Hanford Groundwater Modeling - Statistical Methods for Evaluating Uncertainty and Assessing Sampling Effectiveness

**Prepared for
Rockwell Hanford Operations**

By

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HANFORD GROUNDWATER MODELING -
STATISTICAL METHODS FOR EVALUATING
UNCERTAINTY AND ASSESSING SAMPLING
EFFECTIVENESS

prepared for

Rockwell Hanford Operations
Richland, Washington

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January 1979
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ABSTRACT

This report is the first in a series of three documents which address the role of uncertainty in the Rockwell Hanford Operations groundwater model development and application program at the U.S. Department of Energy Hanford Site. Groundwater data collection activities at Hanford are reviewed as they relate to Rockwell groundwater modeling. Methods of applying statistical and probability theory in quantifying the propagation of uncertainty from field measurements to model predictions are discussed. It is shown that measures of model accuracy or uncertainty provided by a statistical analysis can be useful in guiding model development and sampling network design. Recommendations are presented in the areas of model input data needs, parameter estimation data needs, and model verification and variance estimation data needs.

FOREWORD

GENERAL CONSIDERATIONS

C. W. Manry, Project Manager
Long Term Management of Low Level Wastes Program
Waste Technology Program

The Hanford Site, located in south-central Washington, has been a site for radioactive waste storage, reactor development, and chemical processing of defense high-level wastes. Since the early operation of the nuclear facilities at Hanford, ground disposal of low-level radioactive wastes has been widely practiced. Liquid discharges and solid waste burial in the 200 Areas have created an inventory of about 1700 kilocuries of fission product activity and 600 kilograms of plutonium in the Hanford soils. It is estimated that the volumes of contaminated soils and sediments could be as high as 50 million cubic meters. To control these radionuclides from entering the biosphere and becoming a hazard to man will require a long-term waste management plan. The final Environmental Statement* (1975) which assessed all waste management operations at Hanford expresses firm commitments to long-term management of radioactive wastes at Hanford. The major commitments are:

- Publish and make available to the public the status of studies and research in the critical areas of geology, hydrology, meteorology and ecology.
- Develop and test high technology predictive models for assessing radionuclide transport mechanisms.
- Develop a data base to ensure the absence of significant changes in patterns which could result in transport of radionuclides away from their current locations.
- Provide control measures where required to assure safe containment of fission products.
- Develop and implement technology for recovery of plutonium discharges to the soils.

* ERDA-1538 (Unclassified) Final Environmental Statement, Waste Management Operations, Hanford Reservation, December 1975.

To meet these commitments, the Long-Term Management of Low-Level Waste Management Program has been initiated. Implementation of the program is planned under three major activities: Technology Development, Waste Assessment, Demonstration of Compliance with the National Environmental of Policy Act (NEPA). The environmental analysis and engineering technology developed under this program will contribute significantly to the development of a comprehensive low-level waste management plan for Hanford.

SPECIFIC CONSIDERATIONS

R. C. Arnett
Rockwell Hanford Operations
Technical Liaison

This particular report supports the goals and objectives of the Technology Development Activity.

Computer models are widely used in environmental and safety assessments such as those being conducted for the Rockwell Hanford Operations' Long Term Management of Low Level Wastes Program. One of the most neglected areas of computer models studies is an integrated, systematic analysis of the uncertainty in the model results caused by uncertainty or limitations in the basic data, physical and/or mathematical theory, computational methods and resources, and methods of estimating distributions of model input parameters. In order to perform a realistic assessment using computer models, the uncertainty of the results as well as the results themselves should be presented. This report is one of a series of reports which present a basic framework and methodology for addressing uncertainties in groundwater modeling.

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LIST OF SYMBOLS

a, b, c	= symbols used to indicate constant coefficients in various applications
$a_\alpha, a_{\hat{\alpha}}$	= gradient vector associated with the function $\bar{z}(\alpha, u, x, t)$
$b(\alpha)$	= bias of the estimate $\hat{\alpha}$ of the parameter α , written as a function of α
$c(x), d(x), e(x_b)$	= polynomial shape or spline functions used in Example 3-2
d_{ij}	= distance between the points x_i and x_j
$f_l(x_i, u)$	= a polynomial included in the trend function $\bar{z}(\alpha, u, x_i)$ of a Kriging algorithm
$h, h_o, h(x, t)$	= hydraulic potential used in Example 3-2
$p(z), p(z; x, t)$	= probability density function of $z(x, t)$
$p(\hat{\alpha}_1, \hat{\alpha}_2; x_1, x_2)$	= second-order (joint) probability density of $\hat{\alpha}_1$ and $\hat{\alpha}_2$
t, t_i	= time
u	= a column vector of model inputs
x, x_i	= a column vector of cartesian coordinates (one, two or three dimensional depending on the application)
x_a	= spatial coordinate associated with a point on the z_a contour line
x_{i1}, x_{i2}	= horizontal and vertical coordinate of point x_i
$y(t), q(t)$	= column vectors of nodal potentials and accretion rates used in Example 3-2
$z, z_i, z(x), z(x, t)$	= dependent variable or measurement of primary interest in a particular modeling study or statistical analysis; a random process

$\bar{z}(\cdot), \bar{z}(\alpha, u, x, t)$	= symbol representing a function intended to reproduce the behavior of the unknown true mean $E[z; x, t]$
$\bar{z}(\hat{\alpha}, u, x, t)$	= the simulated output of a mathematical model based on the parameter estimates in the vector $\hat{\alpha}$
z_a	= value assigned to a particular $z(x)$ contour line
A	= a matrix of model coefficients derived in Example 2-1
$A, A(\eta), B(y), B(y, \kappa) D(q)$	= coefficient matrices used in Example 3-2
$A_o, A_\alpha, A_{\hat{\alpha}}$	= Jacobian matrices associated with the function $\bar{z}(\alpha, u)$
$C[\hat{\alpha}_1, \hat{\alpha}_2]$	= covariance of the two random variables $\hat{\alpha}_1$ and $\hat{\alpha}_2$
$E[\cdot], E[z], E[z; x, t]$	= mathematical expectation (mean) of a random variable (e.g., $z(x, t)$)
F_α	= a test threshold used to test for model lack-of-fit
$G[\cdot]$	= nonlinear potential function defined in Example 3-2
G	= the estimator coefficient matrix derived in Example 2-1
H_α	= Hessian matrix associated with the function $\bar{z}(\alpha, u, x, t)$
I	= the identity matrix having ones on its diagonals and zeros elsewhere
$\bar{K}(x)$	= hydraulic conductivity used in Example 3-2
L_j	= number of replicates available at a particular measurement time t_j
$N(x, t)$	= net accretion rate used in Example 3-2
$P(N)$	= performance index used to compare alternative sampling networks providing N measurements
S_α, S_u	= dimensions of β_α and β_u , respectively
$S_\epsilon(\hat{\alpha})$	= weighted sum-squared error performance function evaluated at the estimate $\hat{\alpha}$
S_ϵ	= the sum-squared residual error
T	= indicates matrix or vector transpose when used as a superscript
$V[\cdot], V[z], V[z; x, t]$	= variance of a random variable (e.g., $z(x, t)$)

W	= weighting matrix used in least-squares estimation
Z	= a vector of N measurements of the dependent variable $z(x,t)$ taken at various times and locations
$\bar{Z}(\alpha,u), \bar{Z}(\hat{\alpha},u)$	= column vectors of true and predicted dependent variable means, respectively, at various times and places
α	= a column vector of true model parameters
$\hat{\alpha}, \hat{\alpha}[Z]$	= a column vector of estimated model parameters computed from the measurement vector Z
$\alpha_\ell, \hat{\alpha}_\ell$	= scalar components of the parameter vector α and parameter estimate vector $\hat{\alpha}$, respectively
$\beta, \beta_\alpha, \beta_u$	= column vectors of boundary conditions defined in Example 3-2
$\gamma(\Delta x), \gamma_{ij}$	= the variogram value associated with two samples of a random process taken at points located a distance Δx apart or at points x_i and x_j
ϵ	= a column vector of N residual errors
$\epsilon(x,t)$	= the measurement residual error at location x and time t
λ_i	= Kriging algorithm weighting factor associated with measurement z_i
μ_ℓ	= a Lagrange multiplier arising in the punctual Kriging algorithm
η, κ	= column vectors of nodal porosities and conductivities used in Example 3-2
$\bar{\eta}_e(x)$	= effective porosity used in Example 3-2
$\omega(x), \omega(x,t)$	= random residual or sampling error at x and t
Ω, Ω_R	= column vectors of sampling errors at various times and locations
ρ_{ij}	= the correlation coefficient between the i and j^{th} components of a random vector (e.g., $\hat{\alpha}$)
σ_ω^2	= the scalar variance of the sampling error $\omega(x,t)$
$\hat{\sigma}_{\omega r}^2, \hat{\sigma}_{\omega p}^2$	= estimates of σ_ω^2
τ, τ_i	= normalized interpolation time in Example 2-1

$\xi(\Delta x)$	= the incremental difference between two samples of a random process taken at points located a distance Δx apart
Δ	= time integration interval used in Example 3-2
$\Sigma_{\hat{\alpha}}$	= covariance matrix of the parameter estimate vector $\hat{\alpha}$
$[\Sigma_{\hat{\alpha}}]_{ij}$	= the scalar element of $\Sigma_{\hat{\alpha}}$ corresponding to row i and column j
Σ_{Ω}	= covariance matrix of the sampling error vector Ω
$\text{DIM}[\cdot]$	= operator indicating the dimensionality of the vector within the brackets
$\max_x[\cdot]$	= operator indicating that the function within the brackets is to be maximized with respect to its argument x
$\text{Prob}\{\cdot\}$	= operator indicating the probability of a random event (or condition) defined by a mathematical expression written within the brackets
$\text{Tr}[\cdot]$	= symbol representing the matrix trace, defined as the sum of the diagonal elements of the matrix within the brackets
$[\cdot]^{-1}$	= symbol representing the inverse of the square matrix within the brackets

1. INTRODUCTION AND OVERVIEW

This report is the first in a series of three documents concerned with groundwater modeling and data collection programs sponsored by Rockwell Hanford Operations (Rockwell), Rockwell International Corporation. The study summarized in these documents was divided into the following basic tasks:

1. A review of groundwater data collection activities at the Hanford Site, with particular emphasis on the application of field data to Rockwell's groundwater model development activities.
2. A review of parameter estimation methods applicable to groundwater models used at Hanford.
3. A review of methods for designing the field sampling programs needed to support groundwater model development at Hanford.

The overall orientation in these reviews was intended, from the the outset, to be statistical and probabilistic, with proper consideration given to both model and data-related sources of uncertainty.

The present report summarizes the results of the first review task listed above and also introduces some basic statistical concepts which are used in the parameter estimation and sampling design reviews described in two companion reports (McLaughlin, 1979, and Moore and McLaughlin, 1979). Particular emphasis is placed on the close connection between the quality (or uncertainty) of the field data used to develop mathematical models and the quality (or uncertainty) of subsequent model predictions. Although this connection is widely acknowledged in groundwater hydrology, it has not generally been analyzed in a systematic way. We shall see that quantification of uncertainty can be quite valuable, particularly to the modeler concerned

with the reliability of predictions used to make policy decisions or to the manager concerned with minimum cost design of a large scale sampling network.

The starting point for our analysis is the relatively obvious fact that observable groundwater variables (such as hydraulic potential, soil moisture, or contaminant concentration) tend to fluctuate significantly over time and space. This observed variability is, of course, due partly to the complex dynamic behavior of the groundwater aquifer and partly to the inevitable measurement errors encountered in any field or laboratory investigation.

We can attempt to explain measured fluctuations in a particular variable (the *dependent* variable) by supposing that they are caused by changes in related *independent* variables which may or may not be observable. This approach seems particularly reasonable in light of the large body of theory available for describing groundwater behavior. It is well known, for example, that the hydraulic potential in a confined, saturated aquifer can be related, through the principles of mass conservation and potential flow, to a relatively small number of boundary conditions and soil properties which are, in principle at least, well defined. Such theoretical explanations, while generally quite useful, rarely explain *all* the temporal and spatial variability observed in the field. Some unexplained and, for all practical purposes, random *residual error* nearly always remains after even the best theory (or model) is used to explain field observations. This error is a tangible measure of the observer's *uncertainty* about the true state of the groundwater system.

As implied earlier, residual errors can result either from deficiencies in the theory or model used to explain aquifer behavior or from various unavoidable measurement uncertainties. Generally, both sources of error are significant. They are, moreover, difficult to separate since model errors are frequently influenced by uncertainties in the field data used to develop the model in the first place. The relationship between data and model uncertainties can, however, be precisely defined *if* a careful statistical representation of measurement variability is adopted. This is the primary

topic of Section 2, which presents a convenient quantitative approach for describing and evaluating uncertainty.

The statistical theory developed in Section 2 is applied more specifically to groundwater problems of interest to Rockwell in Section 3. The two problems selected for detailed discussion are contour estimation (spatial interpolation of well measurements) and impact assessment (prediction of long-term groundwater trends). These problems are closely related from a statistical point-of-view since they are both ultimately concerned with the estimation of unknown groundwater variables from a limited set of scattered field observations. The computational methods outlined in Section 3 provide a consistent quantitative means for comparing the accuracy of alternative estimation techniques and for evaluating the relative efficiency of alternative data collection procedures.

The final section of this report summarizes the results of a review of current Hanford data programs (the original Task 1 review mentioned earlier). Our approach to this review is based largely on the statistical concepts developed and illustrated in Sections 2 and 3. These concepts help to unify a number of diverse comments and recommendations on sampling procedures at Hanford which might, at first glance, appear to be unrelated. The same general viewpoint should be equally useful in future data reviews, as well as in other aspects of model development and sampling design.

2. STATISTICAL DESCRIPTION OF FIELD MEASUREMENTS AND MODEL PREDICTIONS

The Introduction to this report stresses the importance of a consistent quantitative approach for analyzing measurement and model uncertainty. In this section, we consider in more detail statistical methods for describing uncertainty and examine how uncertainty propagates from field measurements through model parameter estimates to model predictions. Most of the statistical concepts required can be conveyed quite easily with a minimal amount of matrix algebra. The mathematical expressions we use are intended primarily to clarify definitions of important terms and to show how specific quantitative analyses could be carried out in practice. Readers wishing further background in basic probability and statistics or in matrix algebra are referred to the texts by Papoulis (1965), Benjamin and Cornell (1970), and Lipschutz (1968).

RANDOM PROCESSES, PROBABILITY DENSITIES, AND MATHEMATICAL MODELS

The qualitative concepts of measurement variability and uncertainty mentioned in Section 1 may be defined more precisely if we adopt some of the methods of classical probability theory. In practice, groundwater variables do not fluctuate over an unbounded range but, rather, tend to remain in a more or less well-defined range of "reasonable" values. Observations typically cluster about a central or average value as illustrated in Figure 2-1. The bell-shaped curve in this figure indicates the relative frequency of *probability* of the observation values on the horizontal axis--values with large probabilities occur more often (in the long run) than values with small probabilities. To be more precise, we can say that the probability that an observation z lies in the interval between z_l and z_u is given by:

FIGURE 2-1

A TYPICAL FIRST-ORDER
PROBABILITY DENSITY

$$\text{Prob } [z_l \leq z \leq z_u] = \int_{z_l}^{z_u} p(z) dz \quad (2-1)$$

where $p(z)$ = the function plotted in Figure 2-1.

The function $p(z)$ is called the *probability density* of z , and z is called a *random variable* to emphasize the fact that it does not have a single deterministic value but is, instead, defined over a range. When the probability density is a function of time and/or space (as in many groundwater applications) the variable z is often called a *random process* (a more rigorous development of this topic is presented in Papoulis, 1965).

Although probability densities are of considerable interest in their own right, we will generally be concerned only with the first two *moments* of the density function, commonly known as the *mean* and *variance*. These are defined in much the same way as the moments of a rigid body with a density distribution $p(z)$:

$$\text{Mean of } z: \quad E[z] = \int_{-\infty}^{\infty} z p(z) dz \quad (2-2)$$

$$\begin{aligned} \text{Variance of } z: \quad V[z] &= \int_{-\infty}^{\infty} [z - E(z)]^2 p(z) dz \\ &= E\{[z - E(z)]^2\} \end{aligned} \quad (2-3)$$

The operator $E[\cdot]$ is commonly called the *mathematical expectation* of z . If z is a random process, it is sometimes convenient to write $p(z)$, $E[z]$, and $V[z]$ as explicit functions of time and location. For example:

$$E[z; x, t] = \int_{-\infty}^{\infty} z p(z; x, t) dz \quad (2-4)$$

where x = a column vector of cartesian coordinates identifying a particular measurement location (one, two, or three dimensional, depending on the application)

t = measurement time

In many cases, the mean and variance provide all the information needed to characterize the statistical behavior of the random process (see Papoulis, 1965).

The probability density of a particular groundwater variable describes its spatial and temporal fluctuations without any reference to related independent variables or theories of groundwater behavior. If we wish to *explain* the variability described by the probability density, it is convenient to write the random process (dependent variable) z in the following way:

$$z(x,t) = E[z; x,t] + \omega(x,t) \quad (2-5)$$

where $z(x,t)$ = value of z at location x and time t

$\omega(x,t)$ = random measurement residual (or *sampling error*) at x and t

This expression simply divides $z(x,t)$ into its deterministic mean and a residual $\omega(x,t)$ which accounts for random fluctuations away from the mean. The random residual for a particular value of $z(x,t)$ is indicated in Figure 2-1.

The partitioning of $z(x,t)$ provided by Equation (2-5) allows us to distinguish average trends from more local random deviations which vary from sample to example (or from replicate to replicate). For the most part, the physical theories of groundwater hydrology are designed to explain average behavior--mathematical models based on these theories are actually models of the mean term in Equation (2-5). We shall see in our discussion of contour estimation that attempts can also be made to explain the random term but, for the present, we will concentrate on models of the measurement mean.

The simplest useful model of the mean is one which separates temporal and spatial fluctuations in $z(x,t)$ into distinct *effects* represented by separate terms in a linear equation. An example is the following model, which distinguishes between two effects proportional to time and distance, respectively:

$$E[z; x, t] = a + bt + cx \quad (2-6)$$

where a, b, c = constants which do not depend on either x or t

Here the only independent variables included are the time t and location x . Such simple effects models are commonly used in statistical investigations concerned with hypothesis testing and the analysis of variance (see Kendall and Stuart, 1973).

In most groundwater applications, more complex models of mean fluctuations are available and a more general mathematical description is required. If we distinguish between two categories of independent variables, called parameters and inputs, we can express most groundwater models in the following form:

$$E[z; x, t] = \bar{z}(\alpha, u, x, t) \quad (2-7)$$

where α = a column vector of model *parameters* which are, generally speaking, unobservable

u = a column vector of model *inputs* which are, generally speaking, observable

$\bar{z}(\cdot)$ = a complex function relating the independent variables α, u, x and t to the dependent variable mean $E[z; x, t]$

The model's parameters and inputs may themselves depend on time and/or location. A more detailed discussion of the differences between these two types of independent variables will be provided shortly.

It should be apparent that a wide range of mathematical models, from simple effects models to large scale numerical simulations, can be proposed to explain variations in the mean of a particular measured variable. All of these models are, of course, approximations to the "true" mean, which may or may not depend on the particular independent variables selected. Unfortunately, the validity of such approximations is difficult to assess since the dependent variable mean is unobservable (only the *sum* of the mean and the random residual $w(x, t)$ is observable). A practical investigation of

model validity is possible only if certain assumptions are made about the temporal and spatial behavior of the true mean.

The conventional way to proceed is to *tentatively assume* 1) that a particular model structure (i.e., a particular function $\bar{z}(\cdot)$) correctly describes the true mean, and 2) that some of the independent variables of the model are unknown. If the logical implications of these assumptions are followed through, certain statements about the relationship between field observations and model predictions can be made. Statistical tests for checking the validity of these statements can then be used to establish whether or not there is a reasonable chance that the assumed model structure is correct. If the structure does appear to be correct, a number of important expressions relating model and measurement uncertainty can be developed.

Following the traditional statistical approach, let us tentatively assume that a particular model having the form given in Equation (2-7) is structurally correct, so that the dependent variable at time t and location x can be written as:

$$z(x,t) = \bar{z}(\alpha,u,x,t) + \omega(x,t) \quad (2-8)$$

where α, u = the "true" parameter and input values which enable the model $\bar{z}(\cdot)$ to perfectly reproduce the mean $E[z; x, t)$

It is understood here that some of the model's independent variables (the model inputs) are perfectly known while others (the model parameters) are *a priori* completely unknown*. This statistical description of measurement variability is generally called the *Fisher* approach and is discussed in detail in Kendall and Stuart (1973). An alternative description is provided by the *Bayesian* approach, which treats some or all of the independent variables as random variables in their own right. The Bayesian approach is not used in this report but is thoroughly covered by Box and Tiao (1973). A good comparison of the Fisher and Bayesian approaches is presented in

* The term *a priori*, as used here, reflects the state of knowledge about a variable *before* field measurements have been used to estimate its value at a particular time or location.

Schweppe (1973).

In most groundwater applications, some of the independent variables included in the model $\bar{z}(\cdot)$ are used to simulate hypothetical management practices or environmental conditions of particular interest. Well injection rates may be adjusted, for example, to represent a proposed waste discharge strategy (see Arnett et. al., 1977b). Such specified variables are, by definition, well known and may be included in the set of model inputs. Most other independent variables are either estimated from available field data or assigned "physically reasonable" values based on the modeler's judgement. It is convenient to classify these variables into three categories characterized by three corresponding levels of *a priori* uncertainty:

- Variables and coefficients which are either well-known *a priori* (e.g., physical constants) or which may be measured quite accurately (e.g., controlled discharge rates or site topography).
- Variables and coefficients which are less well-known *a priori* but which may be estimated with reasonable accuracy from available field observations (e.g., certain boundary and initial conditions).
- Variables and coefficients which are unknown *a priori*, which are unobservable and which can only be estimated indirectly (e.g., hydraulic conductivities, leakage rates, or sorption coefficients).

The well-known variables in the first category may be included with hypothesized source terms in the model input vector, which can be assumed to be error-free. The poorly-known variables in the third category are significant sources of uncertainty and are appropriately included in the parameter vector. The remaining "gray area" variables in the second category could be considered to be either inputs or parameters, depending on the application. In order to simplify our presentation we will assume that all "gray area" variables are assigned to either the input or parameter categories.

Equation (2-8) provides a way to relate field observations explicitly to a particular mathematical model. The model's predictions cannot, however,

be computed or its validity tested until its unknown parameters are estimated. This is the primary topic of the next subsection.

PARAMETER ESTIMATION AND UNCERTAINTY PROPAGATION

Although engineering judgement and expertise can be (and often are) used to arrive at model parameter estimates in the absence of data, it seems reasonable to require that such subjective estimates be supported with laboratory or field measurements whenever possible. A variety of methods are commonly used to estimate parameters from field data, some statistical in nature and many others deterministic or *ad hoc* (see McLaughlin, 1979, for a detailed review). All of these methods are similar, however, in that they implicitly define a functional relationship between a particular set of field observations and a particular vector of parameter estimates. This relationship, called an *estimator* by statisticians, may be written mathematically as:

$$\hat{\alpha} = \hat{\alpha}[Z] \quad (2-9)$$

where Z = a column vector of field measurements taken at various locations and times and used to compute the parameter estimate $\hat{\alpha}$.

$\hat{\alpha}$ = uncertain estimate of the true but *a priori* unknown parameter vector α .

The measurements used to compute the estimate $\hat{\alpha}$ may take a number of different forms. Hydraulic conductivity estimates can, for example, be based on laboratory soil column measurements, on piezometric measurements taken during a well pumping test, or on water table measurements from a regional well sampling program. For the present, we will assume that the parameters of interest are estimated from measurements of the dependent variable predicted by the model $\bar{z}(\cdot)$ (other cases can be handled with appropriate modifications of the model structure). If, for example, the model is designed to predict the mean hydraulic head, we presume that its conductivity estimates

will be computed from head observations.

The functional interpretation of the estimation process given in Equation (2-9) allows us to investigate in detail the effect of measurement uncertainties on parameter estimates. In particular, we can generalize the scalar measurement equation presented earlier (Equation (2-8)) in the following way:

$$Z = E[Z] + \Omega \quad (2-10)$$

where $E[Z]$ = a column vector of measurement means evaluated at $(x_1, t_1), (x_2, t_2), \dots, (x_N, t_N)$

Ω = a column vector of random sampling errors at $(x_1, t_1), (x_2, t_2), \dots, (x_N, t_N)$

(x_i, t_i) = the location and time of measurement i

N = the number of measurements in the vector Z

The dependence of $\hat{\alpha}$ on the sampling error vector Ω can now be written explicitly as:

$$\hat{\alpha} = \hat{\alpha} \{E[Z] + \Omega\} \quad (2-11)$$

This rather abstract equation can be readily understood when illustrated with examples. The following example describes a simple time-dependent interpolation model which has no inputs and only two scalar parameters, but is general enough to convey some important statistical concepts.

Example 2-1

A convenient procedure for interpolating successive monthly measurements of pan evaporation may be based on the standard linear interpolation equation:

$$\bar{z}(\hat{\alpha}, t) = \hat{\alpha}_1 + \hat{\alpha}_2 \tau \quad 0 \leq \tau \leq 1$$

where $\bar{z}(\hat{\alpha}, t)$ = predicted evaporation rate at time t
 $\hat{\alpha}_1, \hat{\alpha}_2$ = estimated interpolation parameters
 $\tau = (t - t_1) / (t_2 - t_1)$
 t_1, t_2 = observation times prior to and subsequent to time t , respectively

Normally, the parameter estimates are selected as follows:

$$\hat{\alpha}_1 = z_1$$

$$\hat{\alpha}_2 = z_2 - z_1$$

where $z_i \triangleq z(t_i)$ $i = 1, 2$

The estimator may in this case be written as a simple matrix product:

$$\hat{\alpha} = GZ$$

where $\hat{\alpha} = [\hat{\alpha}_1 \quad \hat{\alpha}_2]^T$
 $Z = [z_1 \quad z_2]^T$
 $G = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}$

The superscript T represents the matrix transpose (i.e., $\hat{\alpha}$ and Z are column vectors).

This example illustrates how a simple linear parameter estimator can be compactly represented with vector and matrix notation. If we make the tentative assumption that the interpolation model is structurally correct (i.e., that $\bar{z}(\hat{\alpha}, t)$ can predict $E[z; t]$ perfectly if $\hat{\alpha}$ is selected properly), we can relate the parameter estimates more directly to measurement sampling errors. This is illustrated in the continuation of Example 2-1.

Example 2-1 (continued)

If the interpolation model is structurally correct, there is some set of "true" parameters which will give a perfect match to the mean evaporation, as indicated by the following version of Equation (2-7):

$$E[z;t] = \bar{z}(\alpha, t) = \alpha_1 + \alpha_2 \tau$$

where α_1, α_2 = the "true" interpolation parameter values being estimated

This expression may be written as a simple vector product:

$$E[z;t] = \bar{z}(\alpha, t) = a^T \alpha$$

$$\text{where } a = [1 \quad \tau]^T$$

$$\alpha = [\alpha_1 \quad \alpha_2]^T$$

since a^T is a row vector and α is a column vector, their product is a scalar.

It follows from Equation (2-8) that an evaporation measurement at any time t_i may be written as:

$$z_i = \bar{z}(\alpha, t_i) + \omega_i = a_i^T \alpha + \omega_i$$

$$\text{where } a_i = [1 \quad \tau_i]^T$$

$$\tau_i = (t_i - t_1)/(t_2 - t_1)$$

Since $\tau_1 = 0$ and $\tau_2 = 1$, the parameter estimates derived earlier may be written as:

$$\hat{\alpha}_1 = z_1 = \alpha_1 + \omega_1$$

$$\hat{\alpha}_2 = z_2 - z_1 = \alpha_2 + \omega_2 - \omega_1$$

These equations may be summarized in vector form as:

$$\hat{\alpha} = \alpha + G\Omega$$

$$\text{where } \Omega = [\omega_1 \quad \omega_2]^T$$

The model's prediction at time t was defined earlier to be:

$$\bar{z}(\hat{\alpha}, t) = \hat{\alpha}_1 + \hat{\alpha}_2 \tau$$

or, in vector notation:

$$\bar{z}(\hat{\alpha}, t) = a^T \hat{\alpha}$$

If the expression for $\hat{\alpha}$ derived above is substituted into the prediction equation, the following result is obtained:

$$\bar{z}(\hat{\alpha}, t) = E[z; t] + a^T G \Omega$$

Note that both the parameter estimate vector $\hat{\alpha}$ and the prediction $\bar{z}(\hat{\alpha}, t)$ are affected by the sampling error vector Ω .

The above example illustrates what might be called the *propagation of uncertainty*--sampling errors corrupt the measurements used to compute parameter estimates and the resulting estimation errors corrupt the model's predictions. A reasonably general description of uncertainty propagation is given in Figure 2-2. The shaded elliptical area surrounding the sampling error mean (assumed zero) defines the region of probable ω_1 and ω_2 values. The actual sampling error vector Ω is represented by a point in this region. The sampling error influences, successively, the measurement vector Z , the parameter estimate vector $\hat{\alpha}$, and the model prediction $\bar{z}(\hat{\alpha}, t)$. Each of these variables is random by virtue of its ultimate dependence on Ω . In each case, the degree of randomness is illustrated schematically by an appropriate shaded region.

In order to examine the statistical behavior of random parameter estimates and model predictions in more detail, we must briefly review *multivariate* statistical theory. A first-order probability density such as $p(z; x, t)$ provides, with its associated moments, a reasonably complete statistical description of a scalar random process at a particular time or location. It does not, however, describe relationships or correlations between values of the same random process taken at different times and locations. In general, measurements taken at nearby times and locations or parameters estimated from the same data set will be correlated. The most

FIGURE 2-2

Propagation of Uncertainty
in the Modeling Process

comprehensive description of such correlations is provided by the *second-order* (or joint) probability density of the random variable in question. In the case of two time-invariant scalar parameters, $\hat{\alpha}_1$ and $\hat{\alpha}_2$, the joint probability density may be written $p(\hat{\alpha}_1, \hat{\alpha}_2; x_1, x_2)$. This density specifies a two-dimensional range of likely values for the correlated variables $\hat{\alpha}_1$ and $\hat{\alpha}_2$ similar to the shaded regions shown in Figure 2-2.

The correlation between two jointly distributed random variables is usually measured by the second-moment or *covariance* of the second-order density. The definition is analogous to the expression already presented for the first-order variance:

$$c(\hat{\alpha}_1, \hat{\alpha}_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\hat{\alpha}_1 - E(\hat{\alpha}_1)][\hat{\alpha}_2 - E(\hat{\alpha}_2)] p(\hat{\alpha}_1, \hat{\alpha}_2; x_1, x_2) d\hat{\alpha}_1 d\hat{\alpha}_2 \quad (2-12)$$

$$= E\{[\hat{\alpha}_1 - E(\hat{\alpha}_1)][\hat{\alpha}_2 - E(\hat{\alpha}_2)]\} \quad (2-13)$$

Note that when $x_1 = x_2$, the covariance is equal to the scalar variance $V[\hat{\alpha}]$.

In certain geological applications, random field observations may exhibit erratic and irregular spatial variations which result in unbounded variances and covariances. When this occurs, say in a measurement process $z(x, t)$, the following *incremental process* may be better behaved:

$$\xi(\Delta x) = z(x + \Delta x, t) - z(x, t) \quad (2-14)$$

The expected squared error of this incremental process divided by 2 is commonly called the variogram of $z(x, t)$ and symbolized by $\gamma(\Delta x)$:

$$\gamma(\Delta x) = \frac{V\{\xi(\Delta x)\}}{2} \quad (2-15)$$

The numerous variances and covariances encountered in a multi-parameter analysis of uncertainty propagation may be conveniently combined in a single parameter estimate *covariance matrix*, which is defined in much the same way as the scalar covariance:

$$\Sigma_{\hat{\alpha}} = E\{[\hat{\alpha} - E(\hat{\alpha})][\hat{\alpha} - E(\hat{\alpha})]^T\} \quad (2-16)$$

where the superscript T indicates vector transposition (the quantity in brackets is a column vector post-multiplied by a row vector). If there are p scalar parameters in the vector $\hat{\alpha}$, then $\Sigma_{\hat{\alpha}}$ is a p x p symmetric positive definite matrix. Similar covariance matrices may be defined for other random vectors such as Ω and Z .

The elements of the parameter estimation covariance matrix are related in a natural way to the scalar variances and covariances discussed earlier. These relationships may be summarized as follows:

$$\text{Diagonal elements:} \quad [\Sigma_{\hat{\alpha}}]_{ii} = V[\hat{\alpha}_i] \quad i = 1, \dots, p \quad (2-17)$$

$$\text{Off-diagonal elements:} \quad [\Sigma_{\hat{\alpha}}]_{ij} = C[\hat{\alpha}_i, \hat{\alpha}_j] \quad i \neq j \quad (2-18)$$

The covariance matrix contains all second-order information about the vector random process of interest (in this case $\hat{\alpha}$), and is sufficiently informative to be a generalized measure of overall variability or uncertainty.

Statisticians often find it convenient to measure the degree of correlation between two parameter estimates with the *correlation coefficient*, which is defined, for parameters i and j, as:

$$\rho_{ij} = \frac{[\Sigma_{\hat{\alpha}}]_{ij}}{\{[\Sigma_{\hat{\alpha}}]_{ii}[\Sigma_{\hat{\alpha}}]_{jj}\}^{1/2}} \quad (2-19)$$

This coefficient ranges in magnitude from zero (for uncorrelated estimates) to one (for completely correlated estimates).

The second-order statistical concepts outlined above allow us to derive convenient analytical expressions for the moments of random parameter estimates and model predictions and, therefore, to describe uncertainty propagation more precisely. This is best illustrated if we return to Example 2-1.

Example 2-1 (continued)

The following expressions for the random parameter estimates and predictions of the evaporation interpolation model were derived earlier:

$$\hat{\alpha} = \alpha + G\Omega$$

$$\bar{z}(\hat{\alpha}, t) = E[z; t] + a^T G \Omega$$

Since the sampling errors are, by definition, zero mean and the true parameter vector α is deterministic, the estimate and prediction means are:

$$E[\hat{\alpha}] = \alpha$$

$$E[\bar{z}(\hat{\alpha}, t)] = E[z; t]$$

On the average, the parameter estimates and model predictions are equal, respectively, to the true parameters and the true measurement mean. Such estimates and predictions are said to be *unbiased*.

The parameter estimate covariance matrix may be derived from a systematic application of the definition given in Equation (2-16):

$$\Sigma_{\hat{\alpha}} = G \Sigma_{\Omega} G^T$$

where $\Sigma_{\Omega} = E[\Omega \Omega^T]$ = sampling error covariance matrix

The variance of the model prediction follows directly from Equation (2-3):

$$V[\bar{z}(\hat{\alpha}, t)] = a^T G \Sigma_{\Omega} G^T a$$

As might be expected, estimate and prediction variability are directly dependent on the statistical properties (variances and correlations) of the sampling error.

It is interesting to note the form of the parameter estimate covariance matrix when the sampling errors are uncorrelated and have the same variance. In this case the sampling error covariance matrix is:

$$\Sigma_{\Omega} = \sigma_{\omega}^2 I$$

where σ_{ω}^2 = common sampling error variance

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 2 \times 2 \text{ identity matrix}$$

The estimate covariance matrix is then:

$$\Sigma_{\hat{\alpha}} = \sigma_{\omega}^2 G G^T = \sigma_{\omega}^2 \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}$$

This result indicates, first, that the variance of $\hat{\alpha}_2$ is twice that of $\hat{\alpha}_1$ and, second, that $\hat{\alpha}_1$ and $\hat{\alpha}_2$ are correlated (since the off-diagonal elements of $\Sigma_{\hat{\alpha}}$ are non-zero). The correlation coefficient is given by:

$$\rho_{12} = \frac{-\sigma_{\omega}^2}{\sqrt{2}\sigma_{\omega}^2} = -.71$$

This relatively high degree of correlation occurs because both estimates depend on the measurement z_1 and, therefore, on the sampling error ω_1 .

Variance and covariance equations such as those developed in this example provide a useful way to evaluate a model's uncertainty (or accuracy) before any measurements are actually collected. The modeler can specify what he believes to be a "reasonable" or "likely" level of measurement variability (σ_{ω}^2) and then compute the resulting prediction variance. If this variance is unacceptably high, an effort must be made to improve field instrumentation, collect redundant measurements, modify the parameter estimator, or otherwise reduce the effects of sampling variability. We will consider all of these alternatives in more detail later in this report.

MODEL LACK-OF-FIT

The discussion of parameter estimation and uncertainty propagation provided in the previous subsection allows us to reexamine the question of model structure and validity in more detail. It will be recalled that the classical Fisher approach to statistical analysis *tentatively assumes* that the model of interest, represented by $\bar{z}(\alpha, u, x, t)$, correctly represents the mean of the dependent variable z . When this assumption is made and an appropriate estimator is used to estimate the *a priori* unknown parameter vector α , a complete analysis of uncertainty propagation similar to that illustrated in Example 2-1 may be performed.

The uncertainty analysis obtained subject to the assumption of model correctness may be extended one step further if we consider the *measurement residual error*, defined as the observed difference between measured and predicted dependent variable values at x and t :

$$\varepsilon(x, t) = z(x, t) - \bar{z}(\hat{\alpha}, u, x, t) \quad (2-20)$$

Note that the predicted value $\bar{z}(\hat{\alpha}, u, x, t)$ is computed for a particular estimate $\hat{\alpha}$, as in Example 2-1. If the model is structurally correct, Equation (2-8) holds and the residual error may be written as:

$$\varepsilon(x, t) = \bar{z}(\alpha, u, x, t) - \bar{z}(\hat{\alpha}, u, x, t) + \omega(x, t) \quad (2-21)$$

where α is understood to represent the true but *a priori* unknown parameter value. Once the structure of the model $\bar{z}(\cdot)$ is specified, the statistical behavior of $\varepsilon(x, t)$, which is random by virtue of its dependence on $\hat{\alpha}$ and $\omega(x, t)$, may be readily analyzed. A particularly useful statistical moment is the mean (or expected) sum-squared residual error, which is examined briefly in the extension of Example 2-1 presented below.

Example 2-1 (continued)

Suppose that N evaporation measurements are available at times other than t_1 or t_2 and that N residual errors are computed from these measurements in accordance with Equation (2-20):

$$\epsilon_i = z(t_i) - \bar{z}(\hat{\alpha}, t_i) \quad i=1 \dots N$$

$$t_1 < t_i < t_2$$

If these N errors are squared and summed, the resulting statistic may be written as:

$$S_\epsilon = \sum_{i=1}^N \epsilon_i^2 = \epsilon^T \epsilon$$

where $\epsilon = [\epsilon_1, \epsilon_2, \dots, \epsilon_N]^T$

Note that ϵ^T and ϵ are, respectively, N dimensional row and column vectors and that S_ϵ is a scalar.

If the interpolation model's structure is correct, Equation (2-21) and the expressions developed earlier for $\bar{z}(\hat{\alpha}, t_i)$ and $z(\hat{\alpha}, t_i)$ may be used to write S_ϵ in the following form:

$$S_\epsilon = [AG\Omega + \Omega_R]^T [-AG\Omega + \Omega_R]$$

where Ω_R = a column vector of N sampling errors associated with the evaporation measurements $z_1, \dots, z_N$ used to compute the residual error vector

A = an $N \times 2$ matrix having rows $a_1, a_2, \dots, a_N$, where a_i is defined as in the earlier examples

If all the sampling errors are uncorrelated and have the same variance σ_ω^2 , the mean of S_ϵ is:

$$E[S_\epsilon] = E[\Omega^T G^T A^T AG\Omega] + N\sigma_\omega^2$$

This may be shown after some manipulation (see Kendall and Stuart, 1973) to be equivalent to:

$$E[S_\epsilon] = \sigma_\omega^2 \text{Tr}[G^T A^T AG] + N\sigma_\omega^2$$

where the symbol Tr represents the matrix *trace*, defined as the sum of the diagonal elements of the matrix within the brackets. It follows that the sampling error variance σ_{ω}^2 can be related directly to the expected sum-squared residual error:

$$\sigma_{\omega}^2 = \frac{E[S_{\epsilon}]}{N + \text{Tr}[G^T A A G]}$$

This implies that the following estimate of σ_{ω}^2 is *unbiased* (i.e., has a mean equal to σ_{ω}^2):

$$\hat{\sigma}_{\omega r}^2 = \frac{S_{\epsilon}}{N + \text{Tr}[G^T A A G]}$$

The subscript r indicates that the estimate is based on observed *residual* errors.

The derivation of the estimate $\hat{\sigma}_{\omega r}^2$ outlined in the above example is valid only if the model $\bar{z}(\hat{\alpha}, t)$ is correct (so that Equation (2-21) may be used) and if the sampling errors are uncorrelated and have the same variance. If the model is not correct or the sampling errors have a more complex correlation structure, $\hat{\sigma}_{\omega r}^2$ will no longer be an unbiased estimate of σ_{ω}^2 . The possible bias of $\hat{\sigma}_{\omega r}^2$ can be investigated if an independent estimate of the sample error variance is available. This may be briefly illustrated with our interpolation example.

Example 2-1 (concluded)

Assume, for the moment, that the sampling errors associated with all evaporation measurements in the example are uncorrelated with variance σ_{ω}^2 . Suppose that several *replicate* evaporation measurements (i.e., repeat measurements taken at the same time and place) are available for estimating σ_{ω}^2 . If the replicates are all taken at time t_j (where t_j is unequal to t_1 , t_2 or any of the t_i 's), this estimate may be computed as follows:

$$\hat{\sigma}_{\omega p}^2 = \frac{1}{L_j - 1} \sum_{\ell=1}^{L_j} [Z_{\ell}(t_j) - m(t_j)]^2$$

where $Z_{\ell}(t_j)$ = the ℓ^{th} replicate evaporation measurement taken at time t_j

$$m(t_j) = \frac{1}{L_j} \sum_{\ell=1}^{L_j} Z_{\ell}(t_j) = \text{sample replicate mean at time } t_j$$

L_j = number of replicates available at time t_j

The subscript p indicates that the estimate $\hat{\sigma}_{\omega p}^2$ is based on *pooled* replicate measurements.

If the model $\bar{Z}(\hat{\alpha}, t_i)$ used to derive the residual error estimate of σ_{ω}^2 ($\hat{\sigma}_{\omega r}^2$) is structurally correct, we would expect $\hat{\sigma}_{\omega p}^2$ and $\hat{\sigma}_{\omega r}^2$ to be approximately equal or, equivalently,:

$$\frac{\hat{\sigma}_{\omega r}^2}{\hat{\sigma}_{\omega p}^2} \approx 1$$

If, on the other hand, the model is incorrect, $\hat{\sigma}_{\omega r}^2$ will overestimate $\sigma_{\omega p}^2$. In this case some of the observed residual error will be due *solely* to the model's structural deficiencies (i.e., S_{ϵ} will be non-zero even when σ_{ω}^2 and Ω are zero) and we can expect the following relationship to hold:

$$\frac{\hat{\sigma}_{\omega r}^2}{\hat{\sigma}_{\omega p}^2} > 1$$

The difference between these two alternatives can be conveniently expressed in hypothesis-testing terms:

Hypothesis H_0 :

The model's structure is correct

$$\frac{\hat{\sigma}_{\omega r}^2}{\hat{\sigma}_{\omega p}^2} < F_{\alpha}$$

The model's structure is incorrect

$$\frac{\hat{\sigma}_{\omega r}^2}{\hat{\sigma}_{\omega p}^2} \geq F_{\alpha}$$

where F_{α} is a *test threshold* selected to give a specified probability of correctly detecting model structure errors.

The above example outlines in very brief terms the traditional statistical approach for investigating *model lack-of-fit*. The basic point to be remembered is that sampling error variance estimates based on residual errors and on pooled replicates should be approximately equal when the model's structure is correct (given stated assumptions about the sampling error correlation structure). When these alternative variance estimates are *significantly different*, it is likely that the model's structure is deficient in some way. A precise probabilistic definition of just what constitutes a significant difference is provided by hypothesis-testing theory, which specifies how the test threshold F_α should be selected. Further details on this topic are provided in many statistical texts, including Kendall and Stuart (1973) and Draper and Smith (1967).

It is reasonable to ask just how a model should be modified to give a better fit if hypothesis tests such as the one described in Example 2-1 indicate that structural errors are probably significant. Unfortunately, there is no good general answer to this question. The best approach is for the modeler to reexamine his model's assumptions, using the observed residual errors to identify possible problem areas. Often, structural errors result from theoretical simplifications (e.g., reduced dimensionality) which are made for computational convenience. Lack-of-fit can also be caused by errors in inputs (e.g., boundary conditions) which are assumed to be well-known but which should, in fact, be treated as parameters and estimated from field observations. Each application presents unique difficulties which require a careful review of the entire modeling process.

Once the source of a lack-of-fit problem is identified, the modeler is confronted with the often difficult choice of either modifying his model (sometimes at considerable expense and/or delay) or taking the risk that his predictions will be inaccurate and misleading. A variety of statistical methods are available for quantifying the risks and costs associated with such decisions. These methods can, however, rarely account for all of the institutional and economic considerations involved in model development. At some point, the modeler must reconcile conflicting requirements of accuracy and cost in his own mind and exercise his best professional judgment.

SUMMARY

This section has touched on a number of important statistical concepts which can only be properly appreciated after careful application to practical problems. The simple interpolation example helps to give a general idea of how statistical theory can be used to quantify the propagation of uncertainty from field measurements to model predictions. In order to review this process, it is helpful to recall the following points:

1. The variability observed in groundwater measurements can be conveniently quantified with probability density functions and their associated first or second-order moments (mean, variance, and covariance).
2. The measurement variability described by a probability density can be explained by relating the mean of the observed dependent variable of interest to certain independent variables suggested by hydrologic theory. A mathematical model is a quantitative representation of this relationship.
3. If we tentatively assume that the functional structure of a proposed mathematical model is correct, and that unknown model parameters may be estimated from available field observations, we can derive expressions for the mean and variance of the model's predictions. These expressions depend on the structure of the model and its parameter estimator and on the statistical properties of the random measurement residuals (or sampling errors).
4. Given appropriate assumptions, the variance of random sampling errors may be estimated from either observed residual errors or pooled sample replicates. These alternative variance estimates can be used to verify the tentative assumption of structural correctness which is the basis for any statistical analysis of uncertainty propagation.

We can now turn to some more detailed uncertainty analyses which are particularly relevant to Rockwell's activities at Hanford.

3. GROUNDWATER MODEL ACCURACY ANALYSIS

The statistical concepts outlined in the previous section are applicable to nearly any problem which involves estimation or prediction of groundwater variables from uncertain field measurements. Here we briefly consider two estimation/prediction problems which are of particular interest to Rockwell--spatial interpolation of scattered well measurements and long-term impact assessment. In each case, the primary emphasis is on uncertainty propagation and on the relationship between sampling strategy and model accuracy.

INTERPOLATION AND CONTOUR ESTIMATION

One of the most basic needs in any groundwater management study is for a thorough three dimensional description of existing hydrologic conditions throughout the aquifer(s) of interest. Although this may seem a simple requirement, reliable regional descriptions of important groundwater variables are actually quite difficult to obtain in practice. This is because available measurements of these variables are collected from scattered wells which do not provide adequate information about the basin's overall hydrologic behavior. A satisfactory description of regional groundwater conditions can only be obtained if a good spatial interpolation technique is available, preferably one which augments field measurements with other geological sources of information.

The interpolation or contour estimation problem is defined schematically in Figure 3-1, which shows a rectangular region containing three observation wells at locations x_1 , x_2 , and x_3 . We wish to estimate, from measurements at these wells, the value of a particular regional variable $z(x)$ at some location x_0 where no well is available. When estimates of this variable are computed at many locations, contour lines may be drawn through all

Figure 3-1
SIMPLIFIED DESCRIPTION OF THE
CONTOUR ESTIMATION PROBLEM

points having the same value (see Figure 3-1 for an example). The uncertainty associated with this line (or, equivalently, with the estimates which define it) depends on the configuration of the measurement well network, the natural variability of $z(x)$, and the particular estimation algorithm selected. All of these factors should be accounted for in a statistical analysis of the contouring problem.

The notation developed in Section 2 may be used to define the contour estimation problem more precisely. Suppose we partition a particular observable (dependent) variable into mean and random components, as in Equation (2-8). If the mean component is modeled as a function of specified independent variables, the following measurement equation results:

$$z(x) = \bar{z}(\alpha, u, x) + w(x) \quad (3-1)$$

where $z(x)$ = "true" (and potentially observable) value of the dependent variable at location x

$\bar{z}(\alpha, u, x) = E[z; x]$ = a model of the dependent variable mean (or "trend") over the region of interest

α, u = the "true" parameter and input (independent variable) values which enable the model $\bar{z}(\cdot)$ to perfectly reproduce $E[z; x]$.

$w(x)$ = random residual at location x

The temporal dependence of this equation is not explicitly noted since we will be concerned only with measurement interpolation at one particular time. Time-varying contour estimation is a natural extension of this simpler and more common steady-state problem.

Note that we are following the classical Fisher approach outlined in Section 2 by assuming 1) that the function $\bar{z}(\alpha, u, x)$ correctly describes spatial variations of the true mean $E[z; x]$, and 2) that the parameter vector α is *a priori* unknown. The input vector u consists, as before, of well-known independent variables.

Equation (3-1) may be generalized to describe a complete set of N well measurements collected at various locations. The resulting vector measurement equation is:

$$Z = \bar{Z}(\alpha, u) + \Omega \quad (3-2)$$

where Z = a column vector of N well measurements collected at the locations $x_1, x_2, \dots, x_n$

$\bar{Z}(\alpha, u)$ = a column vector of N corresponding measurement means $\bar{z}(\alpha, u, x_1), \bar{z}(\alpha, u, x_2), \dots, \bar{z}(\alpha, u, x_n)$

Ω = a column vector of N corresponding sampling errors $\omega(x_1), \omega(x_2), \dots, \omega(x_n)$.

This allows the contour estimation problem to be defined as follows:

Derive an estimator

$$\hat{z}(x_0) = \hat{z}[Z]$$

which computes an estimate $\hat{z}(x_0)$ of the dependent variable $z(x_0)$ at any location x_0 in the region of interest from an N dimensional measurement vector Z described by Equation (3-2).

In our problem formulation the random residual is not treated as an undesirable measurement error (as it was in Example 2-1) but is considered to be the primary source of observed variability in the dependent variable $z(x)$. This is consistent with the relatively empirical nature of contour estimation, which relies more on measured correlations than on sophisticated hydrologic models for explanations of spatial variation.

A review of the literature suggests that the most generally useful contour estimation techniques are spline function and finite element filtering procedures, Thiessen polygon interpolation, and Kriging (see Delhomme, 1976, for a good survey of the alternatives). Generally speaking, the spline, finite element, and Thiessen polygon approaches rely more heavily on the

mean function for a description of spatial variability while Kriging relies more heavily on the statistical moments (e.g., covariance or variogram) of the random residual. In either case, the mean and variance of the computed estimates may be derived with the methods described in Section 2.

The reliance of the Kriging estimator on the statistical moments of $\omega(x)$ (or, equivalently, of $z(x)$) makes its accuracy analysis particularly interesting. The *punctual Kriging algorithm* is described by the following linear equation:

$$\hat{z}_0 = \sum_{i=1}^N \lambda_i z_i \quad (3-3)$$

where $\hat{z}_0 = \hat{z}(x_0)$ = computed estimate of z_0
 $z_0 = z(x_0)$ = true (random) dependent variable at location x_0
 $z_i = z(x_i)$ = well measurement at location x_i
 λ_i = weighting factor associated with z_i (to be determined).

It is apparent from Equation (3-3) that both the mean and variance of the estimate $\hat{z}_0$ depend on the weighting factors of the Kriging algorithm (the λ_i). The mean is, for example, given by:

$$E[\hat{z}_0] = \sum_{i=1}^N \lambda_i E[z_i] = \sum_{i=1}^N \lambda_i \bar{z}(\alpha, u, x_i) \quad (3-4)$$

If the assumed mean function $\bar{z}(\cdot)$ is linear in the parameter vector α , it may be written as:

$$\bar{z}(\alpha, u, x_i) = E[z_i] = \sum_{\ell=1}^p \alpha_{\ell} f_{\ell}(x_i, u) \quad (3-5)$$

where $f_{\ell}(x_i, u) = \frac{\partial \bar{z}(\alpha, u, x_i)}{\partial \alpha_{\ell}}$ = a simple function of x_i which does not depend on α

α_{ℓ} = ℓ^{th} component of the p dimensional parameter vector α

and the estimate mean is:

$$E[\hat{z}_0] = \sum_{\ell=1}^p \alpha_{\ell} \sum_{i=1}^N \lambda_i f_{\ell}(x_i, u) \quad (3-6)$$

It is reasonable to select the λ_i so that the uncertainty associated with the estimate is as small as possible. More specifically, $\hat{z}_0$ should be an *unbiased minimum variance estimate* of z_0 which satisfies the following conditions:

$$\hat{z}_0 \text{ unbiased: } E[\hat{z}_0] = E[z_0] \quad (3-7)$$

$$\hat{z}_0 \text{ minimum variance: } V[\hat{z}_0] \leq V[z^*] \text{ for any estimate } z^* \text{ of } z_0 \text{ computed from } Z$$

If Equations (3-1) and (3-6) are substituted into Equation (3-7), it is easy to show that $\hat{z}_0$ will be an unbiased estimate when the λ_i satisfy the following p constraints:

$$\sum_{i=1}^N \lambda_i f_{\ell}(x_i, u) - f_{\ell}(x_0, u) = 0 \quad \ell=1, \dots, p \quad (3-8)$$

If a Lagrange multiplier approach is used to minimize the estimate variance with respect to the λ_i , subject to the constraints of Equation (3-8), N additional equations are obtained (see Delhomme, 1976, for the details):

$$\sum_{j=1}^N \lambda_i \gamma_{ij} + \sum_{\ell=1}^p \mu_{\ell} f_{\ell}(x_i, u) = \gamma_{i0} \quad i=1, \dots, N \quad (3-9)$$

where γ_{ij} = the *variogram* of $z(x)$ evaluated at the points x_i and x_j (see Equations (2-14) and (2-15))

μ_{ℓ} = the Lagrange multiplier associated with the ℓ^{th} constraint in Equation (3-8)

Equations (3-8) and (3-9) together define $N+p$ equations in $N+p$ unknowns (the N unknown λ_i 's and the p unknown α_ℓ 's). Estimates of the α_ℓ 's are generally not computed explicitly since they are not needed to obtain the desired estimate of z_o (computed from Equation (3-3)).

The appearance of the variogram values γ_{ij} and γ_{io} in the Kriging algorithm is a direct result of the minimum variance condition, which introduces second-order statistics into the estimation problem. In most Kriging applications, the variogram γ_{ij} is assumed to be a simple function of Δx , the distance between the points x_i and x_j . This is equivalent to assuming that $z(x)$ varies isotropically over the region of interest, without any directional preferences. A number of typical variograms are discussed, with physical interpretations, in Delhomme (1976). One of these is used in the simple Kriging example outlined below.

Example 3-1

Suppose that the water table elevation mean in a particular rectangular region (see Figure 3-1) is known to be a constant so that:

$$\bar{z}(\alpha, x, u) = \alpha$$

Interpolated values of $z(x)$ throughout the region are to be computed from unreplicated measurements taken at the three well sites x_1, x_2 , and x_3 , using the following Kriging algorithm (Equation 3-3):

$$\hat{z}_o = \sum_{i=1}^3 \lambda_i z_i$$

In this case, Equations (3-8) and (3-9) become:

$$\sum_{i=1}^3 \lambda_i = 1$$

$$\sum_{j=1}^3 \lambda_j \gamma_{ij} + \mu_1 = \gamma_{io} \quad i=1,3$$

If a water table elevation variogram function $\gamma(\Delta x)$ has been developed for this region (possibly from historical data records) the variogram values γ_{ij} can be readily evaluated. When $\gamma(\Delta x)$ has the simple linear form of Figure 3-2, the Kriging equations become:

$$a \sum_{j=1}^3 \lambda_j d_{ij} + \mu_1 = a d_{i0} \quad i=1,3$$

$$\sum_{i=1}^3 \lambda_i = 1$$

where $d_{ij} = |x_i - x_j| = [(x_{i1}^2 - x_{j1}^2) + (x_{i2}^2 - x_{j2}^2)^2]^{1/2}$

x_{i1}, x_{j1} = horizontal coordinates of points x_i and x_j

x_{i2}, x_{j2} = vertical coordinates of points x_i and x_j

Uncertainty propagates from measurements to estimates in a contour estimation problem in much the same way as in the temporal interpolation problem of Example 2-1. This effect may be quantified with expressions which relate the estimate variance explicitly to the statistical properties of the measurements used in the estimation algorithm. In the case of punctual Kriging, the variance of the estimate $\hat{z}_0$ may be shown to be (see Delhomme, 1976):

$$V[\hat{z}_0] = \sum_{i=1}^N \lambda_i \gamma_{i0} + \sum_{\ell=1}^p f_{\ell} \mu_{\ell}(x_0, u) \quad (3-10)$$

This variance, which is a convenient scalar measure of contour accuracy at x_0 , clearly depends on the well sampling configuration since the coefficients and variogram values appearing in Equation (3-10) are all functions of well location.

FIGURE 3-2

LINEAR VARIOGRAM FUNCTION FOR THE
RECTANGULAR REGION OF FIGURE 3-1 PLOTTED VS. Δx

The dependence of the estimate variance on well spacing suggests that alternative sampling networks may be evaluated by comparing their respective variances. A convenient index of sampling network performance is the maximum estimation variance obtained in the region of interest (i.e., the variance at the point where the interpolation is poorest). This index may be written, for a given number of samples N , as:

$$P(N) = \max_x V[\hat{z}(x)] \quad (3-11)$$

If $P(N)$ is plotted for various well configurations (see Figure 3-3), the resulting distribution of points gives a good feeling for the relationship between sampling strategy and contour accuracy. The curve drawn through the points having the smallest $P(N)$ defines a set of *optimal* sampling designs.

In certain simple cases, the optimal well configuration may be derived analytically. The appropriate equations for our example provide an illustration of this procedure.

Example 3-1 (concluded)

If the variogram of Figure 3-1 and the trend function $\bar{z}(\alpha, x, u)$ defined earlier are substituted into Equation (3-10), the variance of the estimate produced by our simple three well Kriging algorithm may be shown to be:

$$V[\hat{z}_0] = a \sum_{i=1}^3 \lambda_i d_{i0} + \mu_1$$

Note that the estimation variance goes to zero at well locations ($x_0 = x_1, x_2$, or x_3) since $z(x)$ is observable at these points.

The three-well performance index $P(3)$ obtained from the above variance expression is:

$$P(3) = \max_{x_0} V[\hat{z}_0] = \max_{x_0} \left\{ a \sum_{i=1}^3 \lambda_i d_{i0} + \mu_1 \right\}$$

FIGURE 3-3

PLOT OF CONTOUR ESTIMATION PERFORMANCE
FUNCTION VS. NUMBER OF SAMPLES FOR VARIOUS
SAMPLING STRATEGIES (Well Configurations)

This maximum can be found analytically by differentiating $V[\hat{z}_0]$ with respect to x_{01} and x_{02} for a particular set of well coordinates x_1, x_2 , and x_3 . The resulting function can then be minimized with respect to these coordinates to give the optimal three-well design.

Alternatively, a sequential approach can be used to locate first one well, then a second, and finally a third. At each stage, the new well is positioned to minimize the maximum estimation error variance over the region. This approach has computational and logistic advantages which make it particularly attractive in certain applications.

The estimation error variance expressions obtained from interpolation techniques such as Kriging are useful not only for sampling design purposes but also for development of contour confidence limits. These graphical indicators of contour accuracy may be derived directly from the error variance if the first-order probability density $p(z;x)$ is known. When the contour estimate is computed from a large number of relatively uncorrelated measurements, it can be shown that $p(z;x)$ will tend towards a normal (or Gaussian) distribution (see the discussion of the Central Limit Theorem in Kendall and Stuart, 1973). In this case, the estimate $\hat{z}_0$ has a 95 percent chance of lying within approximately two standard deviations of z_0 :

$$\text{Prob } \{\hat{z}_0 - 1.96 \sigma_0 \leq z_0 \leq \hat{z}_0 + 1.96 \sigma_0\} = .95$$

$$\text{where } \sigma_0 = \{V[\hat{z}_0]\}^{1/2}$$

The quantities $\hat{z}_0 \pm 1.96 \sigma_0$ are known as the upper (+) and lower (-) 95 percent *confidence limits* for z_0 .

The z_a contour line may be defined as the set of all points x_a at which the variable of interest is equal to a particular value z_a . Mathematically, this is written:

z_a contour line: $\{x_o\}$ such that $\hat{z}_o = z_a$

It follows that the outer and inner 95 percent *confidence contours* for z_a are:

z_a confidence contours: $\{x_o\}$ such that $\hat{z}_o = z_a \pm 1.96 \sigma_a$

These confidence contours may be plotted on either side of the estimated contour line to give an idea of the probable geographic range of an uncertain contaminant plume or groundwater flow pattern (see Figure 3-4). As might be expected, contour accuracy decreases as the contour lines move further away from monitored well locations.

It is clear from the above discussion that the Kriging technique depends on a knowledge of the variogram function $\gamma(\Delta x)$, since it is this function which describes the inherent variability of the random process $z(x)$. As was shown in Section 2, the variogram is directly related to the variance and autocorrelation properties of $z(x)$ and, by implication, $\omega(x)$. Estimation of the variogram is conceptually equivalent to estimation of sampling error statistics.

In practice, the variogram for a particular groundwater variable is developed from the sample variance of the incremental process $z(x+\Delta x) - z(x)$. When this sample variance is plotted (as a series of unconnected points) vs. Δx , a generally monotonically increasing pattern emerges. This pattern of points may be fit by a simple curve such as a straight line (as in Example 3-1), a quadratic, or some other convenient function. Of course, this approach presumes the availability of enough field measurements to develop a meaningful plot. If few (or no) field samples are available the variogram must be assumed or guessed, with qualitative geological information or historical experience used to arrive at a plausible functional representation.

FIGURE 3-4

CONFIDENCE CONTOURS ASSOCIATED WITH
A TYPICAL CONTAMINANT PLUME

IMPACT ASSESSMENT

One of the primary uses of groundwater simulation models is for assessment of the long-term impacts of alternative management policies. Examples include studies of the impacts of aquifer depletion on groundwater quality, studies of the transport and ultimate fate of injected wastes, and studies of the impacts of surface water projects on related groundwater supplies. In each of these cases, the simulation model to be used is adjusted (calibrated) and tested to insure, as much as possible, that its predictions will be accurate. Various hypothetical management alternatives are then investigated, through manipulation of appropriate model inputs, in "open loop" simulation runs which make predictions many years into the future. A schematic description of the problem is given in Figure 3-5.

This sub-section outlines a statistical analysis of simulation model performance which is intended to quantify the prediction uncertainty illustrated visually in Figure 3-5. The analysis parallels, in many respects, the discussion of uncertainty propagation presented in Section 2 and Example 2-1. It is conveniently divided into three parts concerned, respectively, with the derivation of the mean function $\bar{z}(\alpha, u, x, t)$, estimation of the unknown parameter vector α , and computation of expressions for the mean and variance of the model prediction $\bar{z}(\hat{\alpha}, u, x, t)$. Each of these topics is briefly considered in the following paragraphs.

Derivation of the Dependent Variable Mean Function

The Fisher description of measurement variability described in Section 2 is based on the following equation (Equation (2-8)), which partitions the dependent variable $z(x, t)$ into a mean and a random residual or sampling error:

$$z(x, t) = \bar{z}(\alpha, u, x, t) + \omega(x, t) \quad (3-12)$$

where $z(x, t)$ = the observed value of the dependent variable at location x and time t

a) Prediction of Contaminant Concentration $c(x,t)$ at a Particular Location x

b) Prediction of Contaminant Concentration $c(x,t)$ throughout a Region (from 1978 to 2010)

FIGURE 3-5

SCHEMATIC DEFINITION OF THE IMPACT ASSESSMENT PROBLEM

$\bar{z}(\alpha, u, x, t) = E[z; x, t]$ = a model of the dependent variable mean (or "trend") over the region and time period of interest

α, u = the true parameter and input (independent variable) values which enable the model $\bar{z}(\cdot)$ to perfectly reproduce $E[z; x, t]$

$\omega(x, t)$ = random sampling error at location x

We have taken the Fisher approach here and assumed 1) that the function $\bar{z}(\alpha, u, x, t)$ correctly describes spatial and temporal variations in the mean $E[z; x, t]$ and 2) that the parameter vector α is *a priori* unknown (see Section 2). The input vector u consists of well-known independent variables which are discussed in more detail below.

It is worth noting that impact assessment, as we have defined it here, differs somewhat from contour estimation in its interpretation of the terms in Equation (3-12). Contour estimation (particularly Kriging) treats the random residual $\omega(x)$ as the primary source of observed variability in the dependent variable $z(x)$. It follows that contouring algorithms should estimate $z(x)$, which includes both mean and residual sources of variability, rather than $E[z; x]$, which does not, in itself, account for all observed spatial variations. Impact assessment, on the other hand, considers the random residual to be a source of undesirable measurement error--a noise term--whose effects should be minimized. It is not surprising, then, that simulation models concerned with impact assessment are generally designed to estimate the mean $E[z; x, t]$, which is assumed to account for all "legitimate" spatial and temporal variations in the dependent variable $z(x, t)$. These two estimation approaches are equally valid interpretations of the probabilistic description of variability outlined in Section 2. Statistical theory is flexible enough to accommodate them both.

In practice, the function $\bar{z}(\alpha, u, x, t)$ appearing in Equation (3-12) is usually derived from partial differential equations which are discretized in space and time and then solved recursively. This process may be illustrated with the familiar example presented below.

 Example 3-2

Arnett et. al. (1976) describe a two-dimensional model of saturated groundwater flow which is based on the so-called Boussinesq approximation. This model is summarized by the following equation for water table elevation (or hydraulic potential):

$$\bar{\eta}_e \frac{\partial h}{\partial t} = \nabla \cdot [\bar{K}(h-h_o) \nabla h] + N$$

moisture storage *horizontal* *accretion*
 moisture flux

where $h(x,t)$ = hydraulic potential at location x and time t (m)

h_o = elevation of aquifer bottom (m)

$\bar{\eta}_e(x)$ = vertically averaged effective porosity at x
(m/sec)

$\bar{K}(x)$ = vertically averaged hydraulic conductivity at x (m/sec)

$N(x,t)$ = net accretion rate at x (m/sec)

This partial differential equation is solved over a two-dimensional region with either potential or horizontal moisture flux specified at every point on the boundary. All vertical moisture fluxes are included in the accretion term.

The partial differential equation introduced in this example is typical of the equations used in conceptually-based groundwater models. Most models of flow or contaminant transport are derived from basic principles of mass continuity and potential flow which lead naturally to a continuous partial differential formulation. The coefficients and boundary conditions associated with these models are actually *functions* of location which may be represented in a parametric form. The hydraulic conductivity in the vicinity of a well located at x_o could, for example, be approximated by a three parameter quadratic model:

$$\bar{K}(x) = a + b |x - x_0| + c |x - x_0|^2$$

Similar equations may be used for boundary potentials or fluxes.

A systematic method for developing such parameterized representations of dependent variables as well as of model coefficients, inputs and boundary conditions is provided by the *finite element* spatial discretization technique (see Zienkiewicz, 1977). This technique is conveniently illustrated with our Boussinesq example.

Example 3-2 (continued)

If the triangular network of Figure 3-6 is used to divide a region into several discrete elements, potentials, coefficients and inputs may be defined at particular locations (or *nodes*). A continuous representation of these variables can then be constructed from weighted sums of the nodal values:

$$h(x, t) = c^T(x) y(t)$$

$$N(x, t) = c^T(x) q(t)$$

$$\eta_e(x) = d^T(x) \eta$$

$$\bar{K}(x) = d^T(x) \kappa$$

where $y(t), q(t)$ = Q dimensional column vectors of nodal potentials and accretion rates, respectively

η, κ = R dimensional column vectors of porosities and conductivities, respectively

$c(x)$ = a Q dimensional column vector of polynomial *shape functions* for potential and accretion

$d(x)$ = an R dimensional column vector of polynomial *shape functions* for porosity and conductivity

The T superscript used here represents the vector or matrix transpose.

$$y(t) = [y_1(t), y_2(t), \dots, y_{16}(t)]^T$$

$$c(x) = [0, 0, 0, 0, 0, 0, c_7(x), c_8(x), c_9(x), 0, 0, c_{12}(x), c_{13}(x), 0, 0, c_{14}(x)]^T$$

$$\begin{aligned} c_7(x), c_8(x), c_9(x) \\ c_{12}(x), c_{13}(x), c_{16}(x) \end{aligned} = \begin{aligned} &\text{shape functions associated with} \\ &\text{the nodes of element 5} \end{aligned}$$

a) Detailed Finite Element Discretization for Potential & Accretion

$$\eta = [\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, \eta_7, \eta_8, \eta_9]^T$$

$$d(x) = [0, 0, 0, d_4(x), d_5(x), d_6(x), d_7(x), d_8(x), d_9(x)]^T$$

$$\begin{aligned} d_1(x), d_2(x), d_3(x) \\ d_4(x), d_5(x), d_6(x) \end{aligned} = \begin{aligned} &\text{shape functions associated with} \\ &\text{the nodes of element 2} \end{aligned}$$

b) Coarse Finite Element Discretization for Porosity and Conductivity

FIGURE 3-6

DETAILED AND COARSE FINITE ELEMENT
DISCRETIZATION SCHEMES FOR EXAMPLE 3-2

The shape functions contained in the vectors $c(x)$ and $d(x)$ relate potential, accretion, porosity or conductivity at location x to the adjacent nodal values of these variables, providing a convenient interpolation scheme which has considerable physical appeal. Note that the coefficients $\eta_e(x)$ and $\bar{K}(x)$ need not be discretized at the same level of detail as the more variable potential and accretion functions.

A one-dimensional version of the shape function approach may also be used to parameterize constant boundary conditions. Boundary values of potential could, for example, be written as:

$$h(x_b) = e^T(x_b) \beta$$

where $e(x_b)$ = an S dimensional column vector of cubic spline functions defined for points x_b on the boundary

β = an S dimensional column vector of coefficients which weight the various components of $e(x_b)$

The coefficients in the vector β could be values of potential at boundary nodes or simply parameters selected to give $h(x_b)$ a certain desired shape.

The parameterization provided by the finite element and spline fitting techniques described in the example is applicable to most groundwater modeling problems. When the dependent variable, coefficients, and source terms of a partial differential equation have been discretized on a finite element grid, the original equation may be transformed into a set of coupled ordinary differential equations of the following general form:

$$A \frac{dy(t)}{dt} + B(y)y + D(q) = 0 \quad (3-13)$$

where $y(t), q(t)$ = Q dimensional column vectors of discretized dependent and input variables, respectively

$A, B(y), D(q)$ = $Q \times Q$ matrices which depend, in general, on the discretized coefficients of the original partial differential equation and on the shape functions and finite element network selected for the discretization

In finite-element applications A is often called the *mass matrix*, while B(y) is called the *global stiffness matrix*. A similar equation structure is also obtained if a *finite difference* discretization procedure is used.

Model formulations such as Equation (3-13) are much more amenable to computerized solution techniques than complex partial differential equations since they are easily converted to systems of algebraic equations if an appropriate time integration procedure is used. This may be conveniently illustrated with the Boussinesq example.

Example 3-2 (continued)

When a finite element approach is used to discretize potential, porosity, conductivity and accretion, the two-dimensional Boussinesq equation may be transformed into the following matrix expression (see Zienkiewicz, 1977, for details):

$$A(\eta) \frac{dy(t)}{dt} + B(\kappa, y)y(t) + D[q(t)] = 0$$

Various time integration techniques may be used to generate a recursive solution for y(t). A wholly implicit technique would give, for example, the following equation:

$$\left\{ \frac{1}{\Delta} A(\eta) + B[\kappa, y(t_k)] \right\} y(t_k) = \frac{1}{\Delta} A(\eta) y(t_{k-1}) - D[q(t_{k-1})]$$

where Δ = time integration interval (sec)

Since $y(t_{k-1})$ and $q(t_{k-1})$ are known at time t_k , the above expression is a nonlinear algebraic equation in the unknown variable $y(t_k)$. This may be solved with iterative numerical methods such as the Newton-Raphson algorithm.

The spatial and temporal discretization procedures outlined above provide the information needed to derive the mean function $\bar{z}(\alpha, u, x, t)$. The independent variables of this function, the parameter and input vectors, may be constructed from the various coefficients and source terms appearing in the discretized model equations using the criteria outlined in Section 2.

This is illustrated with the following continuation of our example.

Example 3-2 (continued)

If the recursive equation for hydraulic potential developed earlier is solved repeatedly from the initial time t_0 to the final time t_k , then $y(t_k)$ may be written as:

$$y(t_k) = G[y(t_0), q(t_0), q(t_1), \dots, q(t_{k-1}), \Delta, \eta, K, \beta]$$

where $y(t_0)$ = hydraulic potential initial condition

$q(t_0), \dots, q(t_{k-1})$ = accretion rate vectors at the times $t_0, \dots, t_{k-1}$

η, K = unknown porosity and conductivity vectors

β = vector of time-invariant hydraulic potential boundary conditions

This "closed form" non-recursive expression emphasizes the fact that $y(t_k)$ depends on all previous accretion rates as well as on the initial condition vector $y(t_0)$, the hydraulic parameter vectors η and K , and the boundary condition vector β .

The hydraulic potential at any point x in the discretized region of Figure 3-6 may be computed directly from the weighted interpolation expression given earlier:

$$h(x, t_k) = c^T(x) y(t_k)$$

This is the dependent variable mean at time t_k :

$$\bar{z}(\alpha, u, x, t_k) = c^T(x) y(t_k)$$

The vectors α and u are composed of the independent variables $y(t_0), q(t_0), \dots, q(t_{k-1}), \eta, K$, and β .

In many applications, the hydraulic coefficients and boundary conditions of the Boussinesq model are poorly known, while the accretion rates and initial conditions are well known (or assumed to have hypothetical values corresponding to particular management strategies). This suggests that the parameter and input vectors be defined as follows:

$$\alpha = [\eta, \kappa, \beta_\alpha]$$

$$u = [y(t_0), q(t_0), q(t_1), \dots, q(t_{k-1}), \beta_u]^T$$

where $\beta_\alpha = S_\alpha$ dimensional column vector of poorly known boundary condition parameters

$\beta_u = S_u$ dimensional column vector of well-known boundary condition parameters

The dimensions of α and u are given by:

$$\text{DIM}(\alpha) \triangleq p = 2R + S_\alpha$$

$$\text{DIM}(u) \triangleq M = 1 + k + S_u$$

With the rather complex procedure for deriving $\bar{z}(\alpha, u, x, t)$ defined, we can now return to the problem of analyzing model prediction accuracy. The basic concepts are quite similar to those used in Example 2-1, although the details are considerably more difficult.

Estimation of Model Parameters

It was pointed out in Section 2 that a variety of methods, both statistical and deterministic, are available for computing estimates of *a priori* unknown model parameters. Most of these methods implicitly define a functional relationship between field observations and the parameter estimate vector which has the following form (see Equation (2-9)):

$$\hat{\alpha} = \hat{\alpha}[Z] \tag{3-14}$$

where Z = a column vector of N field measurements taken at various locations $(x_1, x_2, \dots, x_N)$ and times $(t_1, t_2, \dots, t_N)$ and used to compute the parameter estimate $\hat{\alpha}$

$\hat{\alpha}$ = uncertain estimate of the true but *a priori* unknown parameter vector α

As in the case of contour estimation, the measurement vector may be partitioned into mean and random residual components (see Equation (3-2)):

$$Z = \bar{Z}(\alpha, u) + \Omega \quad (3-15)$$

where $\bar{Z}(\alpha, u)$ = a column vector of N measurement means $\bar{z}(\alpha, u, x_1, t_1), \dots, \bar{z}(\alpha, u, x_N, t_N)$ corresponding to the measurement times and locations associated with the elements of Z

Ω = a column vector of N sampling errors $\omega(x_1, t_1), \dots, \omega(x_N, t_N)$ corresponding to the measurement times and locations associated with the elements of Z

Equation (3-15) is the fundamental measurement equation of classical non-linear regression theory (the input vector u contains the "regressor variables"). Some of the more commonly used estimation procedures based on this equation are discussed in Kendall and Stuart (1973). The most well-known of these is probably the weighted least-squares estimator, which is based on the intuitively reasonable assumption that a model's parameters should be adjusted so that its output fits available measurements as closely as possible. The model/measurement fit for any particular measurement set Z and estimated parameter vector $\hat{\alpha}$ may be conveniently computed from the weighted sum-squared residual error:

$$S_{\epsilon}(\hat{\alpha}) = \epsilon^T W \epsilon \quad (3-16)$$

where $\epsilon = Z - \bar{Z}(\hat{\alpha}, u)$ = an N-dimensional column vector of measurement residual errors (see Equation (2-20)).

W = a specified NxN positive definite symmetric weighting matrix

The *least-squares estimate* of α is simply the parameter vector which minimizes the performance index $S_{\epsilon}(\hat{\alpha})$ subject to appropriate constraints.

Most methods for finding least-squares parameter estimates are based on a well-known theorem of vector calculus which states that local minima of scalar functions are obtained only at points where the gradient is zero (see Wilde and Beightler, 1967). This implies that:

$$\frac{\partial S_{\epsilon}(\hat{\alpha})}{\partial \hat{\alpha}} = 0 \quad \text{when } \hat{\alpha} = \hat{\alpha}_{LS} = \text{least-squares estimate of } \alpha \quad (3-17)$$

Equation (3-17) is actually a set of p scalar equations in the p unknown scalar parameters $\hat{\alpha}_1, \hat{\alpha}_2, \dots, \hat{\alpha}_p$ which form the vector $\hat{\alpha}$. In general, these p equations, which are usually nonlinear and coupled, must be solved numerically with search techniques such as the Gauss-Newton or steepest descent methods (see McLaughlin, 1979, for a more detailed discussion).

The statistical properties of the weighted least-squares estimator may be derived fairly readily when the estimate $\hat{\alpha}$ is sufficiently close to the true parameter α for certain linear approximations to hold (see Appendix A). In this case, the least-squares estimate may be written as a linear function of α and Ω (Equation (A-9)):

$$\hat{\alpha} \approx \alpha + [A_o^T W A_o]^{-1} A_o^T W \Omega \quad (3-18)$$

where the symbol $[\cdot]^{-1}$ indicates the inverse of the square matrix within the brackets and where:

$A_o = \partial \bar{Z}(\alpha_o, u) / \partial \alpha =$ an $N \times p$ dimensional *Jacobian matrix* consisting of the derivatives of the predicted measurement means taken with respect to the elements of the parameter vector and evaluated at a nominal parameter value α_o "near" the true parameter value α

In practice, the assumptions used to derive Equation (3-18) allow the Jacobian matrix to be evaluated at the least-squares estimate $\hat{\alpha}$, in which case it may be written as $A_{\hat{\alpha}}$ rather than A_o . The Jacobian may be computed numerically, from small perturbations of the model's parameters, or it may sometimes be derived analytically from the governing equations.

It is evident from Equation (3-18) that the mean and covariance of the parameter estimate vector are:

$$E[\hat{\alpha}] \approx \alpha \quad (3-19)$$

$$\Sigma_{\hat{\alpha}} = [A_{\hat{\alpha}}^T W A_{\hat{\alpha}}]^{-1} A_{\hat{\alpha}}^T W \Sigma_{\Omega} W A_{\hat{\alpha}} [A_{\hat{\alpha}}^T W A_{\hat{\alpha}}]^{-1} \quad (3-20)$$

These expressions indicate that the least-squares estimate is *unbiased* with a covariance matrix directly proportional to the covariance Σ_{Ω} of the sampling error vector Ω .

The covariance expression of Equation (3-20) applies for an arbitrary positive definite symmetric weighting matrix specified by the modeler. Generally, the elements of this matrix are selected to emphasize "good" measurements and deemphasize "poor" measurements. Equation (3-20) indicates, as might be expected, that some weighting matrices give smaller estimation error covariances than others.* The particular weighting matrix which gives the *smallest* covariance is shown by Kendall and Stuart (1973) to be:

$$W = \Sigma_{\Omega}^{-1} \quad (3-21)$$

The resulting error covariance is:

$$\Sigma_{\hat{\alpha}} = [A_{\hat{\alpha}}^T \Sigma_{\Omega}^{-1} A_{\hat{\alpha}}]^{-1} \quad (3-22)$$

This important result indicates that a weighting matrix equal to Σ_{Ω}^{-1} gives the *minimum variance* unbiased estimate of α if the linear approximations cited in Appendix A are valid. In practice, it is advisable to select a weighting matrix proportional to Σ_{Ω}^{-1} even if these approximations are not *known* to be valid, since better guidelines are rarely available.

The approximate uncertainty analysis summarized in Equations (3-19) through (3-22) is useful when the parameter estimate is thought to be

* A square matrix Σ_1 is "smaller" than another matrix Σ_2 of equal size if $\Sigma_2 - \Sigma_1$ is positive definite.

fairly close to the true parameter value or when the model is linear in α . If these conditions do not apply, the computed estimate may no longer be either unbiased or minimum variance. Although exact expressions for the estimate mean and covariance cannot be derived for the general nonlinear parameter estimation problem, some lower bounds can be developed. Perhaps the best known of these is the *Rao-Cramer lower bound* on the estimate covariance (see Schweppe, 1973, and Kendall and Stuart, 1973, for derivations and detailed discussions). This bound is valid for any estimation procedure, linear or nonlinear, and so gives a reliable indication of the *best possible* accuracy that can be expected in a particular application. When a least-squares estimation approach is taken the Rao-Cramer bound has the following form:

$$\Sigma_{\hat{\alpha}} \geq [I - \frac{\partial b(\alpha)}{\partial \alpha}]^T [A_{\alpha}^T \Sigma_{\Omega}^{-1} A_{\alpha}]^{-1} [I - \frac{\partial b(\alpha)}{\partial \alpha}] \quad (3-23)$$

where $b(\alpha)$ = the estimate bias ($E[\hat{\alpha}] - \alpha$), written as a function of the true (unknown) parameter value α

$$A_{\alpha} = \frac{\partial \bar{Z}(\alpha, u)}{\partial \alpha}$$

I = $p \times p$ identity matrix

Since the derivatives appearing in this expression are evaluated at the unknown true parameter value α , an estimate of α is needed before the right-hand-side of the inequality can be computed. An expression for the bias $b(\alpha)$, or at least the bias derivative $\partial b(\alpha)/\partial \alpha$, is clearly also required.

If the least-squares estimate $\hat{\alpha}$ is substituted for α and the bias is assumed to be relatively independent of α (but not necessarily zero), the Rao-Cramer bound becomes:

$$\Sigma_{\hat{\alpha}} \geq [A_{\hat{\alpha}}^T \Sigma_{\Omega}^{-1} A_{\hat{\alpha}}]^{-1} \quad (3-24)$$

The right-hand side of this inequality is the variance expression obtained from the linear analysis (Equation (3-22)).

This result reinforces our earlier statement that the least-squares estimator is minimum variance (i.e., its covariance attains the Rao-Cramer bound) in linear problems.

Model Prediction Accuracy

The covariance bound given in Equation (3-24) allows us to proceed with our analysis of groundwater model uncertainty propagation for the general nonlinear case. Although we cannot derive exact expressions for the mean and variance of the model prediction $\bar{z}(\hat{\alpha}, u, x, t)$, as we did with the linear models of Examples 2-1 and 3-1, we can at least obtain an optimistic assessment of the model's "best possible" prediction accuracy. This may be done if the model prediction function $\bar{z}(\hat{\alpha}, u, x, t)$ is expanded about the true parameter α in a truncated Taylor series:

$$\bar{z}(\hat{\alpha}, u, x, t) \approx \bar{z}(\alpha, u, x, t) + a_{\alpha}^T (\hat{\alpha} - \alpha) + (\hat{\alpha} - \alpha)^T H_{\alpha} (\hat{\alpha} - \alpha) + \text{higher order terms} \quad (3-25)$$

where $a_{\alpha} = \partial \bar{z}(\alpha, u, x, t) / \partial \hat{\alpha} =$ a p-dimensional gradient vector of the model prediction function, taken with respect to $\hat{\alpha}$ and evaluated at the true parameter α

$H_{\alpha} = \partial^2 \bar{z}(\alpha, u, x, t) / \partial \hat{\alpha}^2 =$ a p x p dimensional *Hessian matrix* composed of scalar second derivatives of the model prediction function, taken with respect to $\hat{\alpha}$ and evaluated at the true parameter α

When the estimate $\hat{\alpha}$ and true parameter α are relatively close, the higher order terms of this expansion may be dropped. If the parameter estimate is unbiased, the model's prediction mean may then be approximated by:

$$E[\bar{z}(\hat{\alpha}, u, x, t)] \approx \bar{z}(\alpha, u, x, t) + \text{Tr}[\Sigma_{\hat{\alpha}} H_{\alpha}] \quad (3-26)$$

where the symbol $\text{Tr}[\cdot]$ indicates the matrix trace encountered earlier (see Example 2-1). This result shows that the model prediction has a bias proportional to the parameter estimate covariance matrix $\Sigma_{\hat{\alpha}}$. The prediction will be unbiased only if the model is linear ($H_{\alpha} = 0$) or the estimation covariance is negligibly small.

If we make, as a rough approximation, the assumption 1) that the prediction bias is small relative to the values of α and $\hat{\alpha}$ and 2) that the second-order term in Equation (3-25) is negligible, the variance of the model prediction is:

$$V[\bar{z}(\hat{\alpha}, u, x, t)] \approx a_{\alpha}^T \Sigma_{\hat{\alpha}} a_{\alpha} \quad (3-27)$$

The gradient vector a_{α} is similar to the Jacobian matrix A_{α} encountered in the Rao-Cramer bound (Equation (3-21)) in that it is evaluated at the unknown true parameter value α . If the estimate $\hat{\alpha}$ is substituted for α (these values are relatively close if our previous assumptions are valid), the prediction variance can be further approximated by:

$$V[\bar{z}(\hat{\alpha}, u, x, t)] \approx a_{\hat{\alpha}}^T \Sigma_{\hat{\alpha}} a_{\hat{\alpha}} \quad (3-28)$$

The gradient vector may be estimated numerically, from small perturbations of the model's parameters, or it may occasionally be derived analytically from the model's governing equations (as in Example 2-1).

It should be evident that the linearized analysis outlined above depends on numerous assumptions which are difficult, if not impossible, to verify in practice. Even if expressions such as Equation (3-26) or (3-28) are valid, their usefulness is compromised if the parameter estimate covariance $\Sigma_{\hat{\alpha}}$ can only be assigned a lower bound. Unfortunately, there is, at present, no satisfactory general method for analyzing the accuracy of non-linear simulation models. Occasionally, mean or variance expressions may be derived without the assumptions we have made, but such results cannot usually be extended beyond particular applications. This is not to say that a linearized approach to uncertainty analysis is useless--it usually gives a better feeling for model prediction accuracy than other less quantitative alternatives and it is reasonably reliable when the estimates are "near" the true parameter values. So long as linearized methods are used cautiously, they can be a valuable aid to the manager seeking an *a priori* measure of the performance of particular models, estimators, or field sampling programs.

It is appropriate to note that the discussion of model lack-of-fit presented at the end of Section 2 applies, in principle at least, to nonlinear models. Residual errors are a useful clue to lack-of-fit problems in any modeling applications, and should be carefully examined when a new model is being tested (see Draper and Smith, 1967, for some simple graphical lack-of-fit tests based on residual error). Although some of the more common hypothesis tests (such as the sum-squared residual error test of Example 2-1) do not apply in the general nonlinear case, Draper and Smith (1967) suggest that independent estimates of the sample variance (such as $\hat{\sigma}_{wp}^2$ and $\hat{\sigma}_{wr}^2$) may still provide a good qualitative feeling for a model's structural validity. Any conclusions reached should, of course, be viewed as tentative and treated with caution. Other authors propose various *non-parametric* lack-of-fit tests which may be useful in particular applications and which merit further investigation (see Kendall and Stuart, 1973). Since no single test is completely dependable, all available alternatives should be tried.

When a linearized analysis of uncertainty propagation and model accuracy is thought to be at least tentatively acceptable, the variance expressions of Equations (3-22) and (3-28) may be used to compare alternative sampling strategies and develop confidence limits in much the same way as was illustrated in our discussion of contour estimation. Figures 3-3 and 3-4 and the associated mathematical expressions apply, in fact, equally well to impact assessment and contour estimation applications. This is a direct consequence of the generality of the concept of uncertainty propagation, which is the basis for any statistical analysis of model accuracy, no matter how simple or complex.

SUMMARY

The contour estimation and impact assessment examples discussed in this section generate a number of mathematical expressions and are based on a number of assumptions which may be difficult to follow on a first reading. The details should not, however, obscure the basic concepts of the analysis, which are summarized at the end of Section 2.

Both contour estimation and impact assessment analyses are based on mathematical models of measurement variability which relate the dependent variable of interest to various model inputs and parameters. In the contour estimation (Kriging) example, uncertainty propagates directly from field measurements to the estimates of interest, since the model and estimation algorithm have particularly simple linear forms (Equation (3-3)). In the impact assessment example, uncertainty propagates first from field measurements to parameter estimates and then to model predictions (as in Example 2-1). The differences in computational complexity observed in these two examples are due primarily to the form of the assumed function $\bar{z}(\alpha, u, x, t)$. Since classical statistics is based largely on linear models, the analysis of the Kriging algorithm (which is linear) proceeds in a straight-forward way to well-defined expressions for the estimation mean and variance. The impact assessment analysis must, on the other hand, be based on a conceptually weaker *quasi-linear* approach which yields approximations and lower bounds rather than the neat formulas of classical linear statistics.

In either case, the measures of model accuracy or uncertainty provided by a statistical analysis can be used to guide model development or sampling network design. If model uncertainty appears to be too large at certain times or locations, a better parameter estimation procedure based, perhaps, on more measurements may be indicated. Or, alternatively, the sampling program used to obtain calibration measurements may need to be improved, well sites moved, or instrumentation modified. Such measures can be evaluated quantitatively in a variety of ways, as illustrated for example by Figure 3-3.

It is important to remember that an uncertainty analysis may be invalid if the underlying model's structure is faulty and the fundamental assumptions of the Fisher approach are violated. When residual error tests indicate that structural problems are likely, it is best to defer uncertainty analysis until model errors can be identified and corrected. So long as these errors are significant, parameter estimation and sampling design will be curve-fitting exercises, which cannot be generalized beyond particular data sets. It is important that the modeler be watchful for signs that his model's structure is faulty. In modeling, there is always a place for a little healthy scepticism.

4. COMMENTS ON THE HANFORD GROUNDWATER DATA COLLECTION PROGRAM

This section presents the results of RMA's review of groundwater data collection programs at Hanford. The review is based on an examination of only a few of the many data reports which are available and is, by no means, a comprehensive survey of all field activities carried out by Rockwell and its contractors. We do believe, however, that the statistical approach we have taken makes many of our comments generally applicable. In any case, the analysis presented here provides a convenient format which we hope will prove useful both now and in the future.

OVERVIEW

Since we are concerned in this review primarily with the data needs of Rockwell's modeling activities, we have decided to evaluate data collection programs at Hanford in terms of their ability to support these needs. This decision does not in any way diminish the importance of other data needs, but is simply a recognition of the fact that the usefulness of a data program can only be properly measured relative to a *particular* application--in this case, mathematical modeling.

A survey of various modeling documents and scenario study reports (e.g., Arnett, et al, 1976; Arnett, et al, 1977a; and Arnett, et al, 1977b) suggests that most Hanford modeling studies are designed to support one of the following broad management objectives:

1. Periodically describe *existing hydrologic and water quality conditions* in the Hanford basin and identify important long-term changes in these conditions.

2. Evaluate the *environmental impacts* of potentially hazardous activities--actual or hypothetical, intentional or accidental--carried out on or near the Hanford facility.

The modeling activities implied by these objectives fall generally into the two categories discussed in Chapter 3--interpolation (or contour estimation) and impact assessment. Some specific examples are listed below:

Analytical Methods Relating to the Description of Existing Conditions

- Computerized techniques for constructing contour maps of contaminant concentration or water table elevation
- Procedures for estimating total volume or mass of a radionuclide in the groundwater basin
- Hypothesis-testing techniques for establishing whether or not observed changes in a groundwater variable are statistically significant

Models Relating to Impact Assessment

- Groundwater flow models--saturated and unsaturated, confined and unconfined--similar to those described in Arnett, et al (1976)
- Contaminant transport models--primarily for radionuclides and nitrate--similar to those described in Arnett, et al, (1976)

Although the data requirements associated with these examples differ, they are not necessarily inconsistent. Any well designed data collection program will provide a good overall picture of groundwater hydrology, geology and chemistry which can support a variety of independent modeling programs.

The conceptual discussion of groundwater modeling presented in Section 2 provides a general definition of modeling terms which applies equally well to the simple trend functions and estimation algorithms used for contouring and the complex numerical simulation models used for impact assessment. In either case, three basic types of data are required:

1. Measured or hypothesized data for defining *model inputs* (which are presumed to be well-known)
2. Measured data for estimating *model parameters* (which are presumed to be *a priori* unknown)
3. Measured data for estimating the covariance matrix (or variogram) of the measurement *sampling errors*

The first two types of data are needed to compute model predictions while the third is needed to test for lack-of-fit and to check hypothetical uncertainty analyses. In commonly used modeling terminology, the three are often simply called input, calibration, and verification data, respectively.

The particular kinds of measurements required to define model inputs, estimate model parameters, or verify model structure depend, of course, on the application. Examples for typical groundwater models used at Hanford are discussed in Arnett, et al (1976) and briefly summarized below:

Input Variables

- Recharge and discharge flow rates at specified locations--particularly at disposal ponds and ditches, cribs, and retention sites in the 200 East and West areas (flow models)
- Contaminant concentrations and/or flux rates at the above discharge locations (transport models)
- Computed moisture flux rates (transport models)
- Well-known potential or flux boundary and initial conditions--including vertical infiltration, evaporation, and leakage (flow and transport models)
- Well-known hydraulic, chemical, and geological constants or coefficients (flow and transport models)

Parameter Variables

- Hydraulic conductivity, effective porosity, and vertical compressibility (flow models)
- Unsaturated soil moisture properties such as curves of pressure vs. moisture content or of permeability vs. moisture content (flow models)
- Poorly known dispersion and soil sorption coefficients (transport models)
- Poorly known potential or flux boundary and initial conditions (flow and transport models)

Dependent Variables

- Hydraulic potential (saturated and unsaturated flow models)
- Contaminant concentration (transport models)
- Moisture content (unsaturated flow models)

Note that we have, in the above list, divided certain "gray area" variables which are neither perfectly known nor completely unknown (e.g., boundary and initial conditions) between the input and parameter categories, in order to be consistent with the Fisher estimation approach taken in Section 2. Generally speaking, time-invariant independent variables should be treated as parameters and estimated if their uncertainties are believed to contribute significantly to model prediction error.

The field data required to define input variables and verify predictions of dependent variables are, of course, measurements (often interpolated or contoured) of these variables themselves. Model parameters must be handled differently since they cannot be measured directly but must be estimated indirectly from measurements of related variables. As a general rule, we believe that measurements of the dependent (i.e., predicted) variable should be used to estimate unknown parameters. The parameters of regional flow models should, for example, be estimated from regional samples of hydraulic potential and the parameters of local transport models from local contaminant samples.

The general concepts outlined above suggest that the Hanford data program may be evaluated with respect to three distinct criteria--model input data needs, parameter estimation data needs, and model verification (or variance estimation) data needs. Each of these is considered in one of the following subsections. The final subsection summarizes specific data program recommendations developed in our review.

MODEL INPUT DATA NEEDS

The preceding subsection suggests that the model inputs for a particular Hanford modeling application will be composed of a set of well defined site-specific discharge and recharge terms as well as certain boundary and initial condition values. Some of these inputs may be manipulated to simulate alternative management practices.

In impact assessment applications at Hanford the primary uncertainty associated with model input data results from the need to specify a time-series of input values extending far into the future. Generally, the inputs which are most likely to vary, waste discharge and recharge rates, are controllable and their values can therefore be assigned as desired. Other model inputs, primarily boundary conditions, may be presumed to be constant or to follow established seasonal trends. Evaporation and precipitation inputs and associated groundwater boundary flows may, for example, be developed from available historical records. The uncertainties associated with such inputs are probably relatively unimportant at Hanford since waste discharges are by far the largest flow source in the basin and will probably continue to be for some time.

The hypothetical nature of the model inputs used for impact assessment requires that all long-term predictions be presented as *conditional* results, subject to a particular set of management practices and hydrologic conditions applying in the future. This approach is used in the scenario studies reported in Arnett, et al (1977a) and Arnett, et al (1977b).

Overall, the input data needs of Rockwell's groundwater flow and transport models seem to be satisfied fairly well by existing monitoring programs. It appears that additional definition of boundary potentials and fluxes (particularly of nitrate) in the western part of the basin might be needed, but this is based on a rather superficial review of existing data. Contaminant discharge and recharge data collected at the disposal sites appear to be quite extensive and more than adequate from a modeling point-of-view. The accuracy of initial condition inputs developed from contour maps depends, of course, on the contouring procedure used as well as on the configuration of the monitoring sites supplying the raw data (see Section 3). Since most contour maps at Hanford appear to be manually drawn and since variograms and other similar measures of spatial correlation are not available, it is difficult to assess the adequacy of existing initial condition estimates. Rockwell should seriously consider adopting a more quantitative approach to contour estimation and interpolation, so that this ambiguity can be resolved.

PARAMETER ESTIMATION DATA NEEDS

If the approach outlined earlier is taken, the unknown parameters to be estimated in a particular impact assessment study will include a variety of discretized initial and boundary conditions as well as nearly all hydraulic and physico-chemical coefficients included in the model. It is obvious both intuitively and statistically that the number of unknowns which can be meaningfully estimated is restricted by the quantity and quality of available *calibration measurements* (potential, contaminant concentration, moisture content, etc.). The most rigorous way to relate the number of estimated parameters to the amount of calibration data required is to carry out an accuracy analysis similar to the one outlined in Section 3. To our knowledge, this has not been done at Hanford. Most parameter estimation has been carried out manually with little or no attempt to quantify the accuracy of the results.

As a general rule of thumb, it is reasonable to require that calibration measurement locations (in both the horizontal and vertical planes) be distributed throughout the basin at about the same density as their associated model parameters. Potential measurements should, therefore, be as abundant as hydraulic conductivity nodal values and radionuclide measurements as abundant as the nodal values of transport dispersion coefficients. A glance at a map of active monitoring sites shows how this rule of thumb limits the permissible level of model detail at Hanford. It is apparent from the well map that Hanford's monitoring programs have more or less followed the contaminant plumes originating from the disposal sites as they have migrated down-gradient over the years. While this is a reasonable way to provide a good description of *existing* basin conditions, it is not necessarily the best way to support an impact assessment study. A historical and policy emphasis on immediate definition of contaminant plume boundaries has somewhat overshadowed the need to develop an accurate *regional* description of basin hydrology and geology for impact assessment purposes.

The above comments are closely related to the issue of *parameter identifiability*--roughly defined as the degree to which a parameter can be successfully estimated from a particular set of data. Obviously, values of hydraulic conductivity or porosity in some remote corner of the basin cannot be accurately estimated if no well samples are available in the vicinity. Such parameters are, for all practical purposes, unidentifiable.

In some cases, hydraulic parameters may not be identifiable even when nearby well measurements are available. If, for example, a particular section of the basin is in a hydraulic steady-state, effective porosities (or storage coefficients) cannot be estimated. In areas where the potential gradient is relatively constant over time and space, the hydraulic conductivity may be very difficult to estimate without well pump tests. Both of these examples are frequently encountered in practical parameter estimation applications.

Although well pump tests provide a way to deal with identifiability problems through an artificial stress on the local groundwater system, such

tests should be used with caution. Groundwater hydrologists sometimes forget that the conductivities estimated from well pump test data are based on a particular, often highly simplified, model of the *local* hydraulic regime. There is no particular reason why the macroscale conductivity values used in *regional* impact assessment models should be equal or even close to the pump test values. This reveals the danger inherent in constructing conductivity or transmissivity contour maps from a number of localized pump test estimates as is done in Cearlock, et al (1975). Unless the localized estimates are based on a large number of closely spaced tests, they can easily be biased by uncharacteristic hydraulic anomalies which should not be extrapolated throughout the basin.

Ideally, a data program to support model parameter estimation should be designed systematically through optimization of a quantitative estimation performance index. An obvious choice for such an index is the estimation error variance or, equivalently, the prediction error variance discussed in Section 3. Such an optimal design approach must be initially based on existing well data and then slowly refined as more information becomes available (see Moore and McLaughlin, 1979, for a detailed discussion of this approach).

As a start, it would be useful for Rockwell to begin quantifying variability through an analysis of the spatial and temporal correlation properties of variables such as hydraulic potential and contaminant concentration. Available well records could be used to construct variograms and conduct time series trend analyses. Simple graphical indications of variability are already available in the form of manually constructed contour and temporal plots provided in the Battelle Northwest Laboratories series of Hanford Environmental Monitoring Reports. A careful analysis of these plots could probably suggest some promising long-term monitoring strategies.

To summarize, we feel that the parameter estimation needs of Rockwell's modeling activities are somewhat less well served by existing and historical data programs than the input data needs discussed in the previous section. Although much of the available field information on hydraulic potential and contaminant concentrations is valuable for parameter estimation, it does not

appear to provide the regional coverage necessary for an accurate long-term input assessment study. Before a final pronouncement on this is made, however, a more detailed analysis of available data should be carried out so that patterns of spatial and temporal variability can be quantified.

MODEL VERIFICATION AND VARIANCE ESTIMATION DATA NEEDS

In the broadest sense, model verification is (or should be) concerned with estimating model accuracy throughout the region and over the time period of interest in a particular impact assessment application. From a statistical point of view it is futile to attempt to prove that a model is correct or "verified."* Instead, an effort should be made to derive accuracy measures (such as those illustrated in Figure 3-5) which can be used to evaluate the confidence to be placed in a model's predictions.

The information needed to develop confidence intervals and contours for model predictions is discussed in Chapter 3. Confidence bounds depend on estimation means and variances which may be evaluated once the model's structure, inputs and estimated parameters have been precisely defined. These means and variances depend, in turn, on the statistical properties of the random residuals (or sampling errors) associated with the model's calibration measurements.

In practice, the assessment of model accuracy usually reduces to an investigation of residual errors which are indicators of the likely magnitude of the sampling error covariance as well as of possible lack-of-fit errors. Section 2 briefly discusses some of the alternatives, which include construction of dependent variable variograms from available well samples and evaluation of residual error sum-of-squares components to test for model lack-of-fit. Although these error analyses can be based on the data set used to estimate unknown model parameters, many investigators feel that an accuracy analysis is more credible if it is based on an independent data set

* We prefer "model accuracy analysis" to "model verification" but concede that the latter term is more widely used in water resource modeling.

reserved solely for "verification." In reality, the best approach is probably to combine the information obtained from two accuracy analyses--one derived from an *estimation data set* and one derived from a *test data set*. Statistical methods for doing this are available but are probably too advanced for short-term application at Hanford.

It follows from the above discussion that the data needs for model verification are essentially the same as those for parameter estimation. There are, however, some important differences which are worth noting. First, most statistical procedures for testing model lack-of-fit require an independent estimate of sampling error variance based on replicated samples. It is important, therefore, that a verification data program collect enough replicates to provide such an estimate. Second, the optimal distribution of verification measurements is not constrained by parameter identifiability but, rather, by the desired accuracy of the computed estimation error variances. A certain minimal amount of data is needed to derive variance estimates that are good enough to support a meaningful accuracy analysis.

It is important to note that sample replication procedures carried out for quality control purposes are not necessarily adequate for variance estimation and lack-of-fit analyses. While two or three "split samples" may provide an acceptable spot check on laboratory reliability they give a poor, in fact practically useless, estimate of sampling error variance. At least four or five replicates are needed to support reliable lack-of-fit checks in most modeling applications. It is better to take several replicates at only a few locations than two at every location. In the former case at least a few good variance estimates are obtained while in the latter case the replicates have little or no value.

The question of defining just how much field information is needed for a valid accuracy evaluation is an interesting one which can really only be answered with a rigorous statistical analysis. As is pointed out in Example 2-1, estimates of sampling error variances or correlations are themselves random variables which are distributed about unknown "true" values.

Given certain assumptions, it is possible to derive unbiased sampling error variance estimates and to compute the variance of these estimates.

Generally, the variance of an unbiased sampling error variance estimate varies inversely with the number of samples used to compute the estimate. In principle, then, an accuracy analysis can be made as good as desired if a large enough verification data set is used. Conversely, an analysis based on only a few verification data points will be of little value. Even if a model's simulated output goes through every one of three or four data points, its predictive accuracy will be, for all practical purposes, unknown.

It is worth noting that most traditional "model verifications" are based on an inspection, nearly always qualitative, of the same observed residual errors used in a rigorous statistical analysis. The subjectivity of the traditional approach conveniently allows the modeler to *assert*, usually without significant opposition, that his model has been "verified." A more sophisticated version of this approach utilizes a single carefully selected hypothesis test to check, for example, whether or not the overall residual error mean is different from zero. The only statistically valid way to establish whether or not a model's fit is acceptable is to conduct a *series* of different tests on the residual errors. Confidence contours and prediction accuracy assessments should be accepted only after *all* of these statistical tests have failed to demonstrate significant lack-of-fit.

It is apparent from a review of available reports that there have been practically no rigorous statistical accuracy analyses of the groundwater models used at Hanford. This is not unusual in the groundwater field where statistical concepts have only recently begun to influence modeling (in contrast to surface water hydrology where statistical methods have seen wide application.) Rockwell should, in any case, put a high priority on the development of objective model evaluation procedures and should begin to associate model verification more closely with the accuracy evaluation approach advocated in this report. Efforts should be made to include replication as a standard feature in field operations where sampling uncertainties can be significant (particularly in radionuclide measurement). Also, more

careful consideration should be given to the type of accuracy measures (variances, confidence intervals, confidence contours, probability densities, etc.) which will be most useful from a decision-making viewpoint. This will help to define more clearly just what should be expected from a good model verification study.

SUMMARY OF DATA PROGRAM RECOMMENDATIONS

The following list summarizes the major recommendations developed in our review of Hanford groundwater data collection programs.

1. Develop a means for identifying poorly-known boundary and initial condition variables needed in the groundwater models used by Rockwell. Include these variables in the generalized parameter estimation procedure mentioned below.
2. Carry out a systematic quantitative analysis of the spatial and temporal variability of observable model variables, including precipitation/evaporation, contaminant concentrations, hydraulic potential, and soil moisture properties. This analysis should be based on variograms and temporal autocorrelations estimated from available field data.
3. Develop a statistically based approach to groundwater model parameter estimation which accounts for unavoidable sampling errors and which considers parameter identifiability. Relate this approach to a rigorous accuracy analysis which can be used to design cost-effective and informative sampling networks.
4. Devote more effort to analyses of sampling variability based on replicate measurements and evaluate potential model lack-of-fit errors more carefully.

5. Define more precisely the type of model accuracy measures which are most useful from a decision-making viewpoint. Use these measures to formulate an accuracy-oriented model verification program.

We believe these general recommendations provide a sound basis for a more specific quantitative assessment of groundwater modeling data needs at Hanford.

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Appendix A

APPROXIMATE EXPRESSION FOR THE GENERAL WEIGHTED LEAST-SQUARES ESTIMATE IN THE VICINITY OF THE TRUE PARAMETER VALUE

The solution to the least-squares minimization condition (Equation 3-17) can be derived analytically if the measurement mean vector is linearized about a nominal parameter value α_o near the "true" value α :

$$\bar{Z}(\alpha, u) = Z(\alpha_o, u) + A_o(\alpha - \alpha_o) \quad (A-1)$$

where $A(\alpha_o) = \partial \bar{Z}(\alpha_o, u) / \partial \alpha$ = an $N \times p$ dimensional *Jacobian* matrix consisting of derivatives of the measurement mean taken with respect to the elements of the vector α and evaluated at α_o .

The measurement equation (Equation 3-15) may then be written:

$$Z = \bar{Z}(\alpha_o, u) + A(\alpha_o)(\alpha - \alpha_o) + \Omega \quad (A-2)$$

and the residual error obtained for any estimate $\hat{\alpha}$ is:

$$\epsilon = Z - \bar{Z}(\hat{\alpha}, u) = \bar{Z}(\alpha_o, u) - \bar{Z}(\hat{\alpha}, u) + A(\alpha_o)(\alpha - \alpha_o) + \Omega \quad (A-3)$$

If this residual error expression is substituted into Equation (3-16) and the minimization condition (Equation (3-17)) applied, the result is:

$$\frac{\partial S_{\epsilon}(\hat{\alpha})}{\partial \hat{\alpha}} = - 2A(\hat{\alpha})^T W[\bar{Z}(\alpha_o, u) - \bar{Z}(\hat{\alpha}, u) + A(\alpha_o)(\alpha - \alpha_o) + \Omega] = 0 \quad (A-4)$$

where $A(\hat{\alpha}) = \partial \bar{Z}(\hat{\alpha}, u) / \partial \hat{\alpha}$ = Jacobian evaluated at $\hat{\alpha}$

If $\hat{\alpha}$ is sufficiently close to α_o , the following linear expansion can be used to represent $\bar{Z}(\hat{\alpha}, u)$:

$$\bar{Z}(\hat{\alpha}, u) = \bar{Z}(\alpha_o, u) + A(\alpha_o)(\hat{\alpha} - \alpha_o) \quad (A-5)$$

and Equation (A-4) may be written as:

$$A^T(\hat{\alpha}) W[A(\alpha_o)(\hat{\alpha} - \alpha_o) + \Omega] = 0 \quad (A-6)$$

If $A(\hat{\alpha})$ is a continuous function of $\hat{\alpha}$, the following approximation will hold when $\hat{\alpha}$ and α_o are close:

$$A(\hat{\alpha}) \approx A(\alpha_o) \quad (A-7)$$

In this case, Equation (A-6) may be solved for $\hat{\alpha}$:

$$\hat{\alpha} \approx \alpha + [A_o^T W A_o]^{-1} A_o^T W \Omega \quad (A-8)$$

where $A_o = A(\hat{\alpha})$

This is the expression given in Equation (3-18).

RHO-C-18

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