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A Geostatistical Approach to the Inverse Problem In Groundwater Modeling (Steady State) and One-Dimensional Simulations

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The problem of estimating hydrogeologic parameters, in particular, permeability, from input-output measurements is reexamined in a geostatistical framework. The field of the unknown parameters is represented as a 'random field' and the estimation procedure consists of two main steps. First, the structure of the parameter field is identified, i.e., mathematical representations of the variogram and the trend are selected and their parameters are established by using all available information, including measurements of hydraulic head and permeability. Second, linear estimation theory is applied to provide minimum variance and unbiased point estimates of hydrogeologic parameters ('kriging'). Structure identification is achieved iteratively in three substeps: structure selection, maximum likelihood estimation, and model validation and diagnostic checking. The methodology was extensively tested through simulations on a simple one-dimensional case. The results are remarkably stable and well behaved. The estimated field is smooth, while small-scale variability is statistically described. As the quality of measurements improves, the procedure reproduces more features of the original field. The results are also shown to be rather insensitive to deviations from assumptions about the geostatistical structure of the field.

1. INTRODUCTION

1.1. *Parameter Estimation in Groundwater Modeling*

One of the most important tools available in the study of groundwater systems is the numerical solution to deterministic models of flow and mass transport in porous media. During the last two decades a great number of solutions have been proposed to models based on a variety of assumptions. The description of the physics of flow and mass transport through porous media leads to the formulation of boundary value problems. The mathematical solutions of the pertinent boundary value problems is performed by groundwater simulation models, usually by employing numerical techniques such as finite differences [*Remson et al.*, 1971] and finite elements [*Pinder and Gray*, 1977].

In the last decade a significant number of these groundwater models have been applied on a regional (or basinwide) basis for prediction or simulation purposes. Examples include the prediction of the system flow and quality responses to given excitations, such as natural and artificial recharge, change of pumping rates and/or patterns, surface or subsurface discharge of pollutants, and saltwater intrusion in coastal aquifers. For this purpose, hydrogeologic parameters such as permeabilities, storativities, and diffusivities must be known. However, in practice, the required distributions of system parameters are very difficult to obtain. This difficulty is recognized to be a major impediment to wider use of groundwater models and to their full utilization [*Frind and Pinder*, 1973]. *Freeze* [1972] called the estimation of parameters the 'Achilles' heel' of groundwater models.

The problem arises because of the scarcity of available direct measurements of the hydrogeologic parameters. But even in the cases where measurements do exist, they reflect conditions at the point of measurement and cannot be considered representative of regional conditions [*Freeze*, 1972]. In practice, the main source of information about the hydrogeologic parameters is extracted from pumping tests, that is, from a study of the drawdown curve at a well being pumped at a known rate. However, this method of parameter estimation is based on several assumptions, such as homogeneity of the aquifer (or groundwater system) in a large region around the well, negligible influence of pumping or recharge around the well, etc. Consequently, the results of pumping tests reflect local conditions and are not considered the most appropriate for use in regional groundwater simulation models.

To overcome the very real data limitations, current methods of hydrogeologic parameter estimation rely heavily on the extraction of information from measurements on the input-output behavior of the system. This is accomplished through the selection of a set of parameters in such a way that measurements of the water table elevations, the concentration of solutes, and other variables describing the system can be reproduced through the model. This method has been widely applied as a manual trial and error procedure, but recently a large number of systematic and computerized methods, based on formal mathematical procedures, have been proposed. In general terms, in the direct problem the parameters are treated as known constants. If the input or excitation function and the corresponding response function are considered known, the parameters can be treated as dependent variables in a new formal boundary value problem. The solution of this boundary value problem is called the inverse problem of groundwater modeling.

Reviews of the extensive literature on the inverse problem can be found elsewhere [e.g., *Kitanidis*, 1976; *Neuman and Yakowitz*, 1979] and will not be repeated here. The approach

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which will be described in the work is related to statistical approaches to the inverse problem [*Gavalas et al.*, 1976; *Kitanidis*, 1976; *Dogru et al.*, 1977; *Cooley*, 1977, 1979, 1982; *Shah et al.*, 1978; *Wilson et al.*, 1978; *Neuman and Yakowitz*, 1979; *Neuman et al.*, 1980; *Neuman*, 1980; *Yeh and Yoon*, 1981; *Clifton and Neuman*, 1982; and others].

1.2. *Parameter Identifiability*

A serious problem encountered in the estimation of parameters of groundwater models stems from their overparametrization or the inclusion of 'unidentifiable' parameters. Lack of identifiability is simply the lack of sufficient information to distinguish between alternative parameter sets [*Rothenberg*, 1971]. *Gavalas et al.* [1976, p. 337] epitomize the problem as follows:

> ... in a given problem, many different sets of property estimates may provide satisfactory and essentially indistinguishable data fits. Some of these parameter estimates can be grossly in error with respect to the actual properties and as a result can lead to erroneous prediction of future reservoir behavior. To reduce the statistical uncertainty one must either decrease the number of unknowns or utilize additional information (about the parameters).

The problem of overparametrization manifests itself as ill-conditioning in the computation of maximum likelihood or other estimates. Overparametrization is at least partly responsible for algorithmic problems and values of estimated parameters which are physically implausible and consequently unacceptable.

Regional groundwater models are numerical solutions to discretized partial differential equations. For the application of these models it is necessary to have the values of the parameters, such as transmissivities and porosities at each node. If the groundwater basin is nonhomogeneous, the most general approach is to assume that the parameters vary independently at each element or node of the numerical scheme and to estimate each parameter separately from the available prior information and the input-output data. This approach has been followed in many previous groundwater model calibration studies. However, this approach does not lead to better modeling. The amount of information about the parameters which can be extracted either from direct, in situ measurements or from input-output measurements is limited. Consequently, the estimation of hundreds of independent parameters entails considerable uncertainty which adversely affects the accuracy of the 'calibrated' model in evaluating the response to given excitations.

The severity of the overparametrization problem has been recognized in a number of studies as the core of the parameter estimation problem, and several interesting approaches have been proposed. The most common method for reducing the number of independent parameters is the method of zonation, which groups the node parameters into zones. *Jahns* [1966], for example, suggested a stepwise optimization of a quadratic fitting criterion. The detail of the reservoir description is increased from step to step to improve the convergence of the algorithm. *Shah et al.* [1978] utilized sensitivity and error analysis to suggest appropriate levels of parametrization. *Emsellem and DeMarsily* [1971, p. 1269] argued that 'permeability is a parameter with no punctual value but with an average value in a region of a given size.' They suggested a formulation which makes the problem of estimation of aquifer transmissivities well posed by introducing a requirement of regularity for the regional distribution of transmissivity. *Neuman* [1980] suggested a procedure to test against overfitting or underfitting the parameters to the observations. Another interesting approach has been advanced by *Yeh and Yoon* [1981] who represent the spatially distributed transmissivity as the sum of known basic functions with unknown coefficients. The optimal number of basic functions to be used is selected in a stepwise regression fashion. However, trend surfaces and zones, although useful in representing large-scale variability, cannot account for smaller-scale variability and for the local erratic features which are so pronounced in the analysis of core samples. Consequently, they may not be adequate for the combined study of, say, point measurements of head and permeability.

In this work the problem of parametrization will be studied as an integral part of the parameter estimation methodology and in conjunction with the use of all available information. To describe the spatial distribution in a way which is not too restrictive and can account for variability at various scales, the theory of random fields will be employed. The number of independent parameters describing the aquifer properties can be dramatically reduced by employing geostatistical concepts. The geostatistical parameters of, for instance, transmissivity are estimated from point measurements of transmissivity (a common procedure in geostatistics) and point measurements of piezometric head, pumping rate, recharge, etc. The latter is achieved through the application of the theory of stochastic differential equations. The technique allows flexibility in the selection of the appropriate (given all available information) geostatistical structure. After the geostatistical structure has been identified, the best linear unbiased estimate of the hydrogeologic parameter at any 'point' of interest is obtained using linear estimation theory or 'kriging.'

1.3. *Spatial Variability of Hydrogeologic Parameters and the Inverse Problem*

The parameters of the aquifer are distributed in space and can thus be called regionalized variables. On a regional scale these parameters have a relatively regular structure which is amenable to deterministic representation through smooth functions. However, on a more 'local' scale they vary in a rather erratic manner. Direct measurements of hydrogeologic parameters, whenever available, exhibit wide scatter [*Freeze*, 1972, 1975]. According to *Dagan* [1976]: 'Hydrologists do not generally rely on determining the properties of aquifers from small cores, no matter how numerous, but prefer to evaluate the properties of aquifers by pumping tests.' The purpose of the pumping test is to determine 'effective' properties, i.e., the properties of an idealized homogeneous aquifer which responds 'the same way' as the actual nonhomogeneous aquifer.

This approach raises a number of questions. To what extent can a nonhomogeneous formation (or a finite element of a formation) be represented through an equivalent homogeneous formation? How do the parameters of the equivalent idealized formation relate to the hydrogeologic parameters which are measured in situ or in the geotechnical laboratory? To what extent do the estimates of the idealized formation depend on hydrologic conditions, such as boundary conditions, accretion, and rate of pumping? How dependent are the idealized parameters on the assumed criterion of equivalence? How do the parameters employed in a distributed parameter model of homogeneous elements vary with the level of discretization and what is the appropriate level of discretization? What are the implications in the solution of the inverse problem?

Problems related to spatial variability of groundwater parameters were recently addressed in the important works of *Freeze* [1975], *Smith and Freeze* [1979a, b], *Bakr et al.* [1978], *Dagan* [1979, 1981, 1982], *Chirlin and Dagan* [1980], *Smith and Schwarz* [1980], *Gutjahr and Gelhar* [1981], and others. However, the emphasis of these works was not on the solution of the inverse problem.

This study examines the inverse problem from a geostatistical viewpoint. The term geostatistics is employed here both as a generic term, meaning the application of the theory of random fields in the earth sciences, and as the name given to methodologies developed by G. Matheron and his group [e.g., *Matheron*, 1971; *Journel and Huijbregts*, 1978]. Although the emphasis of this research is on the inverse problem, it is recognized that other modeling questions associated with the regionalized character and spatial variability of hydrologic parameters cannot be neglected. For this reason we believe that the study of the inverse problem must begin with relatively simple problems which must be solved as completely as possible before proceeding to the solution of more complex problems.

In this paper the general methodology will be presented and one-dimensional flow problems will be analyzed and simulated. The limitations of one-dimensional problems are, of course, well known [see *Dagan*, 1976; *Gelhar et al.*, 1977]. However, these models are still useful and their analysis has been the topic of recent research [*Freeze*, 1975; *Gutjahr et al.*, 1978; *Smith and Freeze*, 1979a; and others]. An even more important consideration here is that one-dimensional flow problems are more amenable to analytical solutions which can provide valuable insight and illustrate principles which apply to two- or three-dimensional problems.

2. Hydrogeologic Parameters as Random Fields

The parameters of a given geologic formation can conveniently be represented as realizations of random variables which form random fields (or random functions). The reasoning for representing geologic formations as random fields is elucidated in the references which have already been cited, as well as in numerous publications in the area of geostatistics. Let it be emphasized again that this representation is only a convenient mathematical description of the spatial variability of the parameters. The large-scale variability of the aquifer is usually amenable to description through deterministic functions. However, the variability of the aquifer parameters at smaller scales is rather erratic and it is neither possible nor useful to attempt to describe in a deterministic way the distribution of the aquifer parameters beyond a certain level of detail; it is more expedient to describe the parameters in a probabilistic fashion through their average properties, such as mean values, average intensity of fluctuations, and correlations. In this sense, the parameters can be regarded as random variables, one random variable for each point in space. Of course, it is very important to describe the relations among random variables because of their relative position in space, (i.e., the 'structure' of the field), for example, through their joint moments. Hence the applicability of the theory of random fields. To establish notation and for the sake of completeness, we will briefly review some basic geostatistical concepts.

A random field $f(x)$ can be described as a set of random variables, each variable corresponding to a point x in space. To every outcome of a probabilistic 'experiment' there corresponds a set of sample values of random variables. These sample values can be conveniently summarized through a function of space, denoted again by $f(\mathbf{x})$, which will be called a sample or a realization of the field. All possible realizations of the field form the ensemble. (It is the ensemble variability of parameters, head, and seepage velocity which will be examined in this work, consistently with all past work. By employing appropriate ergodicity assumptions, this ensemble variability represents spatial variability as well.)

For the complete probabilistic characterization of the random field $f(\mathbf{x})$, one would need to determine the joint probability density function of any set $f(\mathbf{x}_1), f(\mathbf{x}_2), \ldots, f(\mathbf{x}_n)$ for any n and for $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ arbitrary points in the spatial domain of interest. A partial but useful, practical, and manageable characterization of a random field is through its first two joint moments: the mean function $m(\mathbf{x}) = E(f(\mathbf{x}))$ and the autocovariance function

$$R_{ff}(\mathbf{x}_1, \mathbf{x}_2) = E[(f(\mathbf{x}_1) - m(\mathbf{x}_1))(f(\mathbf{x}_2) - m(\mathbf{x}_2))] \quad (1)$$

Associated with the autocovariance function are the variance

$$\sigma_f^2(x) = R_{ff}(x, x) \quad (2)$$

the autocorrelation function

$$\rho(x_1, x_2) = R_{ff}(x_1, x_2)/(R_{ff}(x_1, x_1)R_{ff}(x_2, x_2))^{1/2} \quad (3)$$

and the variogram

$$2\gamma(\mathbf{x}_1 - \mathbf{x}_2) = \mathrm{Var}\,(f(\mathbf{x}_1) - f(\mathbf{x}_2)) \quad (4)$$

In the framework of second-moment characterization, a random field will be called stationary (or wide sense stationary or statistically homogeneous) when

$$m(\mathbf{x}) = m \quad (5)$$

$$R_{ff}(\mathbf{x}_1, \mathbf{x}_2) = R_{ff}(\mathbf{x}_1 - \mathbf{x}_2) \quad (6)$$

A length scale associated with the autocovariance of a stationary field is the integral scale, defined roughly as the distance at which $f(\mathbf{x}_1)$ and $f(\mathbf{x}_2)$ cease to be correlated. In this work, for isotropic and statistically homogeneous formations, the following definition will be adopted

$$l_f = \frac{1}{\sigma_f^2} \int_0^\infty R_{ff}(|\xi|)\, d|\xi| \quad (7)$$

According to field data reviewed by *Freeze* [1975], the probability density function of permeabilities estimated from point samples is approximately lognormal. For this reason in this work it will be assumed, in agreement with past research,that the natural logarithm of permeability (for brevity to be called log permeability) is normally distributed. There appears, however, that less is known about the form of the autocovariance function of the log permeability.

This work emphasizes the application of linear minimum variance estimators, and consequently we will concentrate on second-moment characterization of random fields. Whenever a distributional assumption is needed, we will go one step further and assume Gaussian distributions. The wide sense stationarity assumption can be relaxed in two ways. First, instead of a constant mean it can be assumed that the mean is a sum of given deterministic functions with coefficients to be determined from the data. Second, the assumption of stationary fluctuations from the mean can be generalized to the assumption of stationary increments (such as Matheron's intrinsic random fields).

For the inverse problem we can consider the following sources of information: (1) point measurements of the piezo-

metric head and pumping rates and miscellaneous estimates of boundary conditions, accretion, etc.; (2) point measurements of hydrogeologic parameters such as permeability or storativity. (3) general prior or additional information about the aquifer properties. The piezometric head can be measured at a number of pumping or observation wells. Similarly, the pumping rates at the pumping wells can be considered known. We can also obtain estimates, although usually with less accuracy, of boundary conditions and accretion or leakage rates.

Estimates of permeability and transmissivity can be measured directly from small cores in situ or in the geotechnical lab. These estimates of permeability refer to the 'support' scale of the order of centimeters. This scale is much smaller than the scales (of the order of kilometers) of interest in regional groundwater management. As will be discussed later, we neither can describe nor are usually interested in describing variability at scales smaller than the scale of small core samples, and consequently, we can consider these direct measurements as point measurements. Another type of measurement can be obtained from pumping tests. These estimates can sometimes be considered as point measurements, since they represent conditions around a well [see *Delhomme*, 1979]. However, they actually refer to a support scale of the order of hundreds or thousands of meters. Consequently, they should not be confused with point measurements from small core samples.

In reality, as very clearly stated by *Emsellem and DeMarsily* [1971], permeability and other hydrogeologic parameters are not point processes but medium properties which always refer to a certain volume or support. However, at a regional scale the permeability of the medium with a small support level h_m resembles a point property of the medium [*Matheron*, 1967]. Scale considerations lead to the useful concept of 'nested variability structures' [*Journel and Huijbregts*, 1978], as follows.

1. At a scale smaller than the smallest support of interest, h_m, the variability is integrated over h_m. The effect of this microstructure appears as white noise or, in the geostatistical terminology, as a 'nugget effect.' If the measurements have support h_m, then the effect of random measurement errors cannot be distinguished from the effects of microstructure.
2. At the intermediate scale which is larger than h_m but smaller than the size of the aquifer there is a variability which can be viewed as stationary.
3. At a scale comparable to the size of the aquifer the properties vary in a fashion which can be described through a drift or a nonstationary process.

In linear second-moment analysis the variogram of the process is the sum of the variograms of the nested structures:

$$\gamma(h) = \tfrac{1}{2}E\{[z(x+h) - z(x)]^2\} = \gamma_0(h) + \gamma_1(h) + \gamma_2(h) + \cdots \tag{8}$$

An expression general enough for our purposes is the following:

$$\gamma(h) = C_0 + \gamma_s(h) + \gamma_i(h) \tag{9}$$

where C_0 is the variance of the white noise term, $\gamma_s(h)$ is the covariogram of the stationary process representing variability at the intermediate scale, and $\gamma_i(h)$ is the intrinsic variogram of the nonstationary intrinsic process representing variability at the regional scale. However, as numerical results illustrate, the use of complex multiparameter models is very seldom statistically justified.

In a usual geostatistical application, the point measurements of, say, permeability would be used to determine the variogram. The permeability data would be employed, first, to select the appropriate functional representation of the variogram and, second, to estimate its parameters. In the inverse problem, however, head and discharge data, as well as permeability data, will be combined, for the first time, to determine the variogram of the permeability field. To achieve this task, the properties of the head and discharge must be derived in terms of the parameters of the permeability variogram. Since we are interested in linear minimum variance estimators, it is sufficient to derive the first two moments of the head and discharge fields. This problem may be called the geostatistical direct problem.

A prerequisite for the solution of the geostatistical inverse problem is to solve the geostatistical direct problem. There is no general method of solution, as there is no general method appropriate for the solution of all deterministic direct problems. Each case will have to be examined separately. Because the developed procedures use linear estimation theory (which has definite computational advantages), we will emphasize in this work the use of linearized analysis.

The proposed geostatistical approach is applied in two main steps. In the first step, all available information is used for the selection of geostatistical structure (such as stationary or nonstationary field, with or without drift) and the estimation of its parameters (such as the variogram and the unknown coefficients of the function which represents the drift). In the second step the minimum variance and unbiased linear estimates and associated estimation variances of the hydrogeologic parameters at any point or area of interest can be estimated. From such estimates on a regular grid, one can develop a map depicting the spatial distribution of the hydrogeologic parameters.

The formal separation of the inverse problem into two steps is probably the most important difference of the present approach from other approaches. However, it must be noticed that this approach is very common in statistical analysis (regression and time series analysis.) (These two steps will be described in more detail in the following sections.) The present approach is also different from other approaches because of its emphasis on the statistical description of lower-scale variability and its efforts to minimize the number of independent parameters which must be estimated from data.

3. Identification of the Geostatistical Structure of the Hydrogeologic Parameter Field

3.1. *Selection and Validation of Geostatistical Structure*

The developed geostatistical model contains two parts: (1) model structure, i.e., stationary or nonstationary field and functional representation of the variogram and the drift, and (2) parameter values, i.e., numerical values of the parameters of variogram and the drift. Estimation of the parameters from available data given the structure of the model is a well-defined algorithmic problem and will be discussed in the next section. In contrast, the problem of selecting the most appropriate model structure remains to some extent in the realm of engineering judgment. In practice, attention is usually restricted to certain classes of models. These classes are chosen on the basis of their practicability and versatility as well as their performance in past applications. Within these classes the selection of the most appropriate model is guided by the principle of parsimony, i.e., the selection of the simplest or 'lowest-order' model in agreement with available data. Systematic model discrimination procedures, ranging from selection of the model which optimizes some scalar performance criterion (such as

Akaike's criterion) to Bayesian discrimination techniques, can be found in the estimation and, more specifically, the regression literature. Such methods can be useful as guides (although their use should not obscure the multiobjective nature of model evaluation and selection.)

The most common procedure for the selection of the most appropriate model is iterative. According to *Schweppe* [1978] the use of measurements to develop mathematical models involves four steps:

1. Hypothesize the structure of the model.
2. Estimate the parameters of the model.
3. Test the validity of the model.
4. If a test for validity fails, diagnose what went wrong and try again.

All available prior information, such as known formation geometry and hydraulic properties, should be taken into account in the selection of the most appropriate model for the structure of the hydrogeologic parameter field. To describe parameter variability within a formation, since some type of spatial homogeneity must be assumed, the search may be restricted in the class of fields with stationary increments. This is a general, versatile, and practicable class of models which have found many applications in geostatistical and time series analysis. The presence of deterministic trends can be accounted for. In general, the simultaneous estimations of trend and variogram parameters involves biases. These biases in the structural parameters may have little effect on the estimation of the field of hydrogeologic parameters. Nevertheless, as emphasized in the more recent geostatistical literature, it is often possible to avoid the estimation of deterministic trends.

To test the validity of the assumed geostatistical structure the following procedure will be followed. The error covariance matrix for the estimate geostatistical parameters will be estimated. For simplicity, in most applications it will be approximated by the inverse of the Fisher information matrix which, according to the Cramer-Rao inequality, is its lower bound (for negligible bias). It is also known that for effectively 'large' samples this bound is 'tight.' The significance of the parameter estimates can thus be statistically tested (e.g., through their t statistics or joint confidence areas.) Furthermore, the consistence between the model and the data is tested statistically. On the basis of statistical tests ('diagnostics') the hypothesized structure is either accepted as valid or modified and the whole procedure is repeated (see appendix.)

3.2. *Estimation of Structural Parameters*

The problem is to estimate the parameters of the trend and variogram of the hydrogeologic parameter field under the assumption that the functional forms of the trend and the variogram are given. In this work, the method of maximum likelihood (ML) estimation is employed. ML estimation is widely accepted as one of the most general and powerful identification methods [*Schweppe*, 1973, 1978; *Goldstein et al.*, 1980]. Its advantages include the following.

1. Parameter estimates are unbiased and of minimum variance for large samples.
2. Tests of hypotheses about model structure based upon ML estimates are optimal for large samples.
3. Distributions of the estimation error and test statistics are readily computed.
4. Computation of ML estimates is an optimization problem with many different ways available to take advantage of sparse matrix structures.

For the application of the ML method, the form of the joint probability function of the measurements of the observable quantities must be known. It is commonly assumed to be Gaussian. There appears to be no detailed or rigorous answer to the question whether this Gaussian assumption is crucial in a particular application. A rule of thumb in maximum likelihood estimation is that 'if many observations are available, the Gaussian assumption is not crucial' [*Schweppe*, 1973, p. 442]. Experience has shown that in many cases where the actual distribution is non-Gaussian the ML methodology (with the Gaussian assumption) gave near-optimal (in a quadratic sense) results. This is hardly surprising since the minimization of the negative log likelihood function can be interpreted as approximate minimization of a weighted sum of squares of prediction errors.

The joint probability density function of the N measurement (such as of head and permeability) is given by

$$p(\mathbf{z}|\boldsymbol{\theta}) = (2\pi)^{-N/2}|Q|^{-1/2}\exp\left(-\tfrac{1}{2}(\mathbf{z}-\boldsymbol{\mu})^T Q^{-1}(\mathbf{z}-\boldsymbol{\mu})\right) \tag{10}$$

where $\mathbf{z}$ is the vector of available measurements, $\boldsymbol{\theta}$ denotes the vector of structural parameters, $|\ |$ denotes determinant, and

$$\boldsymbol{\mu} = E[\mathbf{z}|\boldsymbol{\theta}] \tag{11}$$

$$Q = E[(\mathbf{z}-\boldsymbol{\mu})(\mathbf{z}-\boldsymbol{\mu})^T|\boldsymbol{\theta}] \tag{12}$$

The form of $\boldsymbol{\mu}$ and Q and the parameters to be estimated are chosen at the structure selection step. The vector of parameters will be determined through maximum likelihood estimation or the minimization of the negative log likelihood function:

$$L(\mathbf{z}|\boldsymbol{\theta}) = -\ln p(\mathbf{z}|\boldsymbol{\theta})$$

$$= \frac{N}{2}\ln(2\pi) + \frac{1}{2}\ln|Q| + \frac{1}{2}(\mathbf{z}-\boldsymbol{\mu})^T Q^{-1}(\mathbf{z}-\boldsymbol{\mu})$$

In general, the derivative of the negative log likelihood with respect to a scalar parameter θ_j is

$$\frac{\partial L}{\partial \theta_j} = \frac{1}{2}\mathrm{Tr}\left(Q^{-1}\frac{\partial Q}{\partial \theta_j}\right) - \frac{1}{2}(\mathbf{z}-\boldsymbol{\mu})^T Q^{-1}\frac{\partial Q}{\partial \theta_j}Q^{-1}(\mathbf{z}-\boldsymbol{\mu}) - (\mathbf{z}-\boldsymbol{\mu})^T Q^{-1}\frac{\partial \boldsymbol{\mu}}{\partial \theta_j} \tag{13}$$

where the following relations [*Schweppe*, 1973] were used

$$\frac{\partial}{\partial \theta_j}\ln|Q| = \mathrm{Tr}\left[Q^{-1}\frac{\partial Q}{\partial \theta_j}\right] \tag{14}$$

$$\frac{\partial}{\partial \theta_j}Q^{-1} = -Q^{-1}\frac{\partial Q}{\partial \theta_j}Q^{-1} \tag{15}$$

For the solution the 'method of scoring' (or Gauss-Newton) is employed [see *Gupta and Mehra*, 1974]. This is a gradient-based iterative method for the minimization of the negative log likelihood function. The basic iteration is

$$\boldsymbol{\theta}_{i+1} = \boldsymbol{\theta}_i - \rho_i R_i \mathbf{g}_i \tag{16}$$

where $\boldsymbol{\theta}_i$ is the vector of parameters in the ith iteration, $\mathbf{g}_i$ is the vector gradient of the negative log likelihood function, i.e.,

$$\mathbf{g}_i = \left.\frac{\partial L}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i} \tag{17}$$

R_i is an approximation to the second derivative matrix:

$$\left.(\partial^2 L/\partial \boldsymbol{\theta}^2)^{-1}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i} \tag{18}$$

and ρ_i is a scalar step size parameter which can be chosen to

ensure that

$$L(\mathbf{z}|\boldsymbol{\theta}_{i+1}) < L(\mathbf{z}|\boldsymbol{\theta}_i) \tag{19}$$

In the method of scoring, R_i is approximated by the inverse of the Fisher information matrix $R_i = M_i^{-1}$, where the Fisher information matrix is defined by

$$M_i = E\left\{(\partial^2 L/\partial\theta^2)\Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i}\right\} = E\left\{\frac{\partial L}{\partial \boldsymbol{\theta}}\left(\frac{\partial L}{\partial \boldsymbol{\theta}}\right)^T\Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_i}\right\} \tag{20}$$

The (j, k) element of the Fisher information matrix is

$$M(j, k) = E\left(\frac{\partial L}{\partial \theta_j}\frac{\partial L}{\partial \theta_k}\right) \tag{21}$$

which can be computed by making use of Gaussian moment factoring to be

$$M(j, k) = \frac{1}{2}\operatorname{Tr}\left(Q^{-1}\frac{\partial Q}{\partial \theta_j}Q^{-1}\frac{\partial Q}{\partial \theta_k}\right) + \left(\frac{\partial \boldsymbol{\mu}}{\partial \theta_j}\right)^T Q^{-1}\frac{\partial \boldsymbol{\mu}}{\partial \theta_k} \tag{22}$$

It might be useful to reemphasize that maximum likelihood estimation is just used to determine simultaneously the structural parameters of the fields of hydrogeologic parameters (such as transmissivity or storativity) and related fields (such as piezometric head). Point or block-averaged estimates of hydrogeologic parameters can be calculated as described in the next section.

4. Minimum Variance Unbiased Linear Estimators of Hydrogeologic Parameters (Kriging)

After the geostatistical structure of the unknown field has been selected, its parameters estimated, and the validity of the model tested and accepted, point estimates of the hydrogeologic parameters can be obtained in a step known in geostatistics as kriging. Such point estimates on a fine regular grid can be utilized to construct a contour map of permeability or transmissivity, storativity, etc.

In this work, the term kriging will be interpreted somewhat generally as the application of linear minimum variance estimation theory, such as methods described by *Schweppe* [1973], in the case of random fields. Consider the problem of estimating the value of a hydrologic parameter at a certain point given a number of point measurements of hydrogeologic parameters and head, pumping and accretion rate, etc. The problem can be examined under very general conditions for stationary and nonstationary log permeability fields with known first two joint moments. In practice, the field of hydrogeologic parameter of interest is assumed stationary or stationary increment with variogram which has already been determined. Cases with deterministic trend (or 'drift'), also assumed known, can be included.

Consider now the problem of estimating the log permeability at a given point $\mathbf{x}_0$ when m point measurements of log permeability $(Y_1, Y_2, \cdots, Y_m)$ and n point measurements of head $(\phi_1, \phi_2, \cdots, \phi_n)$ are available. This problem has also been addressed by *Gutjahr* [1981] who employed kriging for the combined estimation of transmissivities and head values. The structure of the log permeability field has already been identified. To become more specific, let it be assumed that the log permeability field is stationary.

A linear estimator of the true log permeability Y at $\mathbf{x}$ is

$$\hat{Y} = \sum_{i=1}^{m}\lambda_i Y_i + \sum_{j=1}^{n}\mu_j(\phi_j - H_j) \tag{23}$$

where H_j is the mean of the hydraulic head field at the point of measurement ϕ_j and the circumflex denotes estimated value. The error of estimation is

$$e = Y - \hat{Y} \tag{24}$$

where Y is the true log permeability at $\mathbf{x}_0$. The coefficients λ_i and μ_j must be selected so that

1. The estimate $\hat{Y}$ is unbiased, i.e.,

$$E(e) = 0 \tag{25}$$

2. The estimation error variance is minimum, i.e.,

$$E(e^2) = \min \tag{26}$$

For unbiasedness,

$$E\{\hat{Y}\} = E\{Y\} \tag{27}$$

or

$$E\{Y\} = \sum_{i=1}^{m}\lambda_i E\{Y_i\} + \sum_{j=1}^{n}\mu_j E\{\phi_j - H_j\} \tag{28}$$

and for constant mean Y

$$\sum_{i=1}^{m}\lambda_i = 1 \tag{29}$$

It is noted that in this particular example, which is presented to illustrate the approach, the mean hydraulic head does not need to be calculated from the data. In other cases this assumption may not be warranted and in fact could be removed, introducing constraints on the values of the coefficients. The reader may refer to *Gutjahr* [1981] for alternative formulations of the cokriging equations. The estimation error variance is

$$\begin{aligned}
E\{e^2\} &= E\left\{\left[Y - \sum_{i=1}^{m}\lambda_i Y_i - \sum_{j=1}^{n}\mu_j(\phi_j - H_j)\right]^2\right\} \\
&= E\{(Y-m)^2\} + \sum_{i=1}^{m}\sum_{k=1}^{m}\lambda_i\lambda_k \operatorname{Cov}(Y_i, Y_k) \\
&\quad + \sum_{j=1}^{n}\sum_{l=1}^{n}\mu_j\mu_l \operatorname{Cov}(\phi_j, \phi_l) - 2\sum_{i=1}^{m}\lambda_i \operatorname{Cov}(Y, Y_i) \\
&\quad - 2\sum_{j=1}^{n}\mu_j \operatorname{Cov}(Y, \phi_j) + 2\sum_{i=1}^{m}\sum_{j=1}^{n}\lambda_i\mu_j \operatorname{Cov}(Y_i, \phi_j) \\
&= \sigma_f^2 + \sum_{i=1}^{m}\sum_{k=1}^{m}\lambda_i\lambda_k Q_{YY}(i, k) \\
&\quad + \sum_{j=1}^{n}\sum_{l=1}^{n}\mu_j\mu_l Q_{\phi\phi}(j, l) - 2\sum_{i=1}^{m}\lambda_i \operatorname{Cov}(Y, Y_i) \\
&\quad - 2\sum_{j=1}^{n}\mu_j \operatorname{Cov}(Y, \phi_j) + 2\sum_{i=1}^{m}\sum_{j=1}^{n}\lambda_i\mu_j Q_{Y\phi}(i, j)
\end{aligned} \tag{30}$$

Minimization of the estimation error variance subject to the unbiasedness constraint is equivalent to the minimization of the following function

$$Z = E(e^2) - 2\nu\left(\sum_{i=1}^{m}\lambda_i - 1\right) \tag{31}$$

where ν is a Lagrange multiplier.

Taking derivatives with respect to λ_i, μ_j, and ν leads to the following system of linear equations:

$$\sum_{i=1}^{m} \lambda_i Q_{YY}(i, k) + \sum_{j=1}^{n} \mu_j Q_{Y\phi}(k, j) - \nu = \text{Cov}(Y, Y_k) \qquad k = 1, \cdots, m$$

$$\sum_{i=1}^{m} \lambda_i Q_{\phi Y}(l, i) + \sum_{j=1}^{n} \mu_j Q_{\phi\phi}(j, l) = \text{Cov}(Y, \phi_l) \qquad l = 1, \cdots, n \tag{32}$$

$$\sum \lambda_i = 1$$

The kriging coefficients are determined by solving the system of linear equations and the variance of the estimate $\hat{Y}$ is obtained from (31) after substitution of the kriging coefficients.

5. Application to the One-Dimensional Problem

5.1. *Error-Free Measurements*

The applicability of the described methodology will be illustrated through an application to a rather simple problem. Consider that for steady state flow in a one-dimensional aquifer with prescribed head boundary conditions (see Figure 1) the following measurements are available: (1) m point measurements of the permeability coefficient K_i at locations $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m$, and (2) n point measurements of the hydraulic head ϕ_j at locations $\mathbf{x}(h_1), \mathbf{x}(h_2), \cdots, \mathbf{x}(h_n)$. Let $Y_i = \ln K_i$, $i = 1, 2, \cdots, m$. The field of Y_i (called log permeability) is assumed Gaussian. This assumption is consistent with past work and in reasonable agreement with the available data. The field of Y_i is also assumed in this application to be wide sense stationary with a parametric covariance function or variogram, such as exponential, double exponential, spherical, etc.

The hydraulic head measurements are taken normally distributed jointly with log permeability. The assumption of normality is consistent with first-order analysis, where the hydraulic head is a linear function of Gaussian log permeability, for the estimation of the mean and the covariance matrix of the measurements. Consequently, the assumption of jointly distributed Gaussian hydraulic head and log permeability holds in cases where the application of first-order analysis is appropriate [see *Vomvoris*, 1982]. *Freeze* [1975] also found, through Monte Carlo simulations, that as the integral scale of log permeability fluctuations decreases a larger part of the hydraulic head field is normally distributed.

With these assumptions the joint probability density function of the $(m + n)$ point measurements is given by

$$P(\mathbf{z}/\boldsymbol{\theta}) = (2\pi)^{-(m+n)/2} |Q|^{-1/2} \exp\{-\tfrac{1}{2}(\mathbf{z} - \boldsymbol{\mu})^T Q^{-1} (\mathbf{z} - \boldsymbol{\mu})\} \tag{33}$$

where

$$\mathbf{z} = [Y_1, Y_2, \cdots Y_m, \phi_1, \phi_2, \cdots, \phi_n]^T$$

$$\boldsymbol{\mu} = E[\mathbf{z}|\boldsymbol{\theta}]$$

$$Q = E\{(\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T\} = Q(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m, \mathbf{x}(h_1), \cdots, \mathbf{x}(h_n)|\boldsymbol{\theta})$$

and $\boldsymbol{\theta}$ are the parameters to be estimated.

The covariance matrix can be expressed analytically in terms of the parameters based on the results of first-order analysis [see *Gutjahr and Gelhar*, 1981; *Vomvoris*, 1982; *Dagan*, 1981].

Consider

$$\phi(x) = H_0 - \Delta H \frac{x}{L} - \Delta H \left[\frac{x}{L^2} \int_0^L f(u)\, du - \frac{1}{L} \int_0^x f(u)\, du \right] \tag{34}$$

The mean function of $\phi(x)$ is

$$E\{\phi(x)\} = H_0 - \Delta H \frac{x}{L} \tag{35}$$

The mean vector is

$$\boldsymbol{\mu}^T = [E\{Y_1\}, E\{Y_2\}, \cdots, E\{Y_m\}, E\{\phi_1\}, E\{\phi_2\}, \cdots, E\{\phi_n\}] = \left[F, F, \cdots, F, H_0 - \frac{x(h_1)}{L} \Delta H, \cdots, H_0 - \frac{x(h_n)}{L} \Delta H \right] \tag{36}$$

where F is the mean of the log permeability field. The covariance matrix can be written in partitioned form as

$$Q = \begin{matrix} Q_{YY} & Q_{Y\phi} \\ Q_{\phi Y} & Q_{\phi\phi} \end{matrix} \tag{37}$$

For illustration it will be assumed that the covariance function of Y is exponential. Consequently,

$$[Q_{YY}]_{ij} = R_{ff}(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(-\frac{|x_i - x_j|}{l_f} \right) \tag{38}$$

The $Q_{\phi\phi}$ elements are given by the general relation

$$[Q_{\phi\phi}]_{ij} = E\{[\phi_i - E\{\phi_i\}][\phi_j - E\{\phi_i\}]\} = R_{hh}(\mathbf{x}(h_i), \mathbf{x}(h_k)) = \Delta H^2 \sigma_f^2 \frac{l_f}{L} G\left(\frac{x(h_1)}{L}, \frac{x(h_2)}{L}, \frac{l_f}{L} \right) \tag{39}$$

where

$$\begin{aligned} G\left(\frac{x_1}{L}, \frac{x_2}{L}, \frac{l_f}{L}\right) &= 2 \frac{x_1}{L} \frac{x_2}{L} \left(1 + \frac{l_f}{L} \exp\left(-\frac{L}{l_f} \right) - \frac{l_f}{L} \right) \\ &\quad - 2 \frac{x_1}{L} \left[\frac{l_f}{2L} \exp(-L/l_f) + \frac{l_f}{2L} \exp\left(-\frac{x_2}{l_f} \right) + \frac{x_2}{L} - \frac{l_f}{2L} - \frac{l_f}{2L} \exp\left(-\frac{L - x_2}{l_f} \right) \right] \\ &\quad - 2 \frac{x_2}{L} \left[\frac{l_f}{2L} \exp\left(-\frac{L}{l_f} \right) + \frac{l_f}{2L} \exp\left(-\frac{x_1}{l_f} \right) + \frac{x_1}{L} - \frac{l_f}{2L} - \frac{l_f}{2L} \exp\left(-\frac{L - x_1}{l_f} \right) \right] \\ &\quad + 2 \left[\frac{l_f}{2L} \exp\left(-\frac{x_1}{l_f} \right) + \frac{l_f}{2L} \exp\left(-\frac{x_2}{l_f} \right) + \frac{\min(x_1, x_2)}{L} - \frac{l_f}{2L} - \frac{l_f}{2L} \exp\left(-\frac{|x_1 - x_2|}{l_f} \right) \right] \end{aligned} \tag{40}$$

Also

$$(Q_{Y\phi})_{ij} = \Delta H\, \sigma_f^2 \frac{l_f}{L} J\left(\frac{x_i}{L}, \frac{x(h_j)}{l_f}, \frac{l_f}{L} \right) \tag{41}$$

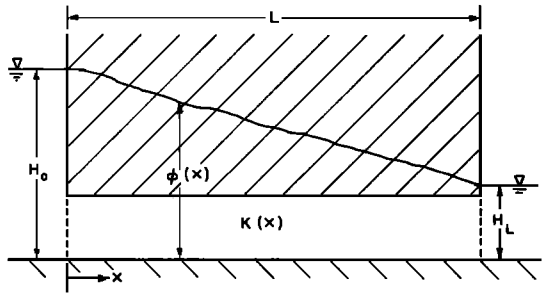

Fig. 1. One dimensional steady flow in horizontal confined aquifer.

where

$$J\left(\frac{x_i}{L}, \frac{x(h_j)}{L}, \frac{l_f}{L}\right) = -\frac{x(h_j)}{L}\left[2 - \exp\left(-\frac{x_i}{l_f}\right) - \exp\left(-\frac{L - x_i}{l_f}\right)\right] + 2 - \exp\left(-\frac{x_i}{l_f}\right) - \exp\left(-\frac{x(h_j) - x_i}{l_f}\right) \qquad x(h_j) > x_i \qquad (42a)$$

$$J\left(\frac{x_i}{L}, \frac{x(h_j)}{L}, \frac{l_f}{L}\right) = -\frac{x(h_j)}{L}\left[2 - \exp\left(-\frac{x_i}{l_f}\right) - \exp\left(\frac{L - x_i}{l_f}\right)\right] - \exp\left(-\frac{x_i}{l_f}\right) + \exp\left(-\frac{x_i - x(h_j)}{l_f}\right) \qquad x(h_j) < x_i \qquad (42b)$$

Finally, $Q_{\phi Y} = Q_{Y\phi}{}^T$. The results of first-order analysis for this case are valid for small $\sigma_f{}^2$ [*Gutjahr and Gelhar*, 1981; *Dagan*, 1982].

These results can be applied for the ML estimation of the log permeability field parameters F, $\sigma_f{}^2$, l_f. If reliable prior information about F is available, this formulation is preferable. Otherwise, the estimation of the mean F introduces bias in the estimation of the other two parameters. Since the value of the mean is not used in the kriging equations, this procedure can be readily modified to avoid the estimation of the mean. Instead of using the original observation vector z of log permeability and head measurements, a modified observation vector is used:

$$\mathbf{z}_{\text{mod}} = [Y_2 - Y_1, \cdots, Y_m - Y_{m-1}, h_1, \cdots, h_n] \qquad (43)$$

Note that $\mathbf{z}_{\text{mod}}$ has zero mean (for stationary field) and dimension $n + m - 1$. The loss of one measurement is acceptable to reduce the bias in the estimates of $\sigma_f{}^2$ and l_f. The complete expressions for Q_{mod} and $\partial Q_{\text{mod}}/\partial \boldsymbol{\theta}$ are given by *Vomvoris* [1982].

5.2. *Measurements Which Include Error*

Available hydraulic head and permeability measurements are usually contaminated by measurement errors. The analysis can be easily extended to account for measurement errors. Observations can be represented as

$$\mathbf{z} = \mathbf{z}_0 + \boldsymbol{\varepsilon} \qquad (44)$$

where z is the vector of the actual measurements, $\mathbf{z}_0$ is the vector of actual (error-free) values, and $\boldsymbol{\varepsilon}$ is the vector of measurement errors. It may be assumed under rather general conditions [see *Schweppe*, 1973] that $\boldsymbol{\varepsilon}$ is independent of $\mathbf{z}_0$ and normal with zero mean and known covariance matrix R. Under certain conditions R can be computed from available data. If then

$$\mathbf{z}_0 \sim N(\boldsymbol{\mu}, Q) \qquad (45)$$

then

$$\mathbf{z} \sim N(\boldsymbol{\mu}, Q + R) \qquad (46)$$

and maximum likelihood estimation can be applied. A common assumption is that measurement errors are independent of one another. For log permeability observations, $\varepsilon_{if} \sim N(0, \sigma_{ef}{}^2)$, and $\varepsilon_{ih} \sim N(0, \sigma_{eh}{}^2)$ for hydraulic head observations. For log permeability data where the differences of log permeability measurements are taken,

$$E(Y_{i+1} - Y_i) = 0 \qquad (47)$$

$$E((Y_{i+1} - Y_i)(Y_{j+1} - Y_j)) = \text{Cov}(Y_{i+1}, Y_{j+1}) - \text{Cov}(Y_{i+1}, Y_j) - \text{Cov}(Y_i, Y_{j+1}) + \text{Cov}(Y_i, Y_j) = (Q_{\text{mod}})_{ii} + 2\sigma_{ef}{}^2 \qquad i = j \qquad (48a)$$

$$E((Y_{i+1} - Y_i)(Y_{j+1} - Y_j)) = \text{Cov}(Y_{i+1}, Y_{j+1}) - \text{Cov}(Y_{i+1}, Y_j) - \text{Cov}(Y_i, Y_{j+1}) + \text{Cov}(Y_i, Y_j) = (Q_{\text{mod}})_{ij} - \sigma_{ef}{}^2 \qquad |i - j| = 1 \qquad (48b)$$

$$E((Y_{i+1} - Y_i)(Y_{j+1} - Y_j)) = \text{Cov}(Y_{i+1}, Y_{j+1}) - \text{Cov}(Y_{i+1}, Y_j) - \text{Cov}(Y_i, Y_{j+1}) + \text{Cov}(Y_i, Y_j) = (Q_{\text{mod}})_{ij} \qquad |i - j| > 1 \qquad (48c)$$

where Q_{mod} denotes the modified covariance matrix with no measurement error.

6. Numerical Simulations

The performance of the developed methodology was tested for the one-dimensional case through simulation as follows. The log permeability field was synthetically generated and the hydraulic head was calculated. The developed methodology was then called to identify the log permeability field from a small number of point measurements of log permeability and hydraulic head (possibly with error). The field of log permeability estimates with their 95% confidence intervals was then compared with the 'actual' log permeability field.

Case 1

Consider a stationary log permeability random field generated synthetically with zero mean and exponential covariance function with $\sigma_f{}^2 = 1.0$ and $l_f = 0.15$. The horizontal and vertical length scales have been chosen in all simulations so that $L = 1$, $H_L = 1$, $H_R = 0$. The spatial statistics of the generated field (i.e., this particular realization) were computed to be $\sigma_f{}^2 = 1.02$ and $l_f = 0.107$. Assume that six error-free observations are available, two point measurements of log-permeability and four point measurements of hydraulic head. The method of scoring was applied for the minimization of the log likelihood function,

and the estimates of the parameters of the geostatistical structure are

$$\hat{\sigma}_f^2 = 0.727 \qquad \hat{l}_f = 0.152$$

The estimation error covariance matrix is approximated by the inverse of the Fisher information matrix:

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.282 & 0.058 \\ 0.058 & 0.048 \end{bmatrix}$$

Although in this simulation experiments the geostatistical structure is known, it is interesting to notice that the approximate t statistics of the parameters are rather low (1.37 and 0.694, respectively) even though there are only two parameters to be estimated from the data and the measurements are error-free. This result is indicative of the usefulness of simple geostatistical structures, described through a small number of parameters.

The measurements employed in the identification scheme are

$$Z^T = [0.37, -0.034, -0.227, -0.257, -0.1]$$

where the first component is the difference of the two log permeability measurements and the other four components are the differences of the measured hydraulic heads from their corresponding deterministic values. The normalized (zero mean, covariance equal to unit matrix) vector of the measurements is (see appendix):

$$y^T = [-1.58, 0.296, -0.347, -1.12, 1.26]$$

Three tests (at the 95% significance level) are

$$-2 < y_i < 2 \qquad i = 1, \cdots, 5$$

$$-2 < y_i y_j < 2 \qquad i, j = 1, \cdots, 5 \qquad i \neq j \quad \text{(approximate)}$$

$$0.22 < \sum_{i=1} y_i^2 = 5.57 < 9.35$$

The normalized residuals pass these tests and provide no reason to doubt the adequacy and validity of the assumed geostatistical structure and the estimated parameters. The estimated σ_f^2 and l_f are next used in the kriging equations to estimate the value of log permeability at 50 uniformly distributed points. The approximate 95% confidence intervals are also constructed assuming that the permeability is normally distributed. These confidence intervals correspond to individual point estimates and do not account for error in the estimated values of the structural parameters.

The results are compared with the actual field in Figure 2. The kriged values reproduce quite adequately the variability of the actual field and the actual values are within the confidence intervals. A note on the interpretation of these results might be useful. The kriged values are the best estimates of the point log permeabilities and the confidence intervals are referring to these point estimates. In simple terms, they are representative of the variability of small core samples. However, much of the variability of these point values is small scale compared to the aquifer dimensions. As has been discussed elsewhere, a deterministic description of small scale variability is of little interest in the estimation of hydraulic head and, we suspect, in most practically encountered problems. Groundwater hydrologists are more interested in determining how parameters vary over scales comparable to the dimensions of the aquifer and are interested in small-scale variability only to the extent that it affects the effective parameters of the aquifer. This important point will be pursued in detail in the presentation of the two-dimensional case study where the effects of spatial variability are more realistically represented than in the one-dimensional case. Meanwhile, note that if one smooths out the highly erratic small-scale variability of the actual field and compares the estimated with the actual field, the comparison will indicate that the results are quite satisfactory. A more detailed and relevant comparison would be to use the results of the analysis to determine 'effective parameters,' as discussed in references dealing with spatial variability of groundwater systems. This will not be pursued in this paper.

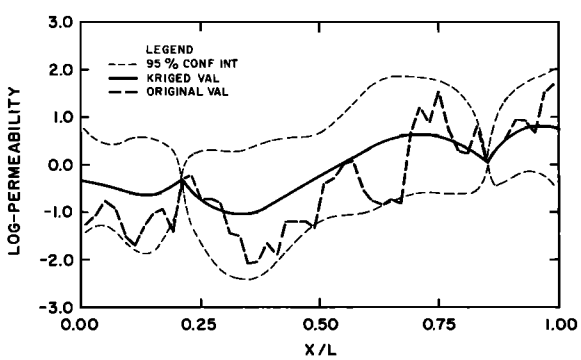

Fig. 2. Kriging on log permeability for case 1. Y measurements at $x/L = 0.21, 0.85$; ϕ measurements at $x/L = 0.10, 0.40, 0.60, 0.88$.

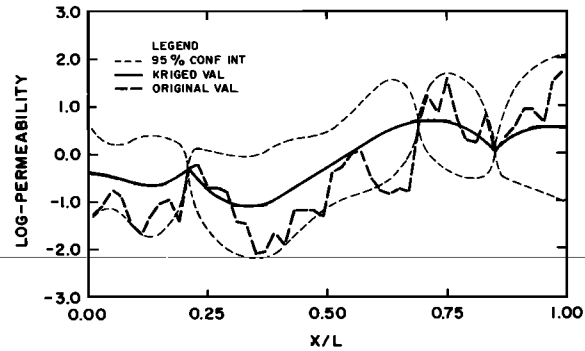

Fig. 3. Kriging on log permeability for case 2. Y measurements at $x/L = 0.21, 0.69, 0.85$; ϕ measurements at $x/L = 0.10, 0.40, 0.60$.

Case 2

For the same log permeability field as in case 1 the developed methodology was applied with six error-free observations, three permeability and three hydraulic head. The estimates of the parameters were

$$\sigma_f^2 = 0.757 \qquad \hat{l}_f = 0.187$$

with approximate estimation error covariance matrix

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.464 & 0.135 \\ 0.135 & 0.077 \end{bmatrix}$$

The results of kriging are given in Figure 3. In this case the kriged field is forced to pass through three fixed points (since kriging is an 'exact' interpolator, i.e., it reproduces error-free measurements). Because of the high-frequency components which are particularly pronounced in this particular realization, some of the actual values near the points of permeability measurements are outside of the confidence interval. It might be noted that kriging gives the best estimates of log permeability, given available data, and as such will be smoother

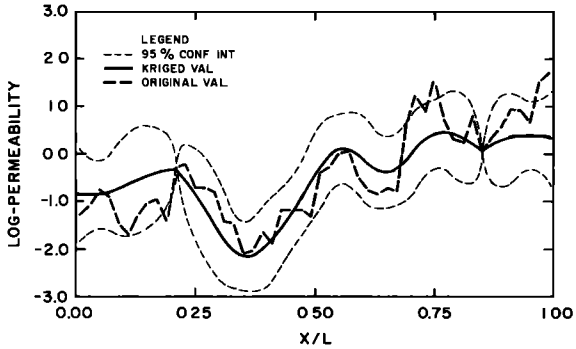

Fig. 4. Kriging on log permeability for case 3. Y measurements at $x/L = 0.21, 0.85$; ϕ measurements at $x/L = 0.10, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90$.

than the actual field. Furthermore, it should be expected that some points of the actual field would be outside of the 95% confidence interval. However, the important feature to note is that the estimates follow the general trend of the actual field; the high-frequency components are adequately described statistically with $\sigma_f^2 = 0.757$ and $l_f = 0.187$, (conditional on the measurements).

Case 3

With the same parameter field as in the previous two cases, the number of measurements was increased to 10 (two permeability and eight hydraulic head). The estimates of the parameters are

$$\hat{\sigma}_f^2 = 0.937 \qquad \hat{l}_f = 0.172$$

with estimation error approximated by the inverse of the Fisher information matrix at the final estimates of the parameters:

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.536 & 0.112 \\ 0.112 & 0.037 \end{bmatrix}$$

The results of kriging are shown in Figure 4. As more measurements were made available the degree of detail of describing parameter variability was improved.

Case 4

Another log permeability field was examined with (estimated) spatial characteristics variance 0.539 and integral scale 0.029. Two point permeability measurements and eight head measurements were assumed given. The estimated parameters are

$$\hat{\sigma}_f^2 = 1.80 \qquad \hat{l}_f = 0.019$$

with approximate covariance matrix

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 1.94 & -0.0227 \\ -0.0227 & 0.00042 \end{bmatrix}$$

The results of kriging are given in Figure 5. Despite the apparent error in the estimation of the structural parameters (which affects the description of the high-frequency variability), the kriged estimates reproduce the actual field remarkably well. The confidence interval is rather wide, a result of the overestimation of σ_f^2.

Case 5

The same field and the same type of observation as in Case 4 were used but with different points of observations the estimated structural parameters were

$$\hat{\sigma}_f^2 = 1.16 \qquad \hat{l}_f = 0.039$$

with Cramer-Rao lower bound:

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.391 & -0.0118 \\ -0.0118 & 0.0015 \end{bmatrix}$$

The kriged values compare quite well with the actual values, as shown in Figure 6, and illustrate the relative insensitivity of the kriging estimates to errors in the geostatistical parameters. On the other hand, it is obvious that errors in the estimation of geostatistical (structural) parameters affect the accuracy of the confidence intervals.

Case 6

In this case the effects of measurement errors will be studied. Consider the setting of case 3, with the only exception being that there are measurement errors with known variances $\sigma_{ef}^2 = \sigma_{eh}^2 = 0.02$. (The 'intensities' of the measurement error σ_{ef}^2 and σ_{eh}^2 could, in theory, be considered as additional parameters to be estimated in the maximum likelihood identification. In practice, one can usually obtain some estimates of how large the measurement errors are expected to be and the final result can be shown to be rather insensitive to the exact assumed value of σ_{eh}^2 and σ_{ef}^2.) The estimators of σ_f^2 and l_f are

$$\hat{\sigma}_f^2 = 0.834 \qquad \hat{l}_f = 0.152$$

with covariance matrix

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.784 & 0.059 \\ 0.059 & 0.085 \end{bmatrix}$$

It is obvious that measurement errors increase the estimation error (as indicated by the covariance matrix) of the geostatistical parameters. The t statistics of the parameter estimates are low, which indicates that it would be rather meaningless to try more complicated structures (for example, account for trend or stationary increments). The results of kriging are shown in Figure 7. It is obvious that when it is recognized that there are measurement errors, the kriged values become smoother and the confidence intervals become wider than in the case of error-free measurements (Figure 4). Note that even though the generated errors in the hydraulic head measurements are rather large, they did not cause 'instability' [*Yakowitz and Duckstein*, 1980] and the results are very smooth.

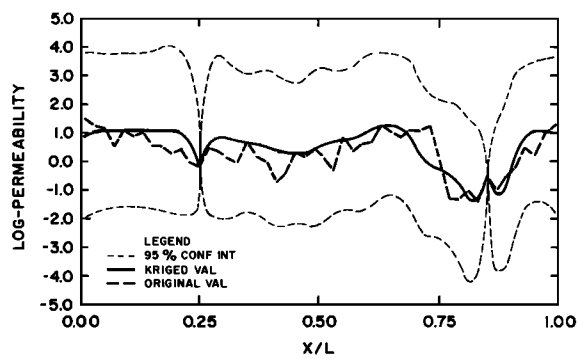

Fig. 5. Kriging on log permeability for case 4. Y measurements at $x/L = 0.25, 0.85$; ϕ measurements at $x/L = 0.20, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90$.

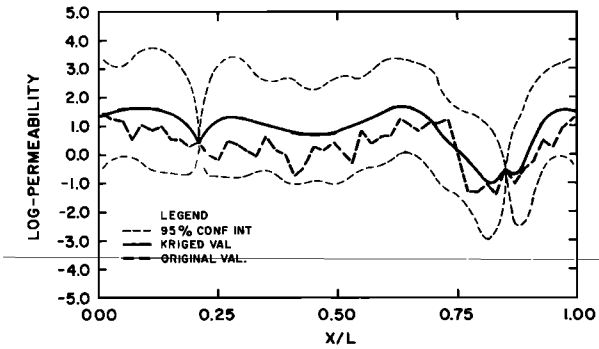

Fig. 6. Kriging on log permeability for case 5. Y measurements at $x/L = 0.21, 0.85$; ϕ measurements at $x/L = 0.10, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90$.

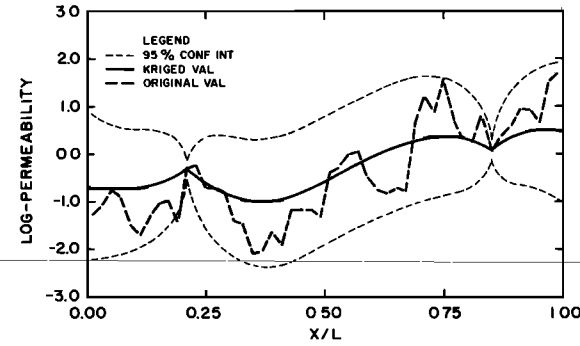

Fig. 8. Kriging on log permeability for field 1, when measurements include error. Case 2: $\sigma_{eh}^2 = \sigma_{ef}^2 = 0.01$. Y measurements at $x/L = 0.21, 0.85$; ϕ measurements at $x/L = 0.10, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90$.

When $\sigma_{ef}^2 = \sigma_{eh}^2 = 0.01$, the estimated parameters are

$$\hat{\sigma}_f^2 = 0.811 \qquad \hat{l}_f = 0.210$$

with

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.811 & 0.204 \\ 0.204 & 0.178 \end{bmatrix}$$

and the results of kriging are shown on Figure 8.

Note that a basic feature of the geostatistical approach is that it does not attempt to reproduce characteristics which cannot be identified from available data and thus, unlike some conventional methods, gives smooth results. In this sense, this approach has important similarities to *Emsellem and DeMarsilly*'s [1971] approach. In addition to giving smooth and stable estimates of the parameters, the present approach provides a statistical description of low-scale variability. Conditional simulations can be used to obtain the range of variations which are expected to exist, given all available measurements.

Sensitivity of Results to the Assumed Geostatistical Structure

Of course, in practice the actual structure of the hydrogeological parameter field can neither be known with certainty nor can be expected to conform to any simple model. The important practical question is whether, on the basis of available information, the geostatistical structure can be adequately (for the purpose of parameter estimation) described through simple geostatistical models characterized by a small number of parameters.

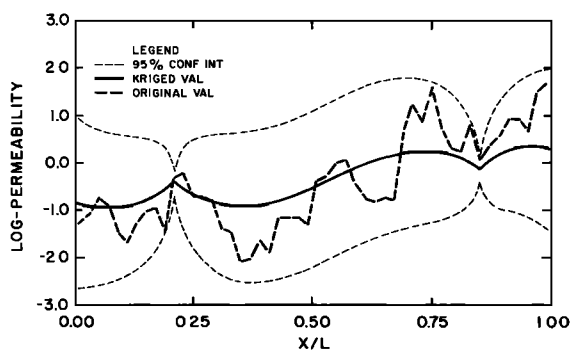

Fig. 7. Kriging on log permeability for field 1, when measurements include error. Case 1: $\sigma_{eh}^2 = \sigma_{ef}^2 = 0.02$. Y measurements at $x/L = 0.21, 0.85$; ϕ measurements at $x/L = 0.10, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90$.

Note that in the reported simulation experiments two log-permeability fields were employed. Field 1 (cases 1, 2, 3, and 6) is ostensibly nonstationary and has a trend. Field 2 (cases 4 and 5) appears stationary and has significantly smaller variance and integral scale than field 1. Yet both fields are realizations of the same stationary random field with zero mean and exponential covariance function (with $\sigma_f^2 = 1.0$ and $l_f = 0.15$). In this sense, these two fields, even though seemingly very different (in a deterministic sense) from one another, can be described by the same statistical model, as verified in the presented results. We believe that this versatility of simple geostatistical structures is a definite advantage over deterministic descriptions (such as zonation and trend surfaces) of the structure of hydrogeologic parameter fields.

To further test the sensitivity of the results to the assumed geostatistical structure, consider a formation consisting of two blocks, each block with constant permeability (see Figure 9). The head at the point of discontinuity is given by

$$H_i = \left(\frac{K_1}{b_1} H_0 + \frac{K_2}{b_2} H_L\right)\left(\frac{K_1}{b_1} + \frac{K_2}{b_2}\right)^{-1}$$

The head at any other location is given as a linear function of the distance from the boundaries. The following case was examined:

$$b_1 = 0.7$$

$$b_2 = 0.3$$

$$K_1 = 0.223 \qquad \ln K_1 = -1.5$$

$$K_2 = 1.65 \qquad \ln K_2 = 0.5$$

Four permeability and six head measurements were taken, as

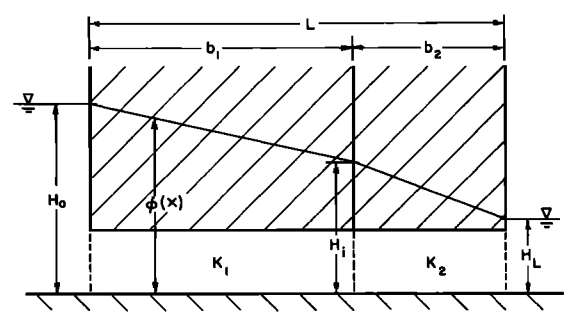

Fig. 9. The one-dimensional two-block field for testing the sensitivity of the model.

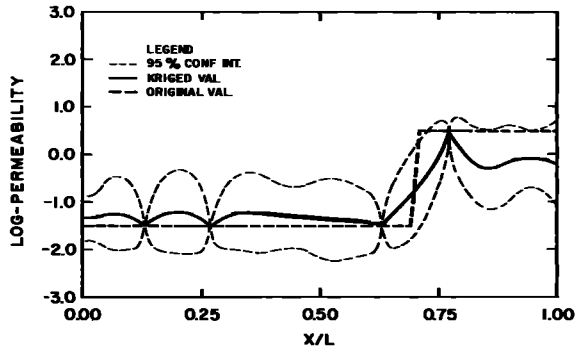

Fig. 10. Kriging on log permeability for the two-block field. Y measurements at $x/L = 0.13, 0.27, 0.63, 0.77$; ϕ measurements at $x/L = 0.04, 0.20, 0.36, 0.52, 0.70, 0.88$.

shown in Figure 10. Assuming that the field is Gaussian, stationary, and with exponential covariance function, the developed methodology estimated the following parameters

$$\hat{\sigma}_f^2 = 0.554 \qquad \hat{l}_f = 0.145$$

with Cramer-Rao lower bound

$$P(\hat{\sigma}_f^2, \hat{l}_f) = \begin{bmatrix} 0.146 & 0.040 \\ 0.040 & 0.024 \end{bmatrix}$$

The results of kriging are shown in Figure 10. The estimated field is remarkably close to the actual field, even though the choice of geostatistical structure was obviously poor. Of course, diagnostic checking or even simple inspection of the final result might suggest in this particular case a more expedient structure and thus further improve the accuracy of the procedure. However, this example illustrates the important fact that the kriging estimates are rather insensitive to deviations from the assumed geostatistical structure (such as normality, stationarity, and type of covariance function). From the viewpoint of applications, this is a very important feature of the developed geostatistical approach. Nevertheless, it must be noted that a proper description of the geostatistical structure is important in calculating estimation errors.

7. Summary and Conclusions

A methodology for the solution of the inverse problem, i.e., estimation of the hydrogeologic parameters of the aquifer from head and discharge measurements, has been presented. The problem is treated in a geostatistical framework which recognizes the distributed parameter nature of groundwater systems. The main advantage of the proposed methodology is that it avoids the problem of large dimensionality which characterizes many existing methods, by drastically reducing the number of independent effective parameters to be estimated. In the developed methodology this number is not determined by the discretization scheme but depends on the amount and quality of available information as well as the actual properties of the formation.

The method consists of two main steps.

1. The structure of the parameter field is identified, i.e., mathematical representations of the variogram and the trend are selected and their parameters are established. This step is equivalent to 'model estimation' in time series [e.g., *Box and Jenkins*, 1976] and to 'structural analysis' in mining geostatistics [e.g., *Journal and Huijbregts*, 1978]. In practice, structure identification is applied in an iterative fashion with three substeps: structure selection, parameter estimation, and model validation and diagnostic checking. Simple geostatistical structures with few (two to five) parameters are flexible enough to describe fairly complicated parameter fields. The proposed approach is in sharp contrast with many conventional methods which attempt to estimate scores of independent parameters. The adequacy and validity of the model are tested through statistical diagnostic checking.

2. Kriging is applied to provide minimum variance and unbiased point estimates of hydrogeologic parameters using all available information.

One of the most important advantages of the developed geostatistical approach is that it does not attempt to restore details which cannot be actually extracted from available data. The problems of overparametrization or underparametrization are handled in an objective and systematic way, and the results of the parameter estimation algorithm are statistically stable. We believe that regional groundwater models calibrated following the geostatistical approach are less affected by spurious parameter variability and consequently should be more reliable for use in simulation studies.

Applications presented in this paper are for the estimation of log permeability from noisy point measurements of log permeability and hydraulic head in one-dimensional flow. Although more complicated situations are encountered in practice, this case provides the grounds to test the new methodology.

To incorporate hydraulic head measurements in the structure identification and kriging steps, the direct problem must be solved in a geostatistical framework. Exact solution is usually unattainable. First-order approximation (i.e., linearization) was employed, resulting in mathematically tractable results. The results of numerical simulations demonstrate the applicability of first-order analysis in the geostatistical approach for the solution of the inverse problem. In the developed methodology, structural parameters are determined through maximum likelihood estimation. Normality is assumed in agreement with available data and consistent with the first-order approximation. The method of scoring (Gauss-Newton) is used for the iterative maximization of the likelihood function. The estimation error covariance matrix was approximated by the inverse of the Fisher information matrix at the last iteration. Statistical tests are presented to examine the validity and adequacy of the model. The validated model is finally used for kriging, i.e., optimal linear estimation of log permeability at points or over areas of the formulation from known head and log permeability values.

The performance of the developed methodology was tested through simulation with very encouraging results. Unlike many conventional approaches, the developed estimation procedure is remarkably stable and well behaved. If the measurements are scant and contain error, the final estimates of log permeability form a smooth and nearly uniform field. As the information content of the measurements increases (by obtaining more measurements, improving their position, or reducing measurement error), the procedure reproduces more features of the original field. Perhaps the most interesting results are those which show the versatility of simple geostatistical structures and the insensitivity of final estimates to deviations from geostatistical assumptions. While it is necessary to make certain mathematical assumptions for the development of the algorithm, the usefulness of the method does not appear to be critically dependent on the validity of these assumptions.

The presented results are also indicative of the difficulties associated with obtaining a detailed deterministic description

of the parameter field when observations are few and contain measurement error. For this purpose, many good quality and appropriately distributed measurements must be available [see *Yakowitz and Duckstein*, 1980]. However, in most practical applications the actual purpose is to obtain a deterministic description of intermediate-scale variability of the hydrogeologic parameter field and a statistical description of lower-scale variability. If this is the case, the solution of the inverse problem is much more tractable, and we are optimistic about the feasibility and usefulness of the inverse problem in groundwater modeling.

APPENDIX

Some statistical tests on the residuals which were applied in this work were based on the assumption of Gaussian-distributed measurements. Consider the vector of the measurements minus their expected values:

$$\mathbf{z} \sim N(0, Q)$$

It is convenient to consider the following linear transformation of z:

$$\mathbf{y} = C^{-1}\mathbf{z}$$

where $Q = CC^T$ and, under the hypothesis that the model is valid, the elements of y are independent standard normal variates. The covariance matrix Q can be calculated once the geostatistical structure has been selected and its parameters have been estimated. (The square root of Q, C, and its inverse C^{-1} can be calculated through Cholesky or Householder decomposition in the process of calculating Q^{-1}.)

To test whether y_i are zero normal variates at the 95% significance level,

$$-2 \le y_i \le 2 \qquad \forall i$$

To test for independence, the product $y_i y_{j(i \neq j)}$ has zero mean and unit variance. Thus even though this product is not normally distributed, it is useful to test whether

$$-2 \le y_i y_j \le 2 \qquad \forall i, j \qquad i \neq j$$

Finally, it is necessary to test whether the y_i taken as a whole appear to conform to the hypothesized y distribution. Since y_i are independent $N(0, 1)$,

$$\sum_{i=1}^{N} y_i^2 \sim \chi^2(N - p)$$

where N is the total number of data, the dimension of z and p is the number of parameters fitted from the data. This test is a general (or 'portmanteau') lack of fit test which is useful in guarding against overfitting or underfitting. Experience also indicates that these tests are useful even in cases where the Gaussian assumption is not strictly true. The normality of the y_i residuals may be tested through the Kolmogorov-Smirnov or Filliben [*Filliben*, 1975] tests.

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REFERENCES

Bakr, A., L. W. Gelhar, A. L. Gutjahr, and J. R. MacMillan, Stochastic analysis of spatial variability of subsurface flows, 1, Comparison of one- and three-dimensional flows, *Water Resour. Res.*, *14*(2), 263–271, 1978.

Box, G. E., and G. M. Jenkins, Time series analysis: Forecasting and control, Holden-Day, San Francisco, California, 1976.

Chirlin, G. R., and G. Dagan, Theoretical head variograms for steady flow in statistically homogeneous aquifers, *Water Resour. Res.*, *16*(6), 1001–1015, 1980.

Cooley, R. L., A method for estimating parameters and assessing reliability for models of steady state groundwater flow, 1, Theory and numerical properties, *Water Resour. Res.*, *13*(2), 318–324, 1977.

Cooley, R. L., A method for estimating parameters and assessing reliability for models of steady state groundwater flow, 2, Applications and statistical analysis, *Water Resour. Res.*, *15*(2), 603–617, 1979.

Cooley, R. L., Incorporation of prior information into nonlinear regression groundwater flow models, 1, Theory, *Water Resour. Res.*, *18*(4), 965–976, 1982.

Clifton, P. M., and S. P. Neuman, 'Effects of kriging and inverse modeling on conditional simulation of the Avra Valley aquifer in southern Arizona, *Water Resour. Res.*, *18*(4), 1215–1234, 1982.

Dagan, G., Comment on a stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media by R. A. Freeze, *Water Resour. Res.*, *12*(3), 567, 1976.

Dagan, G., Models of groundwater flow in statistically homogeneous porous formations, *Water Resour. Res.*, *15*(1), 47–63, 1979.

Dagan, G., Analysis of flow through heterogeneous random aquifers by the method of embedding matrix, 1, Steady flow, *Water Resour. Res.*, *17*(1), 107–121, 1981.

Dagan, G., Stochastic modeling of groundwater flow by unconditional and conditional probabilities, 1, Conditional simulation and the direct problem, *Water Resour. Res.*, *18*(4), 813–833, 1982.

Delhomme, J. P., Spatial variability and uncertainty in groundwater flow parameters: A geostatistical approach, *Water Resour. Res.*, *15*(2), 269–280, 1979.

Dogru, A. H., T. N. Dixon, and T. F. Edgar, Confidence limits on the parameters and predictions of slightly compressible, single-phase reservoirs, *Soc. Petrol. Eng. J.*, 42–56, 1977.

Emsellem, Y., and G. De Marsily, An automatic solution for the inverse problem, *Water Resour. Res.*, *7*(5), 1264–1283, 1971.

Filliben, J. J., The probability plot correlation test for normality, *Technometrics*, *17*(1), 111–117, 1975.

Freeze, R. A., Regionalization of hydrogeologic parameters for use in mathematical models of groundwater flow, in *Hydrogeology*, edited by J. E. Gill, Harpell's, Gardenvale, Quebec, 1972.

Freeze, R. A., A stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media, *Water Resour. Res.*, *11*(45), 725–741, 1975.

Frind, E. O., and S. F. Pinder, Galerkin solution to the inverse problem for aquifer transmissivity, *Water Resour. Res.*, *9*(4), 1397–1410, 1973.

Gavalas, G. R., P. C. Shah, and J. H. Seinfeld, Reservoir history matching by Bayesian estimation, *Soc. Petrol. Eng. J.*, 337–350, 1976.

Gelhar, L. W., A. A. Bakr, A. L. Gutjahr, and J. R. MacMillan, Comments on 'A stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media' by R. A. Freeze, *Water Resour. Res.*, *13*(2), 477–479, 1977.

Goldstein, J. D., W. E. Larimore, and R. F. Brammer, Applications of Kalman filtering and maximum likelihood parameter identification to hydrologic forecasting, *Tech. Rep. TR-1480-1*, Anal. Sci. Corp., Reading, Mass., 1980.

Gupta, N. K., and R. K. Mehra, Computational aspects of maximum likelihood estimation and reduction in sensitivity function calculations, *IEEE Trans. Autom. Control*, *AC19*(6), 774–783, 1974.

Gutjahr, A. L., Kriging in stochastic hydrology: Assessing the worth of data, paper presented at the Chapman Conference on Spatial Variability in Hydrologic Modeling, AGU, Fort Collins, Colo., July 1981.

Gutjahr, A. L., and L. W. Gelhar, Stochastic models of subsurface flow: Infinite versus finite domains and stationarity, *Water Resour. Res.*, *17*(2), 337–351, 1981.

Gutjahr, A. L., L. W. Gelhar, A. A. Bakr, and J. R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 2, Evaluation and application, *Water Resour. Res.*, *14*(5), 953–959, 1978.

Jahns, H. O., A rapid method for obtaining a two-dimensional reservoir description from a well pressure response data, *Soc. Petrol. Eng. J.*, 315–327, 1966.

Journel, A. G., and C. T. Huijbregts, *Mining Geostatistics*, Academic, New York, 1978.

Kitanidis, P. K., A unified approach to parameter estimation of

groundwater models, M.Sc. thesis, Dep. of Civ. Eng., Mass. Inst. of Technol., Cambridge, Mass., February 1976.

Matheron, G., *The Theory of Regionalized Variables and its Applications*, Ecole de Mines, Fontainbleau, France, 1971.

Neuman, S. P., A statistical approach to the inverse problem of aquifer hydrology, 3, Improved solution method and added perspectives, *Water Resour. Res.*, *16*(2), 331–346, 1980.

Neuman, S. P., and S. Yakowitz, A statistical approach to the inverse problem of aquifer hydrology, 1, Theory, *Water Resour. Res.*, *15*(4), 845–860, 1979.

Neuman, S. P., G. E. Fogg, and E. A. Jacobson, A statistical approach to the inverse problem of aquifer hydrology, 2, Case study, *Water Resour. Res.*, *16*(1), 33–58, 1980.

Pinder, G. F., and W. G. Gray, *Finite Element Simulation in Surface and Subsurface Hydrology*, Academic, New York 1977.

Remson, I., G. M. Hornberger, and F. J. Molz, *Numerical Methods in Subsurface Hydrology*, Wiley-Interscience, New York, 1971.

Rothenberg, T. J., Identification of parametric models, *Econometrics*, *39*(3), 577–591, 1971.

Schweppe, F. C., *Uncertain Dynamic Systems*, p. 563, Prentice-Hall, Englewood Cliffs, New Jersey, 1973.

Schweppe, F. C., Model identification problems, in *Applications of Kalman Filter to Hydrology, Hydraulics and Water Resources*, edited by C.-L. Chiu, pp. 115–133, University of Pittsburgh, Pittsburgh, Pennsylvania, 1978.

Shah, P. C., G. R. Gavalas, and J. H. Seinfeld, Error analysis in history matching: The optimum level of parametrization, *Soc. Petrol. Eng. J.*, 219–228, 1978.

Smith, L., and R. A. Freeze, Stochastic analysis of steady state groundwater flow in a bounded domain, 1, One-dimensional simulation, *Water Resour. Res.*, *15*(3), 521–528, 1979*a*.

Smith, L., and R. A. Freeze, Stochastic analysis of steady state groundwater flow in a bounded domain, 2, Two-dimensional simulations, *Water Resour. Res.*, *15*(6), 1543–1559, 1979*b*.

Vomvoris, E. G., Groundwater parameter estimation: A geostatistical approach, M.S. thesis, Univ. of Iowa, Iowa City, July 1982.

Wilson, J. L., P. K. Kitanidis, and M. Dettinger, State and parameter estimation in groundwater models, in *Applications of Kalman Filter to Hydrology, Hydraulics and Water Resources*, edited by C.-L. Chiu, pp. 657–679, University of Pittsburgh, Pittsburgh, Pennsylvania, 1978.

Yakowitz, S., and L. Duckstein, Instability in aquifer identification: Theory and case studies, *Water Resour. Res.*, *16*(6), 1045–1064, 1980.

Yeh, W. W-G., and Y. S. Yoon, Aquifer parameter identification with optimum dimension in parameterization, *Water Resour. Res.*, *17*(3), 664–672, 1981.

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