

**"UNCERTAINTY" IN UNCERTAINTY ANALYSIS
OF GROUNDWATER TRAVEL TIMES**

by

Williams and Associates, Inc.

DRAFT

1. INTRODUCTION

Uncertainty in the prediction of groundwater travel time can derive from a variety of sources. Uncertainty is inherent in the hydrogeologic conceptual model of the specific site under study, in the spatial variation of hydrogeologic properties of the medium, in the sparseness of field measurements and measurement errors associated with them, and in the numerical accuracy (or inaccuracy) of computer codes used to generate travel times (see e.g. U.S. NRC, 1986, and Hunter and Mann, 1986). Considerable confusion is evident regarding the various meanings of uncertainty and the terms used in defining it in the context of groundwater travel time. Some of this confusion is reflected in the DOE's Final Environmental Assessments (FEA's) and in the documents that support it. The purpose of this paper is to elucidate these sources of uncertainty and to consider their interactions. This discussion of uncertainty is intended for use as a baseline for interpreting analyses of uncertainty in groundwater travel time predictions performed by hydrogeologists studying possible high level waste repository sites. To date these analyses have used Monte Carlo and/or Latin Hypercube selections from somewhat hypothetical distributions of hydrogeologic properties in repeated runs of numerical models of porous media through

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which particles of water move. Details among the studies differ markedly, but the general approach is consistent.

2. UNCERTAINTY

The New Webster's Dictionary (1981) defines uncertainty as, "The quality or state of being uncertain; doubtfulness; hesitation; something not exactly known or uncertain; a contingency." Uncertain is defined as, "Not sure or certain; doubtful; not certainly known; indeterminant; ambiguous; not having certain knowledge; unreliable; not to be depended on; undecided; not having the mind made up; vague; not steady; fitful; fickle; variable; inconstant; capricious." Clearly, the intent of the use of the word in hydrogeological circles is the state of not having certain knowledge or of being variable. Hopefully, our use of the word does not include fitful, fickle, or capricious. Each major source of uncertainty in the context of groundwater travel time is considered below.

2.1. Uncertainty Due to Errors in the Conceptual Model

It is generally agreed among hydrogeologists that mathematical groundwater models that are appropriate for assessing groundwater travel time at specific sites should be based on conceptual models that incorporate specific hydrogeologic features of the site in question. Models used to date in supporting documents for the FEA's generally apply analytic or numerical variations of Darcian type flow through porous media. In some models Darcy's Law has been used to approximate flow through a fractured

medium. Regardless of the actual formulation, any model can be represented in the form

$$\underline{G}(y_t, y'_t, y''_t, \dots, z_t, \underline{\theta}, t) = 0 \quad \text{subject to } y = y_0 \text{ at } t_0$$

where y_t is a vector that represents the state of the flow system at time t (starting at time t_0), y' , y'' , ... are the derivatives of y with respect to t , z_t is a vector of the driving variables (e.g. z_{1t} could be hydraulic head in the Darcy context). $\underline{\theta}$ is a vector of coefficients such as hydraulic conductivity or effective porosity. For reasons that will become apparent below, it is more appropriate to call these quantities coefficients rather than parameters. Suppose that $\underline{G}(\cdot)$ can be solved explicitly for y_t ,

$$y_t = f(y_t, z_t, \underline{\theta}, t)$$

where f is a vector of functions such that $f_i(\cdot)$ does not depend on y_{it} . The state vector, y_t , could contain the cartesian coordinate location of a moving particle or concentrations of chemical ions or other variables describing groundwater movement. In generic terms, we apply z_t to the model $f(\cdot)$ with initial conditions y_0 and obtain outputs y_t (Fig. 1).

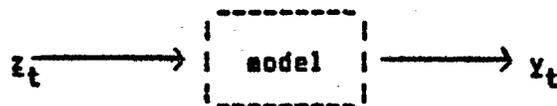


Figure 1. Driving variables produce output y_t

The model can be of many forms. It could be described in terms of a differential equation or a partial differential equation. It can be

solved analytically or numerically. In order to characterize the effect of conceptual model errors (misspecifications) on uncertainty we consider the simple unidimensional linear model

$$dy_t/dt = b$$

or

$$y_t = a + bt.$$

where b (the slope) is the coefficient of the time-space variable and a is the constant of integration determined by initial conditions. This equation is the time term of the first order Taylor approximation of the actual function, $f(\cdot)$. The model is

$$y_t = a + bt + R(t, y_t, y_{2t}, z_t)$$

where the remainder term $R(t, y_t, y_{2t}, z_t)$ includes the effects of omitted variables (y_{2t}) and z_t and the higher order terms in y_t . The size of misspecification, $R(t, y_t, y_{2t}, z_t)$, depends on the nonlinearity of f and how far away t , y_t , y_{2t} , and z_t are from the nominal values used in the Taylor expansion.

For many models, model misspecification can be approximated as

$$y_t = f_0(y_t, z_t, \theta, t) \pm R(y_t, z_t, \theta, t)$$

where $f_0(\cdot)$ is the function approximation used and $R(\cdot)$ is the additive or multiplicative remainder. The remainder cannot be characterized in terms of quantifiable, measurable variables except in

simple cases (such as the Taylor approximation); consequently $R(\cdot)$ often is represented as random variation ϵ giving

$$y_t = f_0(y_t, z_t, \theta, t) + \epsilon.$$

The error term, ϵ , appears to be random because all of the unspecified variables and functions it represents change in ways the modeler cannot see. Uncertainty in model formulation leads to a probabilistic representation of y_t through the ignorance included in the error term ϵ . The magnitude of the error term can be ascertained only by validation of the model by comparing model predictions against field data. Whether or not such field data can even be obtained is questionable.

2.2. Uncertainty Due to the Questionable Stochastic Nature of the Phenomena Being Modeled

Uncertainty due to spatial variation in the hydrogeologic properties could lead us to consider θ to be a random vector. However, the groundwater travel time model can be stochastic due to three other sources as well. In the first instance, the function, $f(\cdot)$, can be described probabilistically. For example, the model could ascribe a 50% chance of a particle being trapped in the immobile liquid phase of the medium (a dead-end pore or fracture). Secondly, since this particular model is applied to a surface and not to a point, the initial condition, y_0 , can be random, thereby representing the initiation of a random pathway. Thirdly, the driving variables, z_t , could be stochastic. In the case of hydraulic head, if steady state conditions are assumed, then randomness, if it occurs, is not in time, but in space. A distribution of head occurs throughout the medium.

We now consider the randomness of θ . In most models in hydrogeology, the components of θ are some combination of hydraulic conductivity, effective porosity, transmissivity, and effective thickness. Recent hydrogeologic literature is filled with articles on the spatial variability and possible stochasticity of these hydrogeologic properties (see Neumann, 1982, for a history of major works; see also Journel and Huijbregts, 1978). Because of this spatial variability and possible stochasticity of these hydrogeologic properties, we refer to effective porosity, permeability, and transmissivity as coefficients rather than parameters. Webster defines parameter as, "Math: In an expression, a constant or variable whose value determines the specific form of the expression; an independent variable other than a coordinate variable in terms of which coordinate variables may be expressed." Thus the intercept, a , and slope, b , given above are parameters that index a family of lines. The coordinate variables are y and t . If a and b (effective porosity, permeability, effective thickness) are not constant in space or if they are used as (coordinate) variables in their own right, then they are not parameters. They in fact are coefficients. The use of the word parameter is a carryover from the days of pure determinism. In current stochastic analysis it is being used incorrectly.

Stochasticity of hydrogeologic properties must be viewed as a possibility, not a certainty, because in fact these properties do not represent stochastic processes in a spatial hydrogeologic sense at our scale of interest. A stochastic process, $S(t)$, is by definition a collection of random variables (S) indexed by an algebraic variable t . The variable t can be a time or space variable, or both. For a particular value of t ,

S(t) is a random variable with a probability distribution. Under this reasoning, effective porosity for example cannot be a stochastic process. If we select a given t (time and space), then the effective porosity at that t is constant in time. In reality it is not a random variable. Effective porosity and other properties do vary over the spatial portion of the variable t. Consequently we can consider effective porosity (or any other hydrogeologic property) to be a regionalized variable, that is, a realization of a spatial stochastic process that may have been created in geologic time at some undefined scale; keeping in mind, however, that even that concept is open to debate. The scale at which geologic stochasticity occurs in particular is open to debate. When we measure these coefficients at a point, we are collecting data produced by such processes. In contrast to spatial stochastic processes as used in other disciplines such as physics or wildlife biology, prediction of future values of hydrogeologic properties is not physically meaningful. The movement of elk in the Bitterroot Mountains of Idaho is a legitimate spatial stochastic process. We can use data (past observations of location) to predict future locations of the elk probabilistically. This movement constitutes a stochastic process. In the case of hydrogeologic properties, except for measurement error our predictions can never change; they will have no probability associated with them. Under steady state conditions the values of hydrogeologic properties are fixed at all points in space. It is important that investigators understand the significance of substituting random hydrogeologic coefficients for randomness in flow pathway (discussed below). From the geologic point of view the product is in fact fictitious. We will deal with measurement error and error due to different sampling scales subsequently.

On the basis of this reasoning, the question arises as to how kriging, trend surface analysis, and inverse prediction, which derive from treating hydrogeologic properties as regionalized variables produced by stochastic processes apply to the prediction of groundwater travel time. Directly they do not. They provide descriptive statistics which help us to characterize the spatial variation and to make estimates of hydrogeologic properties.

In reality stochasticity occurs only in the initial point of entry of a flow line, y_0 . If a particle enters the system at a particular y_0 , it will follow the path of least resistance until it is trapped in dead-end pores or until it exits the flow system, subject to some predefined time scale. In a steady state system, all subsequent particles entering at precisely the same y_0 will follow exactly the same pathway. That is, effective porosity and other hydrogeologic properties are not random, even though the pathways are random at some scale.

Nevertheless, the models currently in use may not be fallacious. These models substitute assumed randomness in the hydrogeologic input coefficients for randomness in the flow path y_0 . From the water particle's point of view the hydrogeologic properties it encounters on its pathway appear to be random as realizations are generated. The hydraulic conductivity and effective porosity along a random pathway appear to the particle to be lognormally distributed and to be spatially correlated; even though, as explained above, effective porosity and hydraulic conductivity in the spatial dimension of t are fixed in nature. As stated above only the initial entry point of the particle, y_0 , and its associated

pathway are random. The existing models that were used to support the FEA's and many of the articles in the literature use this technique. They replace the randomness in y_0 and its associated pathway by presenting the water particle with randomly distributed hydrogeologic coefficients. Whether or not this substitution has true geologic meaning is open to debate. Virtually all of the published papers on this subject deal with the mathematics of the analysis. They do not deal with the validity of the output of these models on a site specific basis. Results of travel time modeling cannot be compared to actual physical measurements; they can be compared only to the results of other models at the same site or the same model at different sites. If one accepts the substitution of random coefficients for random pathways, it is reasonable to view sample data as realizations of effective porosity and other hydrogeologic properties and to use them in defining distributions of hydrogeologic coefficients to present to the particle. This approach may be defensible as long as we remember that the hydrogeologic properties at a specific site are variable in space, but nonstochastic, even though they are being treated as random variables. In nature it is the pathway that is random at some scale, not the hydrogeologic properties. The utility of this approach with respect to sensitivity analyses and to the prediction of data needs will be discussed subsequently.

We then must ask what is the effect of using randomness in θ as a substitute for randomness in y_0 . Consider the effect of random coefficients on our simple linear model with misspecification error,

$$y_t = a + bt + \epsilon.$$

If a and b are random, the variance of y_t is $\sigma_a^2 + \sigma_b^2 + \sigma_\epsilon^2 +$ covariance terms, where σ_x^2 is the variance of x for $x = a$ or b or ϵ . If a , b , and ϵ are uncorrelated (perhaps even independent), then the covariance terms are zero. In our simple model, the variability (a measure of uncertainty) due to misspecification and randomness in the coefficients is additive.

The general effect of randomness in θ is not as simple to gauge because $f(\cdot)$ often is a nonlinear function of θ . However, it is clear that the effect of randomness in θ will be in addition to and distinct from randomness due to misspecification error, ϵ . This reasoning spells out the two sources of uncertainty.

We will not treat randomness in $f(\cdot)$ itself.

2.2.1. Uncertainty or Sensitivity and Error Analysis

Sensitivity analysis is a classical mathematical tool for gauging the effect of changes in f , θ , or z_t on the output, y_t . The most common sensitivity analysis performed is with respect to θ . Techniques for coefficient sensitivity analysis in nonlinear models are outlined in Tomovic (1963) and Tomovic and Vukobratovic (1970). Sensitivity is defined as

$$\frac{\partial y_i}{\partial \theta_j}$$

Typically these sensitivity equations are difficult to solve because of the dependence of $\partial y_i / \partial \theta_j$ on other sensitivities, $\partial y_i / \partial \theta_k$, $k \neq j$.

Consequently, one may define a noninstantaneous sensitivity as the relative change in output, y_i , when θ_j is changed from θ_{j1} to θ_{j2} , i.e.,

$$\text{sensitivity} = \frac{\Delta y_i}{\Delta \theta_j} = \frac{y_{i2} - y_{i1}}{\theta_{j2} - \theta_{j1}} .$$

In order to explore the sensitivity fully, one can perturb the coefficients from a nominal value, θ_1 , to a number of values θ_2 . If the coefficient perturbations are selected at random (Monte Carlo simulation), the sensitivity analysis has been termed "error analysis" (Gardner et al., 1980a,b and Burns, 1975). Statistical experimental designs such as response surface designs (Baker, 1985) and fractional factorial designs (Steinhorst, 1979) have been used to perturb coefficients in useful (but nonrandom) patterns as well.

Statisticians have been quick to analyze statistically the pseudodata that are derived from these perturbations. The use of analysis of variance, regression, partial correlation, and cumulative frequency distributions on the generated y 's does not constitute a valid statistical analysis. The computed measures are valid indices of sensitivity, but they have no meaning in the classical statistical/probabilistic sense.

Most of the groundwater travel time analyses presented in the FEA's and in their supporting documents to date are of this "sensitivity analysis" type. These analyses are appropriate for identifying critical model components that require additional detailed data from subsequent site characterization studies, but the analyses do not constitute probabilistic analyses. Gutjahr (1986) suggests that, "Sensitivity analyses should be

separated from uncertainty analyses* (p.5-34). Because the cumulative frequency distributions generated do not relate to real probability distributions, but only to the relative frequency distributions of the pseudodata, the groundwater travel time distributions could be used for comparisons of different sites only if identical model forms are used at each site.

2.2.2. Uncertainty in Coefficients as a Bayesian Analysis

Another way to consider the coefficient perturbation analyses is to view these analyses as a numerical simulation of a Bayesian analysis. In a classical Bayesian analysis, all prior information about the value of a hydrogeologic coefficient is summarized into a prior probability distribution. Some of this prior information can be quite qualitative and subjective (as is the case in the documents that support groundwater travel time presented in the FEA's). The priors are applied to the probability distributions of new data to generate what are properly called posterior distributions. This approach is a formal way of interjecting prior data and opinion into on-going data analysis. The only difficulty with using Bayesian analysis on groundwater travel time distributions is that only the prior distributions exist. No present probability distributions exist that can be converted to posterior distributions. It seems to be a misapplication of Bayesian analysis to run the priors through a conceptual model and then call the output a posterior distribution.

2.3. Uncertainty Due to Data Collection and Estimation

Data are necessary for conceptual and numerical model formulation and to estimate statistical parameters. We use parameters properly in the sense of means, variances, and autocorrelations of coefficients. There are three sources of uncertainty related to data. These three sources are scale, sampling variation, and measurement error.

Data may be collected at an inappropriate scale. One of the lessons learned from the stochastic groundwater modeling literature is that the results are sensitive to the scale of the model (i.e., the size of the blocks used, Freeze, 1975). In a similar sense, it is apparent that point measurements of effective porosity or hydraulic conductivity, for example, do not represent accurately the effective porosity or hydraulic conductivity at a scale of one to five kilometers. By definition there is no way to characterize hydraulic connectivity or hydraulic continuity at a given site without tests that are large enough in scale to test points that are connected hydraulically at the time scale of the test. Even allowing for a range of values for effective porosity or hydraulic conductivity measured from cores, it is not clear that spatial simulations of point (small-scale) values capture the sense of hydraulic conductivity or effective porosity that operates at the scale of groundwater travel from a repository to the accessible environment. Effective porosity or hydraulic conductivity at a point is a physical concept that is appropriate only at distances of meters. This is the reason that it is difficult to use the (arithaetic or geometric) average of point-source

effective porosities or hydraulic conductivities to derive an equivalent uniform value to apply to a geologic unit (see Neuman, 1982).

When one collects data, uncertainty inevitably is introduced by the design of the sampling regime. Additionally one may be forced to use data that were collected by someone else for other purposes and perhaps without any design at all. Those who accept that hydrogeologic properties are distributed in space (as a realization of some stochastic process in geologic time or for whatever reason) will acknowledge that data collected systematically will differ from those collected as a simple random sample or as a stratified random sample.

Measurement error probably is the least of the uncertainties introduced by data. It can be controlled to a large extent by good field and laboratory techniques and a strong quality assurance program. The variation in data caused by measurement error should be scrutinized carefully, but it probably will be dwarfed by variations introduced by scale of testing and by variations in the sampling program(s) that produced the data set.

We now consider again our simple linear model with misspecification error and random coefficients,

$$y = a + bt + \epsilon,$$

$$\epsilon \sim D(\mu_{\epsilon}, \sigma_{\epsilon}^2),$$

$$a \sim D(\mu_a, \sigma_a^2),$$

$$b \sim D(\mu_b, \sigma_b^2),$$

where \sim means "is distributed as" and $D(\mu_x, \sigma_x^2)$ indicates a generic probability distribution with mean μ_x and variance σ_x^2 . Assume for simplicity that ϵ , a , and b are independent. Since $\mu_\epsilon, \sigma_\epsilon^2, \mu_a, \sigma_a^2, \mu_b,$ and σ_b^2 are unknown parameters, they must be estimated from data collected at the site. The alternative is to take values from the literature or from "expert opinion." Under repeated sampling, the estimators denoted as $\hat{\mu}_\epsilon, \hat{\sigma}_\epsilon^2, \hat{\mu}_a, \hat{\sigma}_a^2, \hat{\mu}_b, \hat{\sigma}_b^2$ are random variables with their own probability distributions. For example, $\hat{\mu}_\epsilon$ will be some function of the random data. If it is an unbiased estimator, it will have a distribution

$$\hat{\mu}_\epsilon \sim g(\mu_\epsilon, \sigma_{\hat{\mu}_\epsilon}^2)$$

where g indicates the sampling distribution of $\hat{\mu}_\epsilon$ with mean μ_ϵ and standard error, $\sqrt{\sigma_{\hat{\mu}_\epsilon}^2}$. A prediction of y is $\hat{y} = \hat{a} + \hat{b}t + \hat{\epsilon}$. Its uncertainty will depend on the model uncertainty ϵ on the use of coefficient uncertainty as a surrogate for pathway uncertainty, and on the uncertainty introduced by using data to estimate unknown parameters that characterize the model and coefficient uncertainty. These three major forms of uncertainty probably are not captured by the random coefficient perturbations used in groundwater travel time analyses that support the FEA's. This technique seems to be more of a representation of coefficient sensitivity as described above and/or the randomness of pathways per se. Furthermore, the uncertainty associated with probabilistic mechanisms that are needed to specify the model $f(\cdot)$ correctly have not been considered. Likewise the uncertainty associated with the driving variables z_t has not been considered. However, uncertainty in the driving variables, z_t , probably is not important in saturated media where steady state conditions can be assumed. External forces like groundwater recharge play a minor role in these deep

groundwater flow systems. On the other hand, these statements will not apply to unsaturated flow regimes such as tuff (Nevada Test Site, Yucca Mountain) where driving variables can change with recharge events.

2.4. Uncertainty Due to Computing

There are uncertainties associated with computer implementation of groundwater travel time models. In any reasonably large computer code there are logical errors and coding errors. In addition there is roundoff error associated with digital computation. If the model is in the form of a system of ordinary differential equations or partial differential equations solved numerically, there are errors due to the numerical approximation of finite difference, finite element, or other solution methods. These sources of uncertainty are dealt with at length in the literature.

Other numerical uncertainties are present in the computing process, but they are less well-defined. For example, some groundwater travel time models do not conserve mass.

3. MODELING ASSUMPTIONS USED IN DOCUMENTS PREPARED IN SUPPORT OF FEA'S

On the basis of the above discussion it is clear that the assumptions implicit in the groundwater travel time modeling analyses (presented to date in supporting documents for the FEA's) include the following:

1. The conceptual model used in each of the calculations is assumed to be known perfectly. No uncertainties in the designation of the conceptual model are incorporated into the output cumulative frequency distributions of groundwater travel time.
2. Randomness in the input coefficients is assumed to be represented accurately and is assumed to be a suitable surrogate for the randomness inherent in a particle's pathway at the 5 or 10 km scale. This assumption is particularly important and should be the subject of considerable future deliberation in the hydrogeologic professional community. Furthermore, combinations of randomly generated hydrogeologic coefficients used in the models are assumed to be physically meaningful at the scale of the test data used in the analysis of groundwater travel time at a given site.
3. Randomness in hydraulic head, the input driving variable, is assumed to be negligible.
4. The test data on which hydrogeologic property input data distributions are based are assumed to be collected at a scale appropriate for analysis at the scale used to simulate groundwater travel times (5 or 10 km).
5. No variation is assumed to exist in the data base due to different sampling programs.

6. Measurement errors in the data are assumed not to exist.
7. The computer codes are assumed to be 100% accurate (verified).
8. No probabilistic mechanisms are assumed to be operating on the particles (such as Brownian motion). The output cumulative frequency distributions of groundwater travel times are assumed to be probability distributions of groundwater travel times.

The earlier discussion has elucidated the importance of these assumptions and has illustrated how they relate to the true uncertainties that are inherent in the outputs of the models. Unfortunately the uncertainty inherent in each of these assumptions is not quantified by the output of the models. By using coefficient randomness as a surrogate for randomness in the water particle's pathway, modelers are providing only a partial representation of uncertainty. Sensitivity analysis relative to the form of the model and to the driving variables may serve to help us understand these additional sources of uncertainty. Uncertainty due to scale of testing, sampling design, measurement error, and probabilistic mechanisms acting on the particles (if any) will be more difficult to quantify but clearly these issues must be approached separately. Numerical inaccuracies in the computer code will be minor if care is taken to use the most modern computational techniques.

Item number 2 above in particular should be the subject of debate in the hydrogeological professional community. The use of randomness in hydrogeologic coefficients in space as a substitute for randomness in flow

paths is not a straightforward, easily understood concept. Whether or not the product is meaningful is not clear. It is clear however that a cumulative frequency distribution of groundwater travel times generated by this procedure need not be expected to contain the true groundwater travel times at all.

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