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Hydrogeology • Water Resource Management • Geological Engineering • Mine Hydrology

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Mr. Jeff Pohle
Division of Waste Management
Mail Stop 623-SS
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Dear Jeff:

Please find enclosed our draft paper entitled "Procedures for Predicting Groundwater Travel Time." We have split the paper into three parts. These parts deal with general aspects of testing hydrogeologic environments and the two types of tests that are required for deterministic modeling and stochastic modeling, respectively. As you will see from our discussion, the nature of deterministic modeling leads the field investigator toward the use of large scale tests wherever the permeability distribution permits. Conversely the nature of the statistical requirements of stochastic modeling lead the field investigator toward small scale tests, regardless of the distribution of permeability in the hydrogeologic environment. In addition to statistical requirements, practical limitations on the number of large scale tests required preclude the use of large scale tests for stochastic modeling. Our investigation of this subject has led us to conclude that it is not technically defensible to mix large scale test results with small scale results as inputs to stochastic models. This conclusion is a consequence of the fact that large scale tests do not test the same geologic domain as do small scale tests when permeability is the objective of the test. Similar reasoning applies to effective porosity.

If you have any questions regarding our paper, please call.

Sincerely,

Roy Williams/sl

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REW:sl

enclosures

PROCEDURES FOR PREDICTING GROUNDWATER TRAVEL TIME

by

Williams and Associates, Inc.

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1. Purpose

The United States Nuclear Regulatory Commission has promulgated rules and regulations which govern the disposal of high level radioactive wastes in the United States. These rules and regulations were promulgated as Title 10, Chapter 1, Code of Federal Regulations--Energy, Part 60. These rules and regulations outline criteria for the disposal of high level radioactive wastes in geologic repositories. The primary criteria of interest for this paper are the criteria concerning groundwater travel time from the disturbed zone to the accessible environment, a distance of 5 km.

Groundwater flow is the principal mechanism by which radioactive wastes might migrate from the repository to the accessible environment. The accessible environment is now established as being no greater than 5 km from the edge of the disturbed zone of the repository. The rules and regulations state under 60.113 Performance of Particular Barriers After Permanent Closure, (2) Geologic Setting that "The geologic repository shall be located so that pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other travel time as may be approved or specified by the Commission." The rules and regulations state further under Section 60.122 entitled Siting Criteria (b) Favorable Conditions, that "(iv) Pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment that substantially exceeds 1,000 years." This paper pertains to sites wherein saturated groundwater flow is the primary mechanism for radionuclide transport. Unsaturated flow is anticipated at the Nevada Test Site but saturated flow is the predominant flow mechanism at all other sites being considered for the disposal of high level radioactive waste. However the concepts outlined in the following report may be applicable, in part, to the unsaturated zone also.

The prediction of groundwater travel time is a multipart process that may use a variety of models. In all cases the initial model that must be formulated is the conceptual model (fig. 1).

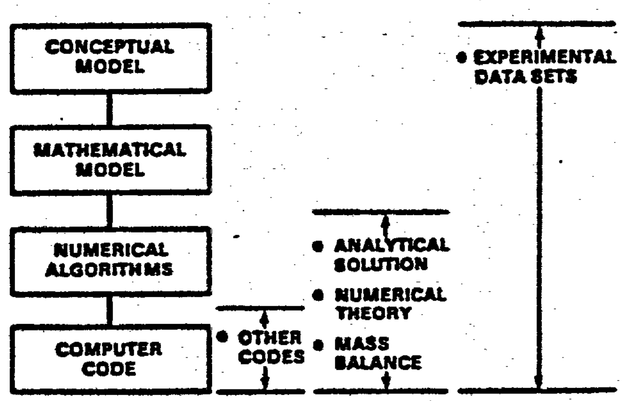

Figure 1. Four Aspects of a Transport Model and Appropriate Model Verification Techniques (Jones and Gee, January 1984, p. 56).

A mathematical model may be applied using the hydrogeologic framework outlined in the conceptual model. Analytical solutions may be used to support the algorithms used in the mathematical model. Jones and Gee (January 1984, p. 55) state that model verification is a simple concept that defies rigorous definition. Jones and Gee provide a clearly stated discussion of the model verification process. Regardless of the model selected experimental data sets are required to verify it. In hydrogeology experimental data sets pertain to data on hydraulic conductivity, transmissivity, hydraulic head, effective porosity and in the transient case, storage coefficient. The acquisition of such data sets requires the use of analytical or numerical models. Such models are deterministic by definition. There are no stochastic models for measuring hydraulic conductivity, effective porosity, transmissivity, or hydraulic head in the field or in the laboratory. The model (analytical or numerical) that is selected determines the scale of the test (both in time and space). The scale of the test in turn determines the volume of rock for which the verification data set is representative.

This paper is directed at the establishment of testing procedures and criteria for the two basic methodologies that are being employed for estimating groundwater travel time. Groundwater travel time analyses are intended to be conducted under the assumption of steady state flow conditions at the sites in question because pre-waste-emplacement groundwater travel times are the primary interest. Testing techniques are discussed herein in general terms for obtaining the necessary hydrogeologic data required for model verification and incorporation into the two prevalent methods of estimating groundwater travel time.

The two methods of predicting groundwater travel time considered herein are referred to as the purely deterministic approach and the stochastic approach. In fact the stochastic approach requires the establishment of a partially deterministic model first so that the geometry of a hydrogeologic framework can be established. Without the geometry of a hydrogeologic framework a stochastic approach cannot be implemented. Hydraulic boundaries and hydrostratigraphic units or zones must be input to a stochastic model. Recent hydrogeologic literature contains many articles on the spatial variability and possible stochasticity of hydrogeologic properties (see Neuman, 1982, for a history of major works; see also Journel and Huijbregts, 1978). Because of this spatial variability and possible stochasticity of hydrogeologic properties, we refer herein to effective porosity, saturated hydraulic conductivity (permeability), and transmissivity as coefficients rather than parameters (as explained in an accompanying paper on uncertainty).

Stochasticity must be viewed as a possibility in hydrogeology, not a certainty because in fact hydrogeologic coefficients do not represent stochastic processes in a spatial hydrogeologic sense at our scale of interest (5 km). The coefficients do vary with position in space but that does not mean that they are stochastic processes. 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 or hydraulic conductivity by definition cannot be a stochastic process. If we select a given t (time and space), then the effective porosity at that t is constant. In reality it is not a random variable. Effective porosity, for example, does vary over the spatial portion of the variable t. Consequently we can consider effective porosity (or any other hydrogeologic coefficient) 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. Probabilists differentiate between a random variable and its realization. When we measure hydrogeologic 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 north Idaho is a legitimate spatial stochastic process. We can use data (past observations of location) to predict future locations of the elk probabilistically. It is for this reason that this movement constitutes a stochastic process. In the case of hydrogeologic coefficients our predictions can never change; they will have <u>no</u> probability associated with them. Under steady state conditions the values of hydrogeologic coefficients are fixed at all points in space. We have pointed out in our paper on uncertainty that regionalized variables are being treated as random variables produced by stochastic processes in lieu of random flow pathways. But it is important that investigators understand the meaning of this substitution. From the geologic point of view the product in fact is fictitious.

The deterministic and stochastic methods differ significantly as outlined in the following discussion. This report elucidates the major differences between the purely deterministic and the stochastic methodologies and their inherent influences on the testing methodologies that must be employed to achieve usable input data bases for each type of analysis.

The detail by which hydrogeologic data are evaluated and collected at a site is directed to a considerable extent by the methodology or approach which will be used to predict groundwater travel time. The purely deterministic approach and the stochastic approach for estimating groundwater travel time create distinctly different requirements pertaining to the hydrogeologic data base. These requirements delineate to a considerable extent the methodologies which must be used for designing a field testing program, for analyzing the data, and ultimately for obtaining the required hydrogeologic data base for predicting groundwater travel time. As explained below, the methodology that is used for predicting groundwater travel time to a large extent directs the scale of testing and the consequent validity of the groundwater travel time predictions when large volumes of rock are involved.

2. Scale

2.1. Conceptual Model Scale

The first step in developing a procedure for estimating groundwater travel time is to develop a conceptual groundwater flow model. Several scales may evolve in the development of a conceptual model(s). The scale of the conceptual model can vary between regional (basinwide) scales and a variety of smaller scales. An intermediate scale perhaps might be referred to as a performance assessment scale. Historically, a groundwater basin or a surface water basin scale has been used to define hydrogeologic environments. The basin scale is helpful in understanding the groundwater flow systems that pertain to predicting groundwater travel times at a site. For the smallest practical scale, a conceptual model may be developed which is pertinent only to the volume of material influenced by a single well hydrogeologic test (a slug test or a test on drill core). A repository scale conceptual model should be of greater value, assuming that the distances involved in groundwater travel time predictions are equal to or less than the 5 km limit to the accessible environment.

The performance assessment scale mentioned above is a more realistic scale of interest. The performance assessment scale may require the use of a basin scale for the delineation of groundwater flow systems and probable groundwater flow paths. The use of the basin scale is especially appropriate for numerical simulation of groundwater flow for the establishment of boundary conditions. Additional conceptual model scales may be of interest depending upon the site in question and on the degree of knowledge which has been obtained about that site. The three scales outlined above are considered to be representative of the scales that will be of interest at any given site.

2.2. Hydrogeologic Testing Scale

Scale is important also with respect to hydrogeologic testing. The single well tests that currently are being used at the sites consist of slug tests or drill stem tests (DST's). Single wells also have been used for very small scale pumping tests; the pumped well and the observation well are coincident in this instance. The scale of the tests varies depending upon the hydrogeologic properties (transmissivity and storativity) of the medium. These two hydrogeologic coefficients, along with hydrogeologic boundaries determine the areal extent of the perturbation caused by the test. The slug or DST types of test characteristically do not influence a large areal or volumetric extent of the rocks being tested. The small areal extent of the test volume results in part from the short duration of the perturbation that usually is created for the test. There are exceptions to this rule in that DST's can be carried out for long periods of time; in such cases the areal extent of the area of perturbation can reach larger distances from the test well. Single well pumping tests also cover longer periods of time than slug type tests. Consequently the areal extent of the test is larger. However, the information derived from such a test is limited due to the absence of separate observation wells.

The scale of the test is increased significantly by the use of multiple well testing techniques. These tests commonly employ a pumping well with more than one observation well. Observation wells may be located at different radial distances from the pumping well; they also may be installed in the confining units above and/or below the pumping unit in order to measure the vertical permeability of the confining layer. These tests frequently are run for long periods of time during which large volumes of fluid are removed from the pumping well. These tests stress a large volume of the hydrogeologic system. Significantly more data and hydrogeologic information are obtained from this type of test due to the larger volume of rock characterized. Analytical or numerical techniques are available for testing anisotropic rocks, bounded aquifers, partially penetrating conditions, leaky aquifers and aquifers whose thicknesses vary in space.

Vertical hydraulic conductivity can be estimated by several techniques. Vertical hydraulic conductivity can be estimated very crudely by a single well test technique which has been outlined by several authors in the petroleum industry literature. The single well vertical permeability test stresses an isolated portion of a permeable layer while monitoring above and/or below the injection horizon so as to measure hydraulic pressure or head perturbations produced by the imposed hydraulic stress.

The state of the art method for estimating vertical hydraulic conductivity involves the use of multiple wells. Wells are located both within the pumped zone or aquifer as well as in the confining units above and/or below the pumped aquifer. The data from all the wells ordinarily are evaluated by analytical techniques to estimate the vertical hydraulic conductivity. Vertical hydraulic conductivity can be estimated on a scale approximately equal to the areal extent of the cone of depression by using conventional analytical techniques. These conventional analytical techniques evaluate the data derived from the pumped aquifer but they do not entail the use of observation points in the overlying or underlying confining units. Analyses of data from observation wells in the confining units yield results which are representative only of the vertical hydraulic conductivities in the immediate vicinities of the observation wells. Nevertheless this analytical technique constitutes state of the art field measurement procedure.

Effective porosity can be measured in the field by only one method. This method is a tracer test which requires more than one well to measure effective porosity accurately. The state of the art for field tracer tests is not well advanced but tracer tests indeed do constitute the state of the art for this measurement. Methodologies exist for conducting tracer tests in single wells but the representativeness of the data is reduced significantly. The multiple well technique has obvious advantages; it maximizes the scale of the test and the volume of rock being tested. Multiple well tracer tests yield data that can be interpreted for quantifying effective thickness for that zone located along the flow path between the two wells used in the tracer test. As used most commonly effective thickness is the product of contributing zone thickness and effective porosity but at least one other definition exists. The scale of the value obtained by this method is constrained by the distance between the two wells. Extending the distance between the two wells or incorporating the use of multiple source or detector wells for a tracer test increases the scale but it also increases the probability that a detectable amount of tracer will not reach the observation wells. The distance separating the wells in a tracer test can become so great that the travel time between the wells will exceed the practical limits of testing. The field determination of effective thickness (synonymous with effective porosity as used herein) is complicated at several sites by the probable existence of fracture flow and by heterogeneities. Testing to date at the sites has been minimal; two tests have been conducted in one flow top at one site (BWIP). Tracer tests are hampered by the vertical distance(s) that separates the hydrostratigraphic unit of interest from the ground surface. The mechanics of conducting the test become extremely difficult because of the long transit times that occur in the tubing which carries the tracer to the test horizon and back from the test horizon to the sensors which usually are located at the surface.

Effective porosity can be estimated based on the evaluation of geophysical logs; this method of testing is very approximate and indirect. The correlation between effective porosity values determined from geophysical logs and the true effective porosity that controls groundwater movement is not clear.

2.3. Time Scale

Time scale is a significant issue which must be considered during test design. The time scale of most hydrogeologic testing is on the order of days to weeks whereas the regulatory standard noted above for ground water travel time is 1,000 years. It is not practical to conduct hydrogeologic tests even for a duration of a few years. This statement is valid especially for tracer tests. It is only semi-practical to conduct long term (up to a year) hydrogeologic tests for determination of boundary conditions and hydrogeologic coefficients. Mechanical problems usually override hydrogeologic problems in long term tests.

The scale of time is a critical component with respect to the determination of groundwater flow direction and gradient. The rules and regulations as quoted above indicate that the fastest path must be determined for groundwater travel time. Low hydraulic gradients (such as 10^{-3} to 10^{-4} at the BWIP site) create a problem with respect to identifying the fastest path. Transient effects on hydraulic head created by drilling activities and testing activities have created perturbations on the system. These disturbances can influence adversely the determination of the static groundwater potential distribution that is supposed to be unaffected by transients. Construction of the repository must be considered as a potential perturbation to the hydrogeologic system. The direction of groundwater flow and hydraulic gradients should be measured before construction of the repository begins. Conditions of low hydraulic conductivity require long periods of recovery from induced transients. These long recovery periods cause difficulties in identifying the direction of groundwater flow both horizontally and vertically and in the determination of the magnitude of hydraulic gradient both horizontally and vertically. The long recovery periods can create time constraints with respect to meeting deadlines.

The time scale is important with respect to tracer or solute transport. Solute transport over 5 kms cannot be demonstrated on a 1,000 year criteria. It can be inferred but not demonstrated. Tracer tests must be much shorter than the travel time standard. Tracer tests are required for the estimation of effective thickness/effective porosity. This hydrogeologic coefficient is vital to the estimation of groundwater travel time.

2.4. Influence of the Simulation Method on Testing Design

2.4.1. Purely Deterministic Approach

The purely deterministic method of simulating travel time requires the establishment of the most likely groundwater flow path. The identification of the most likely flow path requires that the hydrogeologic system be understood to the extent that the hydraulic gradients can be defined in both the vertical and horizontal directions. The gradients determine the direction of flow which is in part a reflection of the distribution of transmissivity at the site. Consequently a purely deterministic approach requires that the spatial distribution of hydrogeologic coefficients be measured in the horizontal and vertical directions along this most probable fastest flow path. In order to derive hydraulic conductivity along such a path the thickness of the zone(s) of interest must be determined. The prediction of groundwater travel time along the most probable fastest flow path requires that the distribution of effective porosity be obtained along that flow path. It should not be concluded that this most probable flow path is a straight line from the disturbed zone to the limit of the accessible environment (5 km). Instead, the length of flow path and the direction of the flow path may be of a sinuous nature due to the variable distribution of effective porosity and transmissivity at the sites. The sinuosity of the flow path is also a factor in the vertical direction because a substantial component of vertical flow may exist at several of the sites if not at all the sites. Consequently the determination of the most probable flow path is a horizontal and a vertical problem which must be solved prior to the establishment of bounds of hydrogeologic coefficients along the flow path. The treatment of the problem purely deterministically at the scale of 5 km by definition requires large scale tests. Hydraulic continuity at this scale, for example, cannot be demonstrated by small scale tests.

2.4.2. Stochastic Approach

The stochastic simulation of groundwater travel time approaches the problem from a different perspective. This approach defines the distribution of vertical gradients and horizontal gradients at the site but not necessarily in any particular direction. A large number of different flow paths is generated by allowing hydrogeologic properties to vary randomly in space between zone(s) of high head and zone(s) of low head. Some type of deterministic model or at least a geometrically well bounded and well structured conceptual model must be developed first in order to provide a hydrogeologic framework for the stochastic analysis. The hydraulic conductivities in the vertical and horizontal directions still must be defined but the values within the units of interest are allowed to vary randomly a fixed points in space among different "realizations" of the regionalized variables. Effective porosity and hydraulic conductivity must be assigned in some manner along the multiple possible directions of flow, but they are not restricted to the most probable fastest flow path as is the case in the purely deterministic approach because flow paths are allowed to wander randomly within the model as hydrogeologic properties are varied at each point among different realizations. Again the principal interest is the assigned distribution of effective porosity and hydraulic conductivity in a vertical and horizontal sense. It is the distribution of these hydrogeologic properties at each fixed point in space that is of primary interest in the generation of cumulative frequency distributions of groundwater travel time.

A method of estimating travel time stochastically employs multiple simulations based on random choices of hydrogeologic coefficients to be assigned to fixed points in the conceptual model (Monte Carlo technique). This approach uses the resulting hypothetical distributions of hydrogeologic properties at each point in the model to generate travel times which yield a cumulative frequency distribution of simulated travel times. This approach assumes that a large number of possible combinations of the values for these hydrogeologic coefficients can occur within the conceptual model. If real data are used in such a model the statistical requirements of the approach guide the investigator toward the acquisition of large numbers of data points. This requirement implies the use of large numbers of small scale tests. Stochastic analyses can be adapted to the results of large scale tests but large numbers of tests are still required to develop input distributions of hydrogeologic properties. Large numbers of large scale field tests are not feasible due to the constraints discussed above and below. Stochastic theory in combination with applied hydrogeologic experience suggests that hydrogeologic coefficients measured analytically at different scales should not be combined as inputs to a stochastic model. Data sets derived at different scales reflect completely different characteristics for the same rocks. Small scale tests offer no evidence of hydraulic continuity from point to point whereas large scale tests reflect fastest path hydraulic conductivity, for example, between pumping well and observation wells.

3. Defining "Site" Hydrogeology

Any conceptual model for groundwater flow is dependent upon the scale that is of interest for estimating groundwater travel time. A conceptual model can vary in size from that of the scale of a test to that of a basinwide scale as noted above. The principal scale of interest for estimating groundwater travel should be on the order of the performance assessment scale (5 km) to basinwide scale.

The prediction of groundwater travel time is method dependent; as discussed above the two principal methods in use are the purely deterministic method and the stochastic method. Both methods generally assume porous media or equivalent porous media flow. Fracture flow can be accommodated in these methods by various manipulations of the data. Specific fracture flow models are not practical due to their inability to estimate solute transport on a scale of kilometers and secondly due to the nature of the data required about the fractures that cannot be obtained from boreholes. Unfortunately field data acquisition techniques required for verification of or input to any kind of fracture flow modeling effort have lagged behind the sophistication of simulation methods that are available to analyze groundwater behavior in fractured media.

3.1. Defining Geologic Framework

The geologic framework must be defined for both the deterministic and stochastic methods of estimating travel times. The stratigraphy must be defined in order to input the approximate bounds on hydrostratigraphic units. The establishment of a geologic framework is an essential prerequisite to the establishment of a hydrogeologic framework. Geologic structures must be mapped for either approach. Faults, fracture zones (as opposed to individual fractures), discontinuities, anticlines, synclines, facies changes and hydrostratigraphic unit pinchouts (facies changes) must be located for the determination of groundwater travel times because of the necessity for identifying the fastest most probable flow path. The stochastic method can accommodate geologic structures by incorporating the distribution of the hydrogeologic coefficients within the structures into the conceptual model. The groundwater travel time is then "realized" based on the assigned distribution of coefficients at each point in the model and a scenario that incorporates flow paths through such structural features.

3.2. Defining Hydrogeologic Framework

The hydrogeologic framework must be defined for both methods of estimating groundwater travel time. Hydraulic conductivity in the horizontal and vertical directions must be determined for both the stochastic and the purely deterministic methods of estimating travel time. The possible or probable distributions of hydraulic properties must be input for the stochastic method; the absolute value of hydraulic conductivity along the most probable fastest flow path must be input for the purely deterministic method. The hydraulic gradient must be input in both the vertical and horizontal directions for the purely deterministic method and for the stochastic method. The expected range of gradients (based on field measurements) can be bounded. The purely deterministic method requires that the fastest path of radionuclide transport be identified. In order to do so a good distribution of hydraulic head measurements must be obtained in order to define the direction of groundwater flow in the horizontal and vertical dimensions. The determination of the gradient can be complicated by the hydraulic conductivity distributions within the hydrostratigraphic units at the site. Low hydraulic conductivities create long recovery times for water levels perturbed by drilling and testing. Long recovery times complicate the measurement of the head distribution that identifies the fastest path. Additional perturbations caused by subsequent testing also will influence the measurement of the hydraulic gradient adversely; consequently the identification of the fastest path for radionuclide transport will be influenced adversely. The requirements for hydraulic gradient for a purely deterministic approach are much more rigorous and more sensitive to uncertainty because of the additional requirement stated as 'determining the fastest path'. Stochastic methods are not constrained by this requirement because the stochastic analysis generates a large number of paths. The fastest path may or may not be included in the model output.

Effective porosity is required for both the purely deterministic and stochastic approaches. The stochastic approach requires that a distribution of effective porosity be obtained and input for those units considered to be involved in the transport of radionuclides away from the repository. A purely deterministic approach requires that the effective porosity distribution be obtained along the fastest path. The fastest path for radionuclide transport cannot be identified until the hydraulic gradients have been measured to such an extent that the fastest path can be ascertained with reasonable certainty. It should be obvious that the spatial distribution of hydraulic conductivity and effective porosity under the purely deterministic approach will be reflected by the measurements of the distribution of hydraulic head at the site in the early stages of investigation. The hydraulic gradient governs the direction along which the hydrogeologic testing should proceed at a proposed site.

Hydraulic continuity must be demonstrated for the purely deterministic approach. Hydraulic continuity refers to the continuous flow path that must be shown to exist between the repository and the accessible environment along the fastest path of radionuclide transport. It is not necessary to demonstrate hydraulic continuity for the stochastic approach because this approach uses input distributions of hydraulic conductivities, hydraulic gradients, and effective porosities for the prediction of groundwater travel times. However hydraulic continuity is tacitly assumed to exist along all pathways generated by the stochastic approach. This assumption is seldom highlighted but if hydraulic continuity does not exist within a stochastic model the model cannot function.

4. Hydrogeologic Testing Methodology

4.1. Influence of Deterministic Approach on Testing

The purely deterministic approach assumes that equivalent porous media flow is appropriate for the medium of interest. Hydraulic conductivity can be determined by several methods as pointed out above. A predominance of low hydraulic conductivities at a site requires that small scale single well type tests be used for the measurement of hydraulic conductivity for those rocks. Under this set of hydrogeologic conditions a large number of such tests are required in the purely deterministic approach to determine the distribution of hydraulic conductivity along the fastest path.

If state of the art testing is to prevail, rocks with a moderate to high hydraulic conductivity require a different test plan. Multiple well long duration tests can be conducted in the higher hydraulic conductivity (higher transmissivity) units or zones. The number of tests required when using the multiple well technique is smaller than the number required with the small scale single well type tests. Multiple well test results in some respects replace the "averaging" process that statistical analysis of small scale test data attempts to accomplish. The term "averaging" is not quite correct because in fact the multiple well test measures the transmissivity only along those openings that are hydraulically connected at the time scale of the test and at the spatial distance between the pumping well and the observation well. Smaller scale openings are dead ended and not reflected in the test results. A few to several multiple well tests may be required depending on heterogeneities and boundary conditions at a site.

Large scale multiple well test techniques are adaptable to the measurement of vertical hydraulic conductivity for input into deterministic models. The large scale tests require the existence of a hydrostratigraphic unit of sufficient permeability to allow pumping from the unit for extended periods of time, preferably at a constant rate of discharge. Data obtained from observation wells completed in the pumped hydrostratigraphic unit can be analyzed to yield a value of vertical hydraulic diffusivity that reflects the effect of average vertical hydraulic conductivity of the individual confining units or the effects of the confining units both above and below the pumped unit.

The vertical hydraulic conductivity of the confining units also can be estimated from observation wells completed in the confining units. Each well completion in a confining unit yields data that can be analyzed for vertical hydraulic conductivity; each value calculated from the data is representative of the hydraulic characteristics of the media between the observation well (point) completed in the confining unit and the adjacent pumped unit. Multiple observation points yield multiple values of vertical hydraulic diffusivity for the monitored confining units. Such values are essential as data input to a purely deterministic model.

Fault zones must be tested and incorporated along the fastest path in the purely deterministic method of predicting travel times. It is essential that they be identified and characterized along the fastest path if their hydraulic properties differ from those of the rocks they transect. Hydraulic continuity may be created by or interrupted by such zones.

Hydraulic gradient can be measured under most hydrogeologic conditions. As explained above low hydraulic conductivities complicate the measurement of hydraulic gradient due to the necessity for installing essentially permanent measuring facilities. Semi-permanent facilities are required because records of long duration are needed to allow for full recovery from perturbations to the system. Perturbations are caused by the drilling activities required for installing and operating monitoring facilities for collection of samples for chemical analyses or from shaft sinking. Low hydraulic conductivity environments require that perturbations be minimized so that the hydraulic gradients and flow directions can be identified. A moderate to high hydraulic conductivity requires temporary to semi-permanent facilities for measuring the distribution of hydraulic head. Less time is required for delineating the static heads necessary for the determination of hydraulic gradient and flow directions when the hydraulic conductivities are high. Some perturbations can be tolerated under these conditions because the system will recover from the perturbations much faster than it does where low hydraulic conductivities prevail. Low hydraulic gradients confound the measurement of the magnitude and direction of the gradients. Consequently low gradients create difficulties in identifying the direction of flow; measurement accuracy plays a significant role in determining the insitu undisturbed gradients under such conditions. Measurement error can be a significant factor in determining hydraulic gradients when they are on the order of 10^{-3} to 10^{-4}, as apparently is the case at the BWIP site for example.

As noted above effective porosity must be measured by the use of insitu tracer tests. Two well tracer tests currently are being used or are proposed at the sites. The duration and scale of the tests must be controlled by the expected values of hydraulic conductivity at each site and within each zone of interest. Low hydraulic conductivities will create difficulty in measuring effective porosity due to long tracer transit times. Low hydraulic conductivities also make difficult the injection of the tracer and the removal of the tracer from observation wells. The injection and removal of the fluid can create significant perturbations upon the hydrogeologic system. It is not practical to conduct a test at the scale of the accessible environment for a number of reasons. These reasons include length of test, unknown distribution of heterogeneities at the site, and the difficulty of detecting tracer in the observations wells at the time scales required for a test at such a scale. Nevertheless in spite of their inherent problems, tracer tests constitute the state of the art procedure for measuring effective porosity.

Hydraulic continuity must be demonstrated for purely deterministic methods of predicting travel times. Hydraulic continuity can be demonstrated by only one method; large scale multiple well tests are required. Such tests directly and indirectly reflect the presence or absence of hydraulic continuity. Observation wells can provide data which indicate the existence of barrier boundaries due to the nature of drawdown data produced by the tests (image well theory). Observation wells located on opposite sides of a hydraulic discontinuity may yield direct evidence of the presence of that discontinuity. It is obvious that several large scale hydrogeologic tests may be required along the fastest path of radionuclide transport from a repository to characterize such boundaries. It is not likely that a single large scale test can answer the major questions of interest regarding hydraulic continuity along the fastest flow path. These same statements are applicable to the measurement of effective porosity and to the distribution of hydraulic conductivity along the fastest path.

4.2. Influence of Stochastic Approach on Testing

The stochastic approach for estimating groundwater travel time requires that a distribution(s) of hydraulic conductivity be input to a model that portrays the hydrogeologic framework within the area of interest. The statistical nature of this methodology requires that a large number of tests be conducted in order to obtain a valid distribution of values. Otherwise the input data simply must be synthesized. A large number of tests is required in order to obtain a defensible input distribution of the pertinent hydrogeologic coefficient. Consequently the stochastic method tacitly steers the methodology for field testing toward conducting many small scale tests, regardless of the hydraulic conductivity of the units in question. In addition to conformability with statistical analysis small scale tests are advantageous for several additional reasons including cost and the long time periods required for conducting numerous large scale tests. Stochastic methods require a large number of values to establish a distribution for input to the model which is not practical to obtain with large scale tests; consequently small scale tests are necessary even though they may not reflect hydraulic properties at the scale of interest. Interestingly enough all field data for input to stochastic models must be obtained from the application of a deterministic analytical model or numerical model. There are no stochastic methods for obtaining field measurements of hydrogeologic coefficients.

A stochastic method does not require that flow direction be determined by field data. The model itself generates numerous flow paths that are called "realizations." Hydraulic gradient must be established in a horizontal and vertical direction but only at certain end points or at boundaries of hydrogeologic zones or units. The expected range in hydraulic gradients usually is input to the model. The distribution of hydraulic gradient can be obtained using standard test methods. Since no fastest path need be identified fewer measurements are required to establish the gradient within the flow system; however, sufficient values must be collected to develop a distribution or at least a range that can be input to a model.

Effective porosity values must be input to the stochastic model for predicting travel times. Effective porosity must be obtained using a number of tests that is sufficiently large to give a valid distribution of effective porosity in the hydrogeologic units of interest. Effective porosity does not have to be singularly determined along the fastest flow path as is the case with the purely deterministic method. The method assumes that the values constitute a valid distribution. In order to obtain a statistical defensible distribution, large numbers of small scale tests almost by definition must dominate the determination of effective porosity in this methodology. Large numbers of large scale tests are not practical to conduct.

Hydraulic continuity does not have to be demonstrated with the stochastic approach but the method tacitly assumes that it exists along all flow paths that are generated by the model. This approach assumes that the distributions of hydrogeologic properties are valid and that flow paths are continuous in any direction proceeding away from the repository. Demonstrating hydraulic continuity is an additional bonus obtained by conducting large scale tests in the moderate to high hydraulic conductivity environments. The presence of hydrogeologic boundaries which could restrict flow or act as preferential pathways ordinarily would not be reflected in the stochastic approach because the scale of testing would be too small as a consequence of the requirement that a large number of tests be conducted in order to obtain a statistically defensible input distribution for the model.

5. Deterministic Groundwater Travel Time Models

It is not the purpose of this paper to present the rationale used in implementing a purely deterministic model for estimating ground water travel time. The previous discussion compares the general characteristics (and clarifies the differences) of the data requirements for the purely deterministic approach and the stochastic approach. A discussion of purely deterministic travel time predictions is best served by a separate paper.

6. Stochastic Groundwater Travel Time Models

Several stochastic approaches are available for estimating groundwater travel time as shown in current professional practice. All of these approaches are based on a stochastic analysis of the hydrogeologic framework of some groundwater flow model, which by definition is partially deterministic, at least in its geometric framework.

6.1. Mean and Variance of Hydrogeologic Properties Applied to Deterministic Models

The most simple and direct of these methods involves a mathematical combination and propagation of the mean and variance of input hydrogeologic properties to estimate a mean and variance of the output variable (travel time). In this case no assumptions are mandated about the shapes of the distributions for the input random variables. Simplifying assumptions, particularly about geologic conditions and about the conceptual flow model, make this procedure general and very approximate at best. The basic steps involved in such an analysis include the following:

1) Establish or define a deterministic model of the hydrogeologic framework, which typically is described by one equation or a series of equations that relate measurable (or estimable) input random variables (hydrogeologic properties) to the desired output variable (travel time).

2) Measure or predict the mean and variance of each input coefficient that is to be treated as a random variable.

3) Use established theorems, transformations, and relationships among random variables to combine them for predicting the mean and variance of the output variable (travel time). In most cases rearrangement of input terms must occur or simplifying assumptions must be made.

If desired, the sensitivity of the output variable to each of the input variables can be assessed by using a variety of acceptable mathematical methods.

6.2. Linear Combinations of Hydrogeologic Coefficients Applied to Deterministic Models

A second approach is more limited in terms of flexibility of the stochastic model, but it does provide a cumulative frequency distribution of the output random variable. The key restriction in this approach is that the output random variable (travel time) must be considered as a linear combination of the input random variables. This limitation dictates that simplifications be made (such as assuming that some of the input coefficients are constants), which may be unacceptable from a rational technical viewpoint. Basic steps in this stochastic approach are:

1) Construct a mathematical model consisting of one or more equations that contain linear combinations of hydrogeologic coefficients that eventually lead to the prediction of the output random variable (travel time).

2) Estimate the distribution of each input hydrogeologic coefficient that is being treated as a random variable. This process may be accomplished

by collecting a sufficient number of data values that is sufficient to define a defensible distribution.

3) The distribution of the output random variable then may be estimated by using accepted analytical or numerical procedures.

4) Estimate exceedance probabilities for groundwater travel time using the predicted cumulative frequency distribution.

The above stochastic models rely on conceptual flow models that are relatively simple and that infer stationarity and homogeneous conditions throughout the hydrogeologic units in the area of interest. Thus, the hydrogeologic coefficients are treated as random variables that vary throughout the unit, but the variation is similar in all locations. This approach corresponds to a geostatistical range of influence equal to zero distance. Hydrogeologic information from large-scale tests would yield data that correspond to these assumed conditions. Modeling of inhomogeneities and spatial correlations requires input from large numbers of tests, which in essence implies small scale tests.

Unless some complexity is incorporated into the above models (which may not always be possible), there is no capability for modeling multiple hydrogeologic units and the random flow paths that cross their boundaries. In order to include the effects of such flow paths and the effects of hydrogeologic property spatial correlations (nonzero range of influence), some type of computer simulation is needed.

6.3. Simulation Approaches

The type of hydrogeologic simulation, and the associated assumptions on which it is based, is determined by the scale of available hydrogeologic information. Thus, we can distinguish two broad categories of simulations: those related to relatively large-scale test results (on the order of several hundred meters to several kms) and those related to small-scale test results (on the order of a few meters or less).

6.3.1. Simulations Based on Homogeneous Zones

The first category of simulations relies on the assumption of hydrogeologic homogeneity over defined regions or zones. Input data for such simulations are obtained from intermediate scale to large scale tests, provided enough tests can be conducted. There are two general methods of simulation, which are related to respective assumptions on hydrogeologic conditions.

Method 1: Hydrogeologic coefficients (treated as random variables) in a particular hydrogeologic unit are considered to be statistically homogeneous over a large area ("globally stationary"). That is, the estimated distribution of a given random variable is the same throughout the entire area of interest. During the computer simulation process, for a given "pass," or iteration, the sampled value (realization) of the random variable is assumed to be the same everywhere within the hydrogeologic unit within the study area.

Method 2: Hydrogeologic properties in a particular hydrogeologic unit are considered to be statistically homogeneous over sub-regions in the study area ("locally stationary"). That is, the estimated distribution of a given random variable is the same throughout a particular sub-region, but the distribution can vary from one sub-region to the next. During the computer simulation process, for a given "pass," or iteration, a value of the random variable must be sampled for each specified sub-region. One disadvantage of this method is that abrupt changes in values of hydrogeologic coefficients can occur at sub-region boundaries, which is not a typical, realistic situation unless lithologic contacts or major faults have been mapped.

Sophistication can be added to either of the above methods by incorporating the intercorrelations among input random variables and/or the spatial relationships among sub-regions.

6.3.2. Simulations That Incorporate Spatial and Cross Correlations

The second category of simulations also can be divided into two methods based on the amount of information available and the assumptions about hydrogeologic conditions. Each method requires a geostatistical analysis of the pertinent hydrogeologic properties to define their spatial relationships. Such an analysis requires considerable data, realistically which can only be obtained from small scale tests. Usually, this analysis involves the generation of variograms (functions that describe spatial variation) for point variables and the identification of statistical trends. If desired, cross-variograms also can be generated to study intervariable relationships. These spatial correlations and trends are essential inputs for a spatial simulation of input properties.

Method 1: The area of interest is discretized into zones or elements with dimensions that should be on the order of at least the smallest sampling area (determined by scale of test). For each simulation pass a set of values of a given hydrogeologic property is simulated so as to have the proper distribution and variogram. One value is assigned properly to each of the elements. The same is done for each of the other input coefficients that are treated as spatial random variables. Several computer methods are available for this type of two-dimensional simulation, including "turning-bands" type (Journel and Huijbregts, 1978), Fourier-domain type (Tahen, 1980), and random-coin type (Sironvalle, Feb. 1980).

An additional step can make the simulation even more unique to the local setting. The spatial simulation can be "conditioned" to original, known data values. Thus, a conditional simulation provides a set of values that has the proper distribution and variogram, and has values at data locations that agree with the measured data values.

Method 2: If correlations among random variables are to be incorporated in the computer study, then some type of co-simulation is required. In this case a suite of values for several random variables is simulated all at once so that each has its proper distribution and variogram, and each has the proper correlation with the other random variables in the simulation. A vector of properly correlated values (one for each random variable) is thus simulated for each of the discretized elements (or zones). A co-simulation also can be conditioned to the known data values.

The purpose of any of the above simulation methods is to provide a domain (probably two-dimensional) of hydrogeologic coefficients, either based on large scale or small scale information, that can be used in a standard flow model. This flow model should be established so as to describe adequately the in-situ conditions and expected groundwater flow behavior. At present, most flow models assume porous medium flow and use finite element (or finite difference) procedures or particle tracking procedures to predict a distribution of travel times across a simulated hydrogeologic domain (conceptual model or deterministic framework). Each simulation pass provides one realization (calculated value) of groundwater travel time; consequently repeated passes provide a distribution of predicted travel times. This distribution can be plotted as a cumulative frequency distribution curve, which has been interpreted to constitute an estimate of the travel time cumulative probability distribution function (cdf). Whether or not the distribution of simulated values includes the real travel time can never be determined because of the spatial randomness of hydrogeologic data that serve as model inputs and because of the uncertainty about the validity of the conceptual model. At any rate, the generated cumulative frequency distribution curve does not represent all of the uncertainty inherent in groundwater travel time prediction (see companion paper).

7. References Cited

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