in detail in the Section “Geostatistics”) is a method whose principle is to minimize estimation errors. What should be assessed is the validity of the variogram analysis of Jones *et al.* when the inverse distance method performed better than kriging. Nonetheless, the main point of interest of their study is that it showed that inverse distance methods, which are very fast

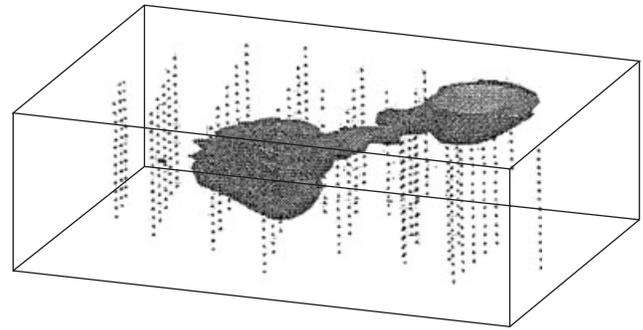


Figure 6 Example of three-dimensional interpolation (kriging) of contaminant concentrations in the cape cod aquifer allowing the location of a contaminant plume to be characterized. The dots represent the data points; the grey zone represents the volume where the interpolated concentrations exceed a threshold (Jones N.L. *et al.*, 2003; reprinted from Ground Water with permission of the National Ground Water Association. © 2003)

and do not require a variogram analysis, perform rather well and can provide an acceptable interpolated map at least in the preliminary stage of a study.

Discrete Smooth Interpolation

A particularly interesting interpolation technique in the framework of geological objects is the so-called Discrete Smooth Interpolation or DSI (Mallet, 2002). The principle of DSI is to construct a discrete representation of an object, a triangulated surface for example, and to impose some constraints on the object. For example, certain nodes are given some fixed positions while others exist, but their location is not known *a priori*. On a node, the orientation of the surface can be defined as a constraint, while its position is unknown. Some constraints such as a minimum distance can be imposed between objects as well. The basis of the DSI algorithm is to minimize the roughness of the discrete object subject to predefined constraints. Generally speaking, the roughness itself is defined as the sum of the squared distance between any point of the graph and the center of gravity of its immediate neighbors.

DSI is an extremely versatile technique. It can be used to interactively model the geometry of complex geological structures including layers and faults. As an example, Figure 7 shows the three-dimensional geometry of the Soûltz horst (Alsace, France). Site characterization is carried out in the framework of a hot dry rock geothermal energy project. In this case, the reservoir geometry was constrained by borehole observations and five seismic profiles. After having identified the different faults and horizons on the seismic profiles, DSI was used to interpolate the triangulated surfaces corresponding to faults and geological boundaries between layers (Renard and Courrioux, 1994).

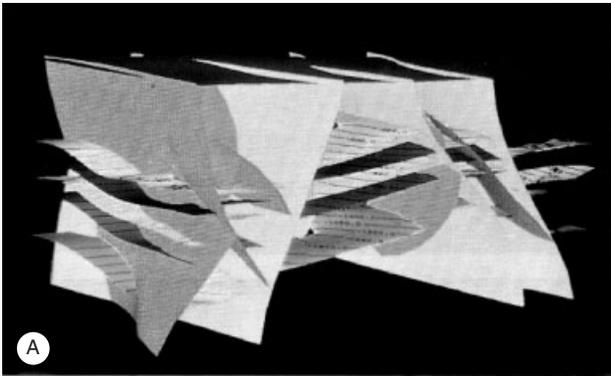


Figure 7 Three-dimensional geometry a network of 18 faults and five stratigraphic layers. The top surface represents the topography, the geometric model extends to a depth of 2 km and has an extension of 6 km by 2 km (Reprinted from Renard and Courrioux 1994. © 1994, with permission from Elsevier) A color version of this image is available at <http://www.mrw.interscience.wiley.com/ehs>

Plausibility Constraints

When interpolating, a common problem is to respect not only the raw data but also some knowledge related to the type of variable that is interpolated. For example, the hydraulic conductivity or the concentration cannot be negative. Another example is the interpolation of the geometry of a three-dimensional surface describing a fault from a series of points in space. In order to be acceptable, it must belong to a certain type of surface such as planes, spheres, cylinders, and surfaces of revolution (Figure 8) as the fault surface has been created by the relative movement

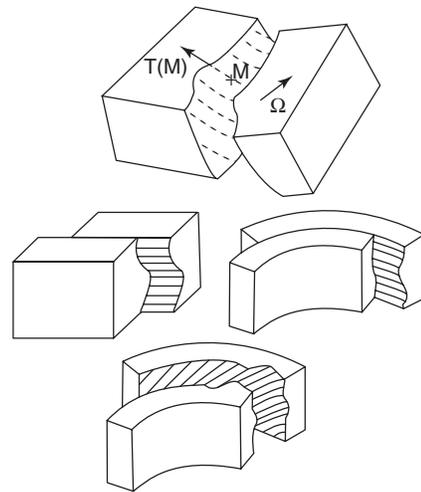


Figure 8 Examples of admissible surfaces for a fault (Reprinted from Thibaut *et al.*, 1996. © 1996, with permission from Elsevier)

of two rigid blocks (Thibaut *et al.*, 1996). Mallet (2002) discusses how to implement such constraints within DSI. As a last example, the interpolation of hydraulic head data must honor boundary conditions. Delhomme (1979) demonstrates how the kriging technique can be modified to account for such constraints (Figure 9).

STOCHASTIC CHARACTERIZATION

Stochastic modeling allows assessing uncertainty. In this section, we present an overview of the statistical models

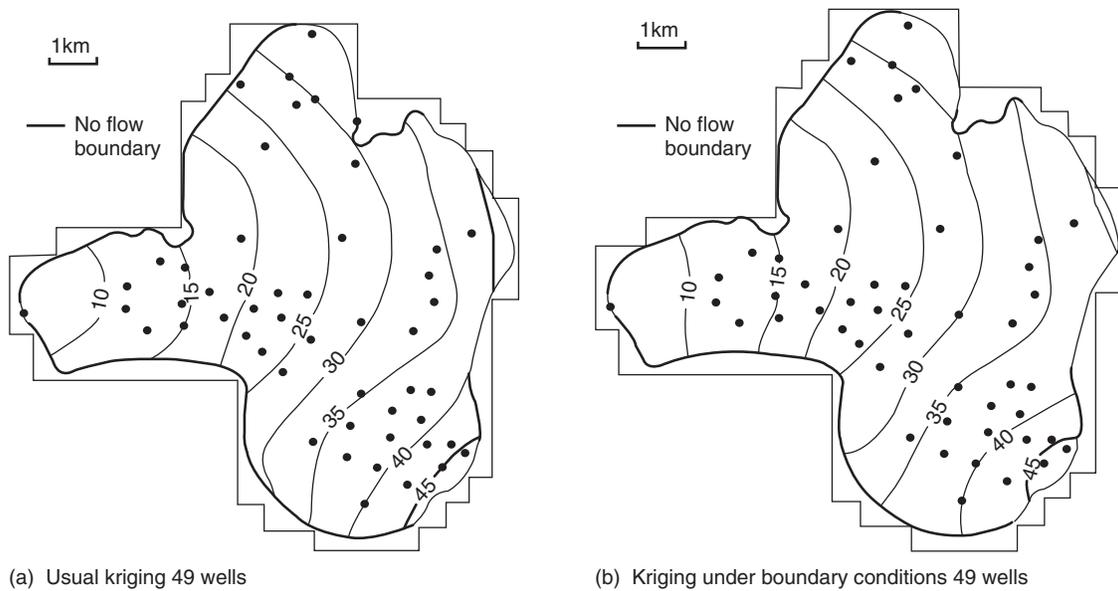


Figure 9 Comparison of (a) standard kriging and (b) kriging under boundary conditions to interpolate piezometric head data (By courtesy of JP Delhomme, 1979)

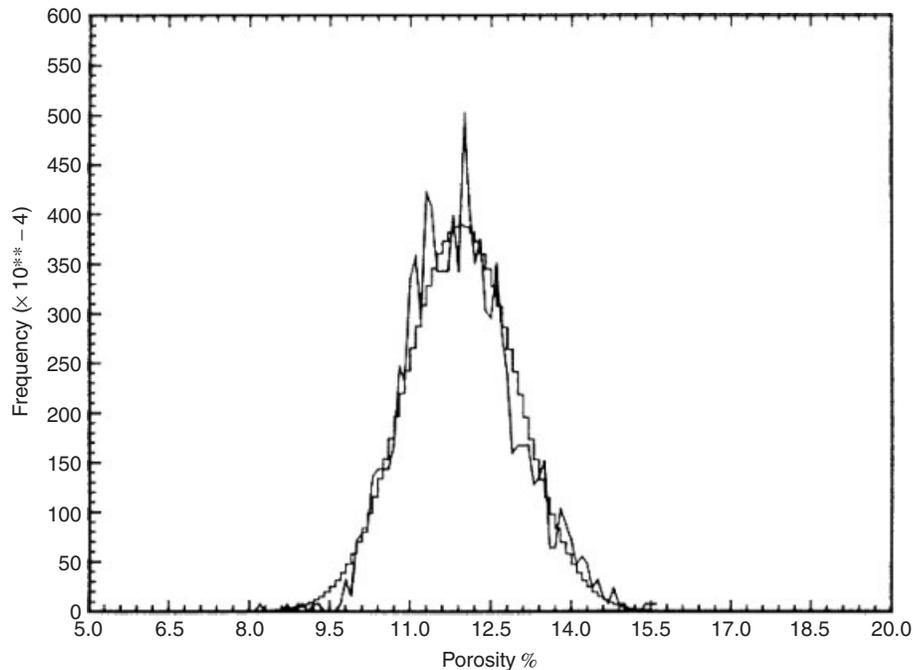


Figure 10 Frequency distribution (experimental and Gaussian model) of porosity of a series of Berea sandstone samples (Reprinted from Bahralolom and Heller 1991. © 1991, with permission from Elsevier)

most currently used for the characterization of porous and fractured media. We start the review with standard statistics, and follow with object-based models, geostatistics, and finally a short overview of the emerging field of multiple points geostatistics.

Statistics

The first kind of stochastic analysis, which is conducted when characterizing a hydrogeological system, is to investigate the univariate and nonspatial statistics. The most simple and complete statistical tool during this first step is to analyze the experimental probability density functions (pdf). The pdf allows the analyst to infer the degree of variability of the property, the type of probability law that would best represent the data, the possible multimodality, and so on. When conducting such analyses, special tools must be used when dealing with data that fall into a finite mathematical space (i.e. compositional data, fracture orientations). In the case of fracture orientation, the field data are a series of orientation angles (strike and dip). The usual way to represent these statistics is a contoured stereographic projection that allows the main families of fractures, their mean orientation, and variability around the mean to be defined (see **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**).

When the experimental statistics have been analysed, simple statistical models can be used to represent the data. For example, Figure 10 shows an example of porosity pdf

taken from a number of sandstone samples. The resulting plot indicates that, in this case, a Gaussian distribution, defined by its mean and variance, can be used to model the porosity distribution.

The statistical analysis of fracture observations along boreholes, tunnel faces, or maps requires some specific tools. For example, the statistics are calculated from data that are usually gathered on 1D or 2D space, but they need to be corrected by stereological techniques in order to estimate the 3D statistics. Chilès and de Marsily (1993) provide an excellent overview of specific statistical (and geostatistical) techniques used to analyze fractures and fracture networks. One of the particular aspects of fracture network statistics is that they often exhibit a very wide range of scales and therefore their statistics can be described by power laws (Figure 11) relating over certain domains (Bonnet *et al.*, 2001; Bour *et al.*, 2002).

A second step of the statistical characterization is to investigate the multivariate statistics to define correlations between them. The variables can be numerical properties and also categorical properties such as lithofacies or hydrofacies indicators. When a large number of numerical variables are available (e.g. geophysical logging), a systematic statistical analysis complemented with the application of a classification algorithm may allow the various relevant litho or hydrofacies identifications in a semiautomatic way. The same statistical techniques are applied to characterize water types within an aquifer (Güler *et al.*, 2002).

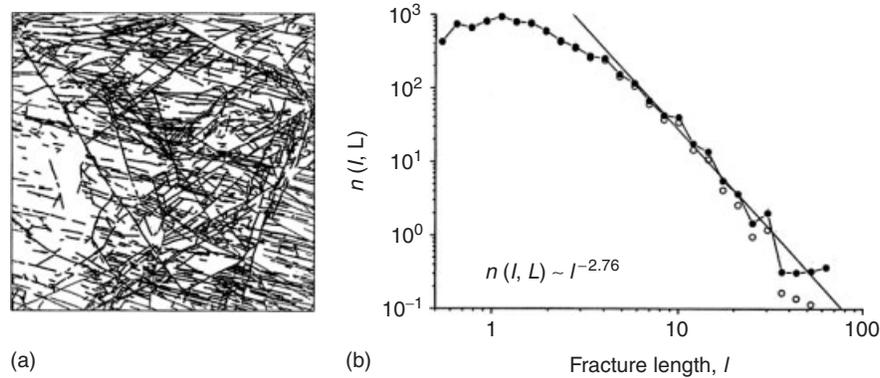


Figure 11 (a) Map of a fracture network in a sandstone outcrop ($90 \times 90 \text{ m}^2$) in Norway and (b) density length distribution. The power law begins when the fracture length is greater than 5 m (Reproduced from Bour *et al.*, 2002 by permission of American Geophysical Union)

Object-based Models

Object-based models attempt to reproduce the geological architecture of the aquifer by locating objects with shapes that resemble geological bodies using rules about their position, size, and shape, and also rules of attraction, repulsion, and spatial proportions. These objects are assimilated to specific geologic facies, which are later assigned porosity and hydraulic conductivity values.

The most common algorithms used in object-based models are Boolean models. These models work with deterministic shapes defined by stochastic parameters. For instance, the early models by Haldorsen and Lake (1984) reproduce sand/shale reservoirs in which shales are included as parallelepipeds with random locations and sizes. Generating such a model starts by randomly drawing a point in space and then drawing at random the three sizes of the parallelepiped (representing a shale inclusion) that is located at the drawn point. This procedure is repeated until a predetermined sand/shale proportion is reached. These models have evolved substantially to include (i) more elaborate shapes, which may better resemble the geological bodies (Figure 12) and (ii) complex rules regarding allowed relative positions of the objects, that is, following a stratigraphic sequence, erosion rules, and so on (Jussel *et al.*, 1994; Scheibe and Freyberg, 1995).

Realizations generated with object-based models are appealing to geologists; however, their main drawback is the difficulty to condition these realizations to large amount of data: it is very difficult to randomly draw objects obeying all rules and honoring borehole information. Other drawbacks are that lithofacies do not conform to the simple geometries used, lithofacies are not randomly distributed in space, and that these algorithms are difficult to generalize and must be custom designed for each depositional pattern. Some of these drawbacks have been addressed by Tyler *et al.* (1994) with different degrees of success.

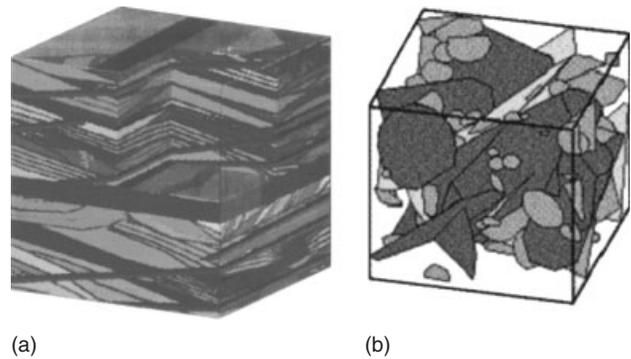


Figure 12 Two examples of object-based models. (a) Simulated structure of a point bar deposits. The dark grey represents low permeability while the light grey represents high permeability region. The cube represents approximately 1 cubic m (Reproduced from Scheibe and Freyberg, 1995 by permission of American Geophysical Union). (b) 3D fracture network. The fractures are assumed to be disks. The network is simulated according to the inferred statistics of fracture orientation, length, and density (Reproduced from Ezzedine, 1994 by permission of American Geophysical Union) A color version of this image is available at <http://www.mrw.interscience.wiley.com/ehs>

Geostatistics

The word geostatistics, or geographical statistics, was defined by Matheron in 1962 to designate a set of statistical techniques used for ore reserve evaluation. The key concept is to quantify, in statistical terms, how the information provided by a sample located in space and/or time influences the statistics of possible values of the same variable at any distance from this data point. This information is quantified with a variogram or a covariance function. The same tools can also be applied to a set of different variables accounting for spatial cross-correlation between variables. These techniques and formulations are described in various references

(Matheron, 1962; Journel, 1989; Goovaerts, 1997; Kitani-dis 1997; Chilès and Delfiner, 1999; *see Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4*).

In practice, dedicated software is available either as interactive packages such as Isatis (<http://www.geovariances.com>), WinGslib (<http://www.gslib.com>), Gocad (<http://www.gocad.com>), Fsstools (<http://www.fssintl.com>), Earth Vision (<http://www.dgi.com>), or as source libraries such as gslib (<http://www.gslib.com>) and the geostatistical template library GsTL (http://pangea.stanford.edu/~nremy/GTL/GsTL_home.html).

Applying geostatistics first involves an exploratory data analysis. If we greatly simplify the procedure, the data exploration consists of analyzing the experimental variogram of the data in order to identify the most appropriate variogram model. The exploratory data analysis can be applied either to a continuous variable or to an indicator variable that represents the presence or absence of a geological object (lithofacies).

When the variogram model is inferred, kriging is used to interpolate at any location conditioned to data within the neighborhood and the variogram. Kriging provides an estimation of the expected value of the variable and its variance that represents the possible error of estimation at the same location. Maps obtained by kriging have already been shown in Figure 6 and Figure 9.

When the characterization process requires an estimation of a property P_1 that does not linearly depend on the property P_2 for which data is available, it is necessary to use nonlinear geostatistical techniques. For example, the statistical expectation $E()$ being a linear operator (i.e. an arithmetic average), and if P_2 is a nonlinear function of P_1 , that is,

$$P_2 = f(P_1) \quad (1)$$

then the expectation of P_2 is not equal to the transform of the expectation of P_1 :

$$E[P_2] = E[f(P_1)] \neq f(E[P_1]) \quad (2)$$

It means that it is erroneous to apply a nonlinear function to a kriged map in order to estimate the expected value of the transform.

To circumvent this problem, the most general nonlinear geostatistical technique is the use of stochastic simulations. Instead of estimating the expected value, the principle is to generate a series of equiprobable realizations that are constructed in order to honor the data points, the variogram, and the pdf of the data. One can then apply the nonlinear transformation to each of these maps and calculate the statistics of the results. Another important aspect is that the kriged field is smoother than the data (Figure 13). The simulated field, instead, has the same spatial structure (variogram) as

observed in the data (Figure 13), as well as the same pdf, but it is only one possible reality, one equiprobable realization. Estimation (kriging) and simulation are therefore not applicable for the same purposes. Kriging is useful to map the expected value and to identify the main trends in a field. Simulations are useful when predictions, such as flow and transport simulations, must be applied on the field.

When applied to generate equiprobable realizations of a continuous variable, some geostatistical models rely heavily on the use of a multi-Gaussian distribution. This multi-Gaussian character has some unwanted side effects that should be carefully considered before use, namely, the lack of connection of the extreme values at the tails of the probability distributions, that is, it is very difficult for multi-Gaussian-based realizations to display flow channels or flow barriers (Gómez-Hernández and Wen, 1998; Wen and Gómez-Hernández 1998).

As an alternative to multi-Gaussian models, indicator-based geostatistical models were developed. In indicator-based geostatistics, the different classes (or categories) in which the range of variability of the parameter under study could be divided, are independently characterized, thus controlling the spatial correlation of all classes, particularly those at the extreme ends of the distribution. Each indicator class is characterized by its own variogram function. One of the earliest applications of indicator-based geostatistics was discussed by Gómez-Hernández and Srivastava (1990) in the context of the simulation of a sand-shale sequence.

The main advantage of all geostatistical methods is their ability to be conditional to parameter measurements. Thus, the realizations not only have the spatial patterns characterized by the variogram function but also honor the parameter data. As a consequence, the larger the number of conditioning data, the more alike are the generated realizations and less the uncertainty on the predictions based on these conditional realizations.

Multiple-point Geostatistics

A recent development of geostatistics that goes beyond the variogram-based geostatistics (whether Gaussian or indicator) deserves a section of its own. The major criticism to geostatistical methods has come from the proponents of object-based simulations criticizing the difficulty in reproducing intricate geological patterns when the only controlling tool is the variogram (a two-point statistics measure). For instance, it is very difficult to generate meandering-like depositional patterns, or realizations respecting certain stratigraphical ordering of the facies generated. A solution to this problem was proposed by Strebelle (2002) that departs from traditional geostatistics. Conditional probability values are computed directly from conditioning data using the exact geometrical pattern of the surrounding data with respect to the point being estimated. (In traditional geostatistics, these conditional probabilities are computed

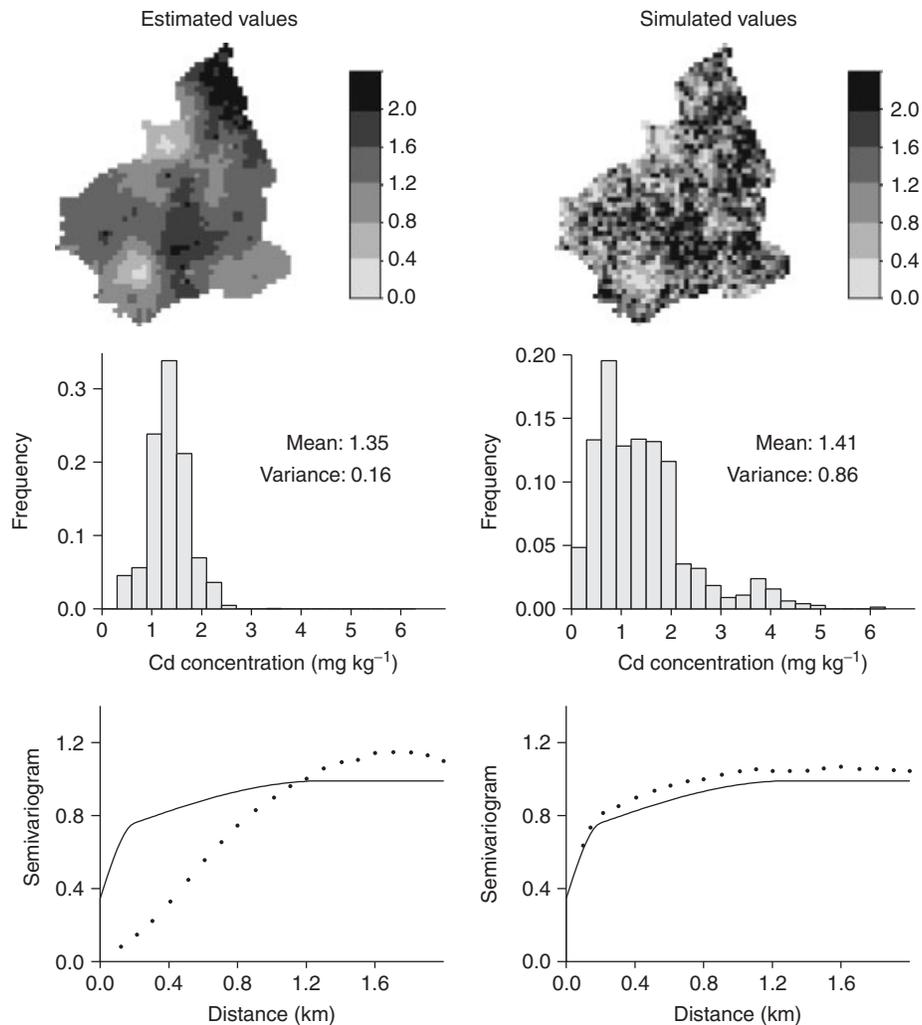


Figure 13 A typical example showing the differences between a map of Cadmium (Cd) interpolated with ordinary kriging (a) and simulation (b). The figure shows the differences in pdfs and variograms calculated *a posteriori* for the two maps. The solid line represents the variogram model and the dotted line represents the experimental variogram calculated *a posteriori* on the interpolated fields (Reproduced from Goovaerts, 1997 by permission of Oxford University Press)

by considering only the separation vectors between each pair of data, and between each datum and the point being estimated.) Evaluating the conditional probability in the way proposed by Strebelle requires establishing the probability distributions for any possible data configuration. Since this is impossible to perform from sample data, Strebelle suggests the use of training images derived from outcrops, expert knowledge, or even a geologist's drawing. He also suggests to only use the nearby data; therefore, reducing the number of conditioning data configurations for which the probability distribution has to be derived.

Multiple-point geostatistics is capable of generating realizations that are very similar to those obtained with object-based algorithms, with the advantage that it can be made conditional by construction, therefore surpassing the main problem of object simulation.

The main criticism to multiple-point geostatistics is the selection of a training image from which to infer the multiple-point statistical model, especially in three dimensions. Outcrops are good for 2D realizations, but there are no three-dimensional outcrops, and it is not trivial to combine multiple 2D training images into a single 3D one. A possible solution to the problem of 3D training images would be to use a genetic model or an object-based model to generate a realization from which to infer the multipoint statistical model. Multiple-point realizations based on such a model will look like the ones obtained from the genetic or object-based models, but will be conditional to well data. Another caveat is that its implementation for practical applications is full of difficulties and computational tricks if CPU-times are to be kept reasonable.

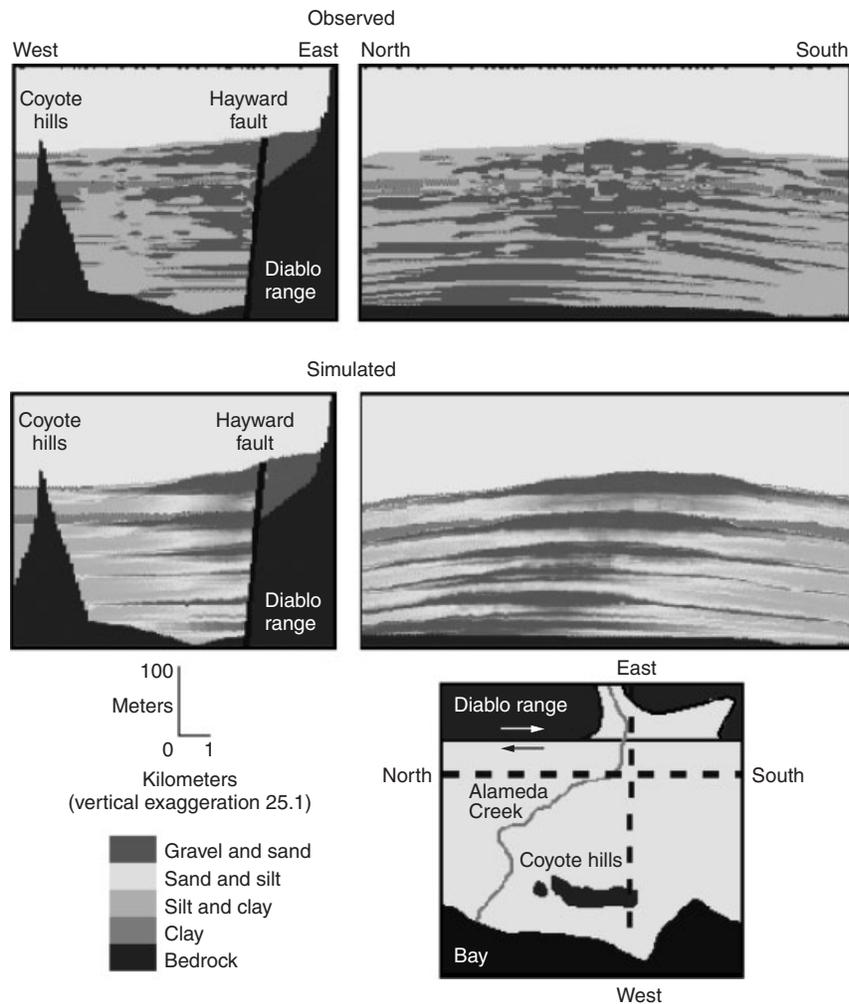


Figure 14 Reconstruction of the internal architecture of the sedimentary complex of the San Francisco Bay, California by a process-imitating model (Reprinted with permission from Koltermann, C. E., and S. M. Gorelick. 1992. Paleoclimatic signature in terrestrial flood deposits. *Science* 256, 1775–1782. © 1992 AAAS) A color version of this image is available at <http://www.mrw.interscience.wiley.com/ehs>

GENETIC MODELS

Genetic models, which should not be confused with the genetic algorithms used in global optimization, assign parameter values to the elements of the model by simulating the genesis of the aquifer. One of the first models capable of generating realizations of facies is SEDSIM. This program was developed by Tetzlaff and Harbaugh (1989), and it simulates the genesis of a sedimentary basin by modeling the processes of erosion, transport, and sedimentation. SEDSIM moves fluid particles over a 2-D grid, in which sediments from multiple types continuously mix. The basic principle of SEDSIM is that a fluid element moves down the slope as velocity increases its capacity to erode and pick up sediments, then when it finishes descending the slope, it slows down, its transport capacity decreases, and the sediments are deposited.

These models are mechanistic, in the sense that they reproduce the mechanical processes involved in the genesis of sedimentary basin. They must be run over tens of thousands of years, and require initial and boundary conditions that are difficult to estimate, as well as identifying of the external stresses that drive the processes. For example, information of the initial spatial distribution of the material that will be eroded is needed, as well as information about pluviometry over the entire simulation time. Because most of these inputs are impossible to determine and, at most, they are drawn from predefined probability distributions, these models cannot be called deterministic, even though they use deterministic models to obtain the spatial representation of the parameters.

One of the successful applications of the method (Figure 14) was performed by Koltermann and Gorelick (1992). They simulated the genesis of an alluvial fan-aquifer

system in north-central California (US). For this purpose, they had to collect local and regional geologic and climatic data, and hydrologic history of the study area. They also had to address sea level change, fault motion, sediment loading, compaction, porosity relations, and paleoclimate-driven fluctuations in floods and sediment loads. In addition, they had to simulate flood events using a stochastic streamflow time series. The geometry and geology of the fan-aquifer was simulated for 6 000 000 years. The output grain size distributions from the process model were transformed into porosity and hydraulic conductivity values using petrophysical relations.

Genetic models such as the ones described here are computationally intensive; however, they produce realistic images of large-scale sedimentary structures provided the model inputs are carefully constrained. The realizations are realistic at a large scale; however, locally it is very difficult to condition them to specific porosity or conductivity values at certain locations. This last caveat of genetic methods could be their major drawback. Lately, some researchers have been working on the problem of conditioning, such as Karssenberg *et al.* (2001). Others have developed agent models in order to trigger the behavior of the sediments while reducing the computational load (Teles *et al.*, 2001).

INVERSION METHODS

Inverse theory is concerned with the problem of making inferences about physical systems from data (directly measured or remotely sensed). Since nearly all data are subject to some uncertainty, these inferences are usually statistical. Further, since one can only record finitely many (noisy) data and since physical systems are usually modeled by continuum equations, no inverse problems are really uniquely solvable: if there is a single model that fits the data, there will be an infinite number of them. Our goal then is to characterize the set of models that fit the data and satisfy our prejudices as well as other information. This section describes how to determine model parameter values. Models are assumed to be valid; the only unknowns are parameter values that define the models. For completeness, we introduce some concepts and terminology commonly used in inverse/forward problem community. Detailed coverage of the inverse problem using deterministic tools and stochastic tools is given in **Chapter 156, Inverse Methods for Parameter Estimations, Volume 4** and **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4** respectively.

Well-posed versus Ill-posed Problem

Prediction based on a given set of parameter values is called *forward modeling*. Determination of parameter

value from observed data is called *inverse modeling*. Inversion requires minimizing the discrepancy between predictions and observations. Inversion can be achieved in two ways. On one hand, a modeler iteratively modifies parameter values (such as hydraulic conductivity), and runs a forward model (i.e. ModFlow, FeFlow) until attaining best “fit” or “match”. This kind of process falls into the trial and error methods. Such forward modeling is sometimes tedious and time consuming. On the other hand, an inverse algorithm can be adopted to automatically or semiautomatically obtain the parameter values from the observed data and an initial set of trial parameters values. The procedure also provides an estimate of parameter uncertainty and resolution.

A well-posed inverse problem requires “existence” of the problem, the “uniqueness”, and the “stability” of the solution or algorithm. Obviously, in view of the observed data and our understanding of a real-world physical system, a problem is presumed to exist, for example, detection of contaminant plume in groundwater suggests that contamination must have happened in the past. The question then is how to relate the observation to the migration history of the contaminant. A cause generally has an effect. Can an effect result from different causes? Is it unique in theory or model? Even if it is, have we counted and resolved all parameters that define a model?

Inverse uniqueness has two levels: the model itself and the model-defining parameters. The latter is related to the stability of a solution algorithm. How sensitive are parameters to uncertainty of observed data? Are the errors amplified during inversion? Is the inversion algorithm efficient in terms of ease of usage and cost of running the inversion program (complexity)?

Deterministic versus Stochastic Inversion

An inverse model attempts to obtain a spatial distribution of the parameter values, so that the simulated state of the system, using forward flow and transport models, reproduce the observed state of the system at those locations. Because the relationship between state variables and parameters is not linear, conditioning parameter realizations to state variable data is not trivial, and, in general involves nonlinear optimization algorithms, in which the objective function and its gradient are very expensive to evaluate.

To address the inverse problem, two main frameworks have been developed and they are either deterministic or stochastic. In the deterministic framework, the structure of the spatial variability of the parameters is fixed. For example, the aquifer is divided into a number of zones, and each zone is supposed to have a constant hydraulic conductivity; then, the algorithm seeks the best hydraulic conductivity values for which the solution of the flow equation reproduces the state data (Carrera and Neuman, 1986).

However in a stochastic framework, the spatial variability of the parameters is statistically mapped. For example, the overall average and variance, and the variogram of the final realization are specified; this characterization is not enough to fully determine the parameter values at every cell. Then, a spatial realization is sought meeting the statistical constraints, conditional to the parameter values, and so that the forward model of the state of the system matches the observed values. Many alternative realizations can meet the statistical constraints and reproduce the state data. The self-calibrating method by Gómez-Hernández *et al.* (1997) was developed for this purpose. To make these inferences quantitative in either deterministic or stochastic framework, one must answer three fundamental questions:

1. How accurately is the data known, that is, what does it mean to “fit” the data?
2. How accurately can we model the response of the aquifer system? In other words, have we included all the physics in the model that contribute significantly to the data?
3. Finally, what is known about the system independent of the data? This is called *a priori* information and is essential since for any sufficiently fine parameterization of an aquifer system there will be unreasonable models that fit the data too. Prior information is the means by which we reject or down-weight unreasonable models.

Examples of Stochastic Inversion Methods

It has already been pointed out that the final hydraulic property realization cannot disregard the measurement data; they are the only factual knowledge available about the aquifer. However, aquifers are systems, the state of which is described by the spatial distribution of piezometric heads, and by the concentration of the solutes dissolved in water. In general, there is more information about the state of the system than about the parameters that controls it. Therefore, it appears necessary to generate spatial distributions of the parameters that are not only conditional to parameter values, but also consistent with the (partial) knowledge about the state of the system. We will illustrate this stochastic inversion by constraint through three examples (*see Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4* for more details).

Cokriging methods. Rubin and Dagan (1987a, b) used the analytical approach to solve the perturbed flow equation. They calculate $h' = h - E[h]$ and $Y' = Y - E[Y]$ at the points of h , head, and Y , log of transmissivity, measurements and determined analytically the covariance function of h' and the cross-covariance (h' , Y') as a function of the covariance of Y . The covariance of Y is function of

a set of parameters q (integral scale of Y and its variance). This is actually sufficient to estimate the transmissivity field by cokriging. The cokriging estimator then gives the optimal estimation of Y at any point as follows:

$$Y(x) = \sum_{i=1}^{n_Y} \lambda_i Y_i + \sum_{j=1}^{n_H} \nu_j (h_j - E[h_j]) \quad (3)$$

where the λ_i and the ν_j are optimal weights that depend on the position x . The cokriging equations that provide the value of the optimal weights simply require that the covariance functions of Y , of h , and of $h - Y$ be known. They are developed by Rubin and Dagan (*see Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4*). Rubin and Dagan then calculate by cokriging all the values of Y at the measurement points where Y is known and where it is therefore possible to compare the known value with the one estimated by cokriging – without using the known value of this point in the cokriging equations. As the cokriging estimator is a function of the q parameters, these parameters can thus be optimized to minimize the errors between the estimated and measured Y values. The Maximum Likelihood method was used for their optimization (*see Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4*). Once the q parameters are known, the cokriging equations give an estimation of Y at all points and a map of Y is obtained (Figure 15).

Bayesian Inversion. For a statistician, an inverse problem is an inference or estimation problem. The data are finite in number and contain errors, as they do in classical estimation or inference problems; the unknown typically is infinite dimensional, as it is in nonparametric regression. The additional complication in an inverse problem is that the data could be directly and indirectly related to the unknown. Bayesian techniques have become more attractive for the hydrogeological communities through the elegant work of Tarantola (1987). One of the fundamental tenets of Bayesian inference is that uncertainty always can be represented as a probability distribution; in particular, the Bayesian approach treats the model as the outcome of a random experiment. The essential defining property of a Bayesian is to talk about the probability $P(H|E)$ of a hypothesis H , given evidence E . Whether one adheres to a Bayesian view, estimators that arise from the Bayesian approach have an attractive property, that is, the posterior pdf is at least as informative as prior one. In this case, the likelihood function is called *diffusive* or totally noninformative, and the prior estimates are exactly equal to the posterior estimates. It is emphasized that the method does not always guarantee better estimates for a couple of reasons. First, the Bayesian approach

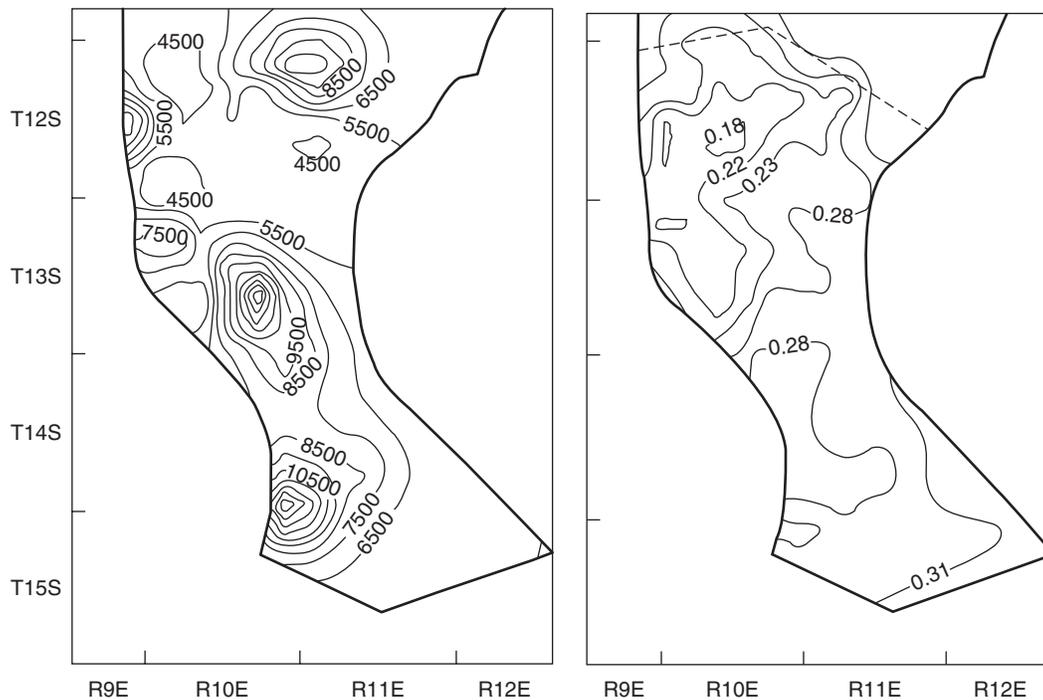


Figure 15 Estimated transmissivity T in $\text{ft}^2 \text{day}^{-1}$ (a) and the conditional variance of $\ln[T]$ (b) based on cokriging and maximum-likelihood estimation (Reproduced from Rubin and Dagan, 1987b by permission of American Geophysical Union)

provides a pdf, not a single-valued estimate. Second, the improvement achieved in the posterior pdf is dictated by the quality of external factors such as the accuracy of the geophysical survey and the petrophysical model in the case of geophysical–hydrogeological stochastic joint inversion.

Bayesian inversion is illustrated in Ezzedine *et al.* (1999). Their hierarchical approach is intended to integrate and transform the well log data to a form in which it can be updated by the geophysical survey, and this tends to be a convoluted process. They started with generating images of the lithology, conditional to well logs. Each lithology image is then used as the basis for generating a series of shaliness images, conditional to well log data. Shaliness images are converted to resistivity images using a site-specific petrophysical model relating between shaliness, resistivity, and lithology, to create the necessary interface with the cross-well resistivity survey. The lithology and resistivity images are then updated using cross-well electromagnetic resistivity surveys. They explored the limits of the approach through synthetic surveys of different resolutions and error levels, employing the relationships between the geophysical and hydrological attributes that are weak, nonlinear, or both. The synthetic surveys closely mimic the conditions at the Lawrence Livermore National Laboratory (LLNL) Superfund site. Ezzedine *et al.* (1999) showed that the proposed stochastic Bayesian approach improves hydrogeological site

characterization even when using low-resolution resistivity surveys (Figure 16).

Self-calibrating Stochastic Inversion

The self-calibrated algorithm (Gómez-Hernández *et al.*, 1997) is the first algorithm specifically aimed at the generation of hydraulic conductivity fields conditional to hydraulic conductivity and transmissivity data without resorting to any approximation of the state equation or linearization of the relationship between head and conductivity. It has been later extended to the generation of realizations conditioned to concentration data by Sahuquillo *et al.* (1999) and Hendricks Franssen *et al.* (2003).

In the self-calibrating approach, multiple realizations of the parameters controlling groundwater flow movement and mass transport, that is, hydraulic conductivity, transmissivity, or specific storage, are generated conditioned to values of the parameters and of the state variables. That the realizations are conditioned to the parameter values means that all realizations display the patterns of variability and cross-correlation observed in the field and modeled by a random function, and, at the same time, each realization honors the measured parameter values at their measurement locations. That the realizations are conditioned to the state variables means that the solution of the groundwater flow and mass transport equations with the parameter realizations generated results in the prediction of the state of the system that

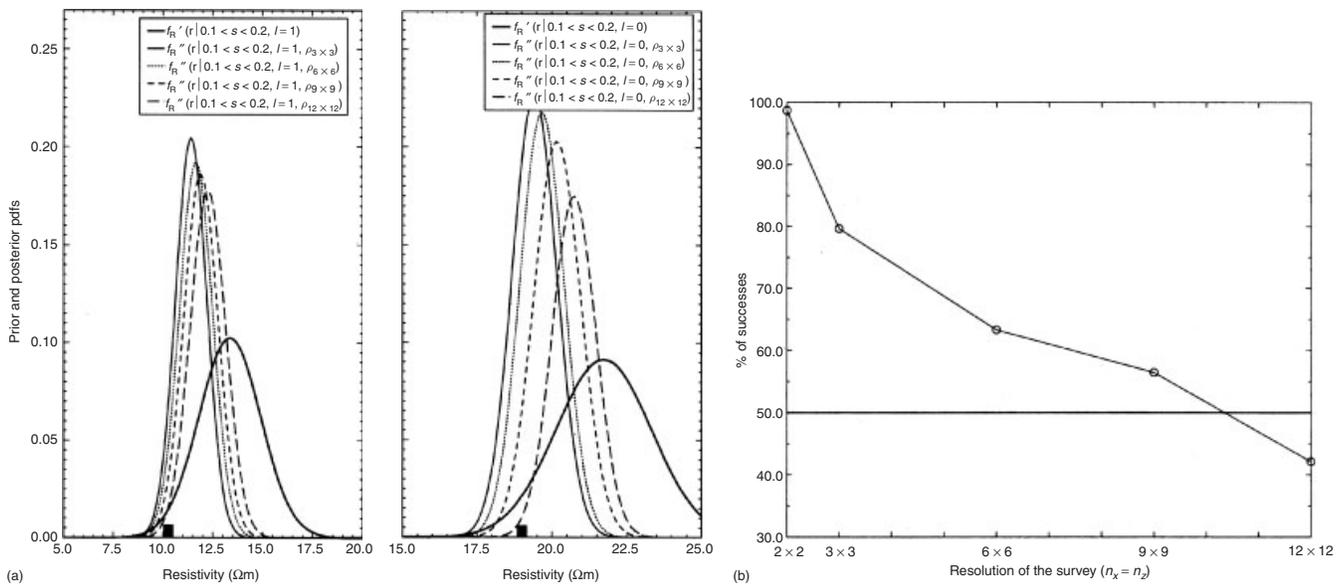


Figure 16 (a) Effect of the block resolution of the $n_x \times n_z$ resistivity survey on the posterior pdf's (prior pdf's are also plotted). The bias in the variance and the mean decrease with the increase of the resolution of the resistivity survey (from 12×12 , 9×9 , 6×6 , to 3×3). The black box denotes "true" resistivity values. Prior and posterior pdf's for shaliness between 0.1 and 0.2 in silt (left) and sand (right). (b) Percentage of number of successes of the Bayesian updating approach for different survey resolutions and different errors in the surveys (Reproduced from Ezzedine *et al.*, 1999 by permission of American Geophysical Union)

honors the spatiotemporal measurements of the state variables. Achieving such a dual conditioning amounts to solve a deterministic inverse problem for each realization, something that can only be done after a careful parameterization of the spatial variability of the realizations and efficient computational algorithms.

CONCLUSION

Looking back at the models described here, it is concluded that the best alternative to characterize the spatial variability of a given parameter is through the use of hybrid models. It is important to capture the architecture of the different facies in the aquifer, as it is to capture the variability of the parameters within each facies. Hybrid models start by using a genetic model, an object-based model, or any of the geostatistically-based models capable to generate facies realizations, to generate the spatial distribution of the different facies present in the aquifer; then a geostatistical model (either Gaussian or non-Gaussian) is used to fill in each facies with spatial distributions of the parameters. An example of this approach can be found in Cox *et al.* (1994), who used the cross-sectional geologic images created with a genetic model to estimate the parameters of an indicator-based spatial statistical model. Then, conditioning and generating multiple realizations of hydraulic conductivity were achieved with a geostatistical model.

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