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DRAFT GENERIC TECHNICAL POSITION ON GROUND WATER TRAVEL TIME (GWTT)

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DWM TECHNICAL POSITION
ON GROUND WATER TRAVEL TIME

1.0 Introduction

One of the NRC performance objectives for High Level Waste repositories, commonly referred to as the "ground water travel time (GWTT) objective", is stated in 10 CFR 60.113 (a)(2) as:

> "The geologic repository shall be located so that pre-waste-emplacement ground water travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years or such other time as may be approved or specified by the Commission."

The "disturbed zone" is defined in 10 CFR 60.2 as:

> "...that portion of the controlled area the physical or chemical properties of which have changed as a result of underground facility construction or as a result of heat generated by the emplaced radioactive wastes such that the resultant change of properties may have a significant effect on the performance of the geologic repository."

The "accessible environment" is defined in 10 CFR 60.2 as the atmosphere, land surface, surface water, oceans and the portion of the lithosphere that is outside of the controlled area. For purposes of this GTP, the "controlled area" is defined (consistent with the Final EPA high level waste rule 40 CFR 191) as extending no more than 5 kilometers from the original emplacement of the waste in the disposal system, with a maximum surface area of no more than 100 square kilometers.

The Disturbed Zone definition and ground water travel time (GWTT) objective were established as part of a multiple barrier approach to high level waste isolation. The Disturbed Zone criterion is intended to prevent the reliance on only the zone directly adjacent to the engineered facility for the major portion of geologic barrier protection, and to avoid the complication of consideration of coupled processes close to the emplaced High Level Waste when demonstrating compliance with the GWTT performance objective. The Disturbed Zone is being addressed by the NRC staff's Generic Technical Position which is presently under review. As the Commission stated when it proposed its technical criteria for licensing activities at geologic repositories (46 FR 35280, July 8, 1981), the GWTT objective should be viewed as a conceptually simple measure of the overall quality of the geologic setting.

It is generally agreed that ground water is the most likely means by which significant quantities of radionuclides could escape a High Level Waste (HLW) repository. Transport of radionuclides to the biosphere then depend on factors which are directly related to the travel time of ground water from the engineered facility to the environment. The 1000 year GWTT objective helps to assure that ground water conditions are favorable, since a repository in compliance with the GWTT performance objective will be influenced by regional hydrogeologic processes (which are characterized by long travel times), rather than any local, relatively fast-moving ground water.

Releases of radionuclides through ground water pathways is limited by the three primary barriers:
(1) the integrity of the waste package and overpack;
(2) the speed of the ground water; and
(3) the geochemical interaction of the radionuclide with the rock along the path of ground water movement.
The present technical position deals only with the second barrier. The concept of ground water travel time encompasses all physical phenomena associated with pre-waste-emplacement water movement along the path, including advective flow, dispersion and diffusion, but not geochemical effects (e.g., sorption). Waste package and geochemical considerations are covered in other technical positions.

The staff has endeavored to present in this Technical Position a workable definition of the pre-waste-emplacement ground water travel time objective to be used for HLW repository licensing. The definition will assist the staff in evaluating compliance of a specific site with the performance objectives of 10 CFR 60. This Technical Position is however intended to be guidance only. It reflects the Staff's interpretation of the GWTT objective, but does not prevent the Applicant or others from advancing alternative interpretations.

2.0 Interpretation of GWTT Objective

Compliance with the GWTT objective in 10 CFR 60.113 (a) (2) requires carrying out the following steps:

- Properly identifying and considering the pre-waste-emplacement environment and its potential spatial and short-term temporal variabilities;
- Identifying the fastest path of likely radionuclide travel; and
- Calculating the appropriate travel time along this path.

The staff recognizes the apparent contradiction in terms between the phrases "pre-waste-emplacement" and "path of likely radionuclide travel" in the definition of the GWTT objective. The staff intends these concepts to mean the paths radionuclides would be likely to take if they were released from the disturbed zone under pre-waste-emplacement conditions, as defined below.

2.1 Pre-Waste-Emplacement Environment

Pre-waste-emplacement pertains to conditions which exist prior to significant disturbance of the geological or hydrological setting by construction activities, or major testing activities capable of seriously disturbing the geologic setting. Restriction of the GWTT requirement to pre-disturbance conditions is in accord with the original intent of 10 CFR 60 to establish a straightforward criterion which is easily defined and determined. The present position does not deny the importance of post-waste-emplacement effects. Evaluation of ground water and radionuclide movement under post-waste-emplacement conditions will be required as part of the demonstration of overall compliance of the repository with the EPA standards (40 CFR 191) as implemented by NRC.

The site must be characterized and understood to the extent that the fastest path of radionuclide travel (Section 2.2) can be identified and the ground water travel time (Section 2.3) can be determined. The determination of GWTT will be for present day environmental conditions only. Short-term changes to the environment, (e.g., tens of years) which can be reasonably inferred from records in the vicinity of the site, such as cycles of wet and dry years, local flooding, changes in ground water and surface water use and irrigation practices, and any other factors that may alter hydraulic heads should be factored into the conceptual model for determining GWTT whenever practicable. Ground water systems which have been demonstrated to exhibit significant transient behavior for the period of record may have to be modeled in a time-dependent rather than a steady-state manner to demonstrate compliance with the GWTT requirement. The determinations do not have to take into account the long-term projections (e.g., thousands of years) of changes to the physical setting of the repository, such as earthquakes, changes to global climate, major changes to surface morphology or use of ground water and land.

2.2 Identification of fastest path of likely radionuclide travel

The paths from the disturbed zone to the accessible environment are to be described in a macroscopic sense. Paths must be potentially capable of carrying a significant quantity of ground water. In crystalline rocks, paths may consist of fractured, weathered or brecciated zones. In porous media, paths will generally consist of layers of porous, permeable sediments. Paths may also consist of fractured zones in consolidated porous media, but not individual fractures unless they carry a significant quantity of ground water. In a uniform medium, a distinct conduit for radionuclide transport may not be evident, in which case the path will be defined by the direction of the gradient. Several examples of paths for generic repositories are covered in Appendix B.

There may be several alternative conceptual models for the repository, each of which might determine a different path for radionuclide transport. For example, the designated location of the underground facility might be a dense rock layer with very low permeability. Although ground water flow might normally be very small in this layer, credible models could be developed indicating that major avenues of transport might exist in adjacent, more permeable layers with consequently shorter travel times. The analysis of GWTT therefore should explore paths for radionuclide transport defined by alternative conceptual models, unless they can clearly be demonstrated to be unlikely, preferably through direct measurements of hydrogeologic properties of the site. Data collection must be focused on identifying and quantifying paths so that there is a high degree of confidence that potentially faster paths have not been overlooked.

2.3 Ground Water Travel Time (GWTT)

Ground water travel time in this position is a random variable rather than a fixed quantity. It will be quantified as a probability distribution of the times of travel for non-reactive, non-decaying, infinitesimal tracer particles from the disturbed zone to the accessible environment along the macroscopic paths. The ground water travel time will be a random variable for several reasons:

- Dispersion - ground water travels only in the open spaces (pores, fractures) in the rock. There would be numerous possible individual particle trajectories within each path, each with a different travel time;

- Molecular diffusion - random movement of the water molecules on a very small scale allows water and solute molecules to diffuse into pores in the rock where there may be no net flow of the water. It is important to note that molecular diffusion is not caused by the tracer, but by the random movement of the water molecules. Therefore molecular diffusion is truly a property of the ground water and can be included in the present definition of GWTT. Molecular diffusion may be important in cases where there is appreciable matrix porosity and generally slow movement of ground water.

- Uncertainty - Measurement error or lack of data necessary to characterize the site adds uncertainty to the travel time estimates for the tracer particles. This uncertainty can be combined into the probability distribution of arrival times for tracer particles.

- Distributed source - The disturbed zone and accessible environment are defined as surfaces rather than points. Tracer particles released at different points along the disturbed zone will reach the accessible environment at different times. The GWTT should be determined for each of the paths representative of likely conceptual models such as those discussed in Section 2.2.

The estimation of GWTT must accommodate spatial variability, temporal variability and uncertainty.GWTT can be presented as a distribution for each of the paths in terms of a Cumulative Distribution Function (CDF), an example of which is shown in Fig. 1. This CDF will combine all spatial variability, temporal variability and uncertainty of the GWTT into a single curve for each of the paths. The CDF itself however is assumed to contain no uncertainty. It is important to note that the CDF does not deny the existence of uncertainty, but that all uncertainty is incorporated into the CDF. Spatial and temporal variability and uncertainty can theoretically be treated separately, but grouping them both into a single CDF has the advantage of simplicity. Compliance with the 1000 year objective would be demonstrated if it could be shown that any tracer particle leaving the disturbed zone has a (100-X)% or greater probability of arriving at the accessible environment in a time greater than 1000 years, where X is a small number. The basis for choice of X% is presented in Section 2.4. The 15th percentile is shown in the figures for illustrative purposes only. In all cases, the basis for the choice of the percentile cutoff must be adequately supported.

Overall, the identification of likely paths and reliable estimation of GWTT is strongly dependent on the adequate characterization of the hydrogeologic conditions between the disturbed zone and the accessible environment. Conceptualizations of paths will likely be simple during the early reconnaissance phase of site characterization. Continued characterization activities will produce more detailed and realistic conceptualizations of stratigraphy and geologic structure, which will lead to improved estimates of GWTT. Further discussion of the concept of GWTT and procedures for its calculation are presented in Appendix A.

2.4 Rationale for Choice of the Percentile of the Cumulative Distribution Function (CDF)

In applying 10 CFR 60.113(a)(2), the staff recognizes that ground water travel time along the paths defined for each conceptual model can be represented by the Cumulative Distribution Function (CDF) rather than a single value, because of uncertainty in understanding the hydrogeology of the site, measurement errors, temporal variations in flow, multiple particle trajectories and a spatially-distributed source. (A single-valued GWTT determined from conservative models and coefficients would also be acceptable to demonstrate compliance with the GWTT objective). Uncertainties in estimating these phenomena are expected to cause the GWTT distribution to span as much as several orders of magnitude. Phenomena leading to the distributed nature of the predicted GWTT are elaborated in Appendix A.

At the upper and lower limits of the GWTT distribution for each of the paths, there will be ground water travel times which, although possible, are so unlikely that they are inappropriate measures of GWTT. Consider for example the two hypothetical cases shown in Fig. 2 for which (1) all particles arrive at the same time, t' or (2) the particles arrive gradually after t'. The two curves in Fig. 2 could represent, for example, flow through a uniform fracture, with Case 1 representing plug flow and Case 2 representing plug flow with diffusion into the matrix (matrix diffusion is discussed further in Section 2.5.2). Case 2 would obviously be more favorable in terms of repository performance, but this fact could not be determined if the "first particle" or very small percentile criterion for GWTT had been chosen.

The choice of a higher percentile would distinguish between Cases 1 and 2 and give credit for the increase in GWTT to the matrix diffusion case. A choice of the percentile which is too high, say the median, T_{50} (the 50th percentile) may be insensitive to the variance. As shown in Fig.3 for the example of a steady, saturated flow field with log-normally distributed hydraulic conductivity, the median GWTT will be exactly the same for zero or infinite spatial correlations used in the computations (Clifton, 1984). Under the median GWTT criterion, sites which exhibit a wide variance of the travel time distribution either because of great spatial variability, dispersion, matrix diffusion, or uncertainty, would be treated as equals so long as they exhibited the same median travel time. In particular, the median GWTT gives little incentive to better characterize the site.

The above rationale limits the range of T to greater than a few percent and less than about 50%. The NRC staff will consider percentiles tending toward the lower end of this range to be satisfactory. Justification for the choice should be provided, considering the factors discussed above.

2.5 Special Considerations

2.5.1 Unsaturated Media

Ground water movement through unsaturated media for pre-waste-emplacement conditions differs from that of saturated media in a number of important ways:

1. In a medium unaffected by boundaries, the gradient and therefore the direction of unsaturated flow is predominantly vertical (confining features such as aquicludes, faults and dikes complicate this general picture). Saturated flow is primarily horizontal, except in areas of recharge or discharge.

2. Unsaturated flow tends to be more responsive to episodes of recharge than saturated flow.

3. Unsaturated flow parameters are highly nonlinear, and depend on the degree of saturation of the medium. This nonlinear dependence could also lead to changes in the flow trajectories for differing levels of saturation, e.g., saturation of fractures or creation of a perched water table.

The transient nature of flow in the unsaturated zone causes a certain difficulty in defining ground water travel time. There is a conceptually important distinction between an episodic recharge event in an unsaturated medium and nearly-steady ground water flow in a saturated medium. Even though there may normally be little downward flow through an unsaturated medium, it is conceivable that unusually heavy precipitation over a period of years could lead to short travel times during that period, at least through the unsaturated portion of the medium. The definition of GWTT as a cumulative distribution function allows the low probability, short travel time events to be fairly weighted with more-typical travel times.

Travel times would be weighted according to the intensity, frequency and duration of the event. The travel time distribution could be estimated, for example, from a transient ground water flow analysis, coupled with the transport of hypothetical tracer particles released at constant time intervals at points along the disturbed zone. The cumulative distribution in this case would incorporate time variability of recharge, as well as the spatial and temporal variability in path lengths. It should be noted however, that the estimation of parameters for unsaturated systems is considerably more difficult than for saturated flow, and may impose increased conservatism on the uncertainty analysis.

2.5.2 Matrix Diffusion

Fractured porous media may exhibit transport behavior characterized by a wide range of ground water travel times. A tracer moving through the medium may pass through the fractures relatively quickly, but will move through the pores in the rock mass between fractures much more slowly. The tracer will also move into and out of dead-end pores by molecular diffusion. The range of transport velocities through the fractured medium can vary by orders of magnitude. The effect of matrix diffusion is probably more significant in media with high matrix permeability and porosity than in relatively tight rocks, especially where ground water movement is very slow (Blencoe and Grisak, 1984). The diffusion of tracer into the rock matrix and dead end pores will also affect the concentration in the fractures, and will impart on the total system a retardation effect similar to "sorption" between the tracer and the rock, even though this is a physical rather than a chemical effect*.

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* This effect is enhanced by the mechanisms of radioactive decay and sorption, but GWTT will measure only the effects on a non-sorbing, non-decaying tracer. Furthermore, the division between chemical and physical effects is not always distinct, e.g., anion exclusion.

Therefore, it would not be correct to characterize the travel time through a dual porosity medium by the speeds at which the water is moving along the fractures alone, although this would undoubtedly produce a conservatively short measure of the ground water travel time. Mathematical models exist which account for the phenomenon of matrix diffusion in fractured media (e.g., Grisak and Pickens, 1980, NRC, 1985). The GWTT distribution could be calculated by looking at breakthrough curves generated for continuous or impulse source functions as described in Section A.4.1 of Appendix A.

3.0 Summary and Statement of Regulatory Position

3.1 Summary

ground water travel time is a measure of the merit of the geologic setting of a high level waste repository. The Staff recognizes that there may be alternative conceptual models of the site because of the inability to completely characterize it with the available data. This inability may lead to a multiplicity of paths for likely radionuclide travel. The ground water travel time along the paths will be a distributed quantity because of spatial variability, temporal variability, the distributed nature of the disturbed zone and accessible environment, and model or data uncertainty. Ground water travel time should therefore be represented as a cumulative probability distribution, although a single-valued GWTT would be acceptable if it were derived from appropriately conservative models and coefficients. The "pre-waste-emplacement ground water travel time along the fastest path of likely radionuclide travel" should be represented as a percentile of all travel times contained in the Cumulative Distribution Function (CDF) for each of the identified paths. Pre-waste-emplacement pertains to conditions at the site prior to any significant disturbance of the hydrological or geological setting such as construction activities or the effects of radioactive waste, and whose spatial and temporal variability can be reasonably inferred from historical records at or near the site. Testing activities capable of altering the pre-waste-emplacement environment should be taken into consideration. The analysis must take into account any information pertaining to preferential points of release from the Disturbed Zone, and consider reasonably likely conceptual models which might lead to transport through other paths.

3.2 Statement of Position

It is the staff's position that in demonstrating compliance with ground water travel time performance objective of 10 CFR 60.113, DOE should do the following:

1. Determine the paths of likely radionuclide travel for the site as described in Section 2.2 and Appendix B.

2. For each of the paths, determine the pre-emplacement ground water travel time as described in Section 2.3 and Appendix A.

3. Select the fastest such travel time so determined.

Appendix A - Calculation of the ground water Travel Time (GWTT)

A.0 Introduction

This section gives guidance on how to calculate the GWTT distributions for each of the identified macroscopic paths defined by conceptual models considered. Section A.1 describes the utility of hypothetical tracer particles and uses the concept to illustrate why there would be a distribution of travel times rather than a single value.

Section A.2 describes several mathematical modeling schemes which could be used to calculate the GWTT distribution. Section A.3 discusses the various methods for estimating parameters, quantifying their uncertainties, and choosing the input for the mathematical models on the basis of the available data. Section A.4 discusses a particular approach to calculating the GWTT distribution by applying a Monte Carlo sampling scheme to a deterministic mathematical model.

Finally, Section A.5 describes how simplified analyses may be used in some cases to satisfy the GWTT performance objective without having to resort to complicated analyses.

A.1 Travel Time Distributions

It is useful in subsequent discussions to think of the radionuclides as consisting of discreet particles, although it should be recognized that these are figurative rather than real. A single "particle" of radionuclide leaving the disturbed zone would generally follow the path traced by the moving ground water, except for phenomena such as molecular diffusion and chemical interaction. Molecular diffusion would cause random motion to be added to the trajectory of the particle, allowing it to move into areas such as pores with little or no net flow. Chemical interaction with the surrounding rock would cause the radionuclide particle to leave the ground water and become fixed temporarily or permanently in or on the surface of the rock. We restrict all subsequent discussion in this Technical Position to transport of the tracer without considerations of geochemical effects. Such effects are covered in another regulatory position (Bradbury et.al., 1985).

Along any "path" as defined in Section 2.2 and Appendix B, there will be natural spatial variability in the properties of the medium; e.g. porosity, hydraulic conductivity. The tracer particles moving in the ground water will follow trajectories governed by the hydraulic properties of the medium and the driving forces at their location. The more uniform the medium, the more parallel will be the trajectory of the tracer particles. Conversely, the tracer particles in a heterogeneous medium may diverge from their neighbors for certain types of heterogeneity, following trajectories of least resistance which are not necessarily the shortest trajectories.

Particles will arrive at the accessible environment at the time determined by the length and velocity along the trajectory along which they are being transported. The GWTT distribution will be determined by the number of particles released at the disturbed zone and their individual travel times.

Unsaturated media are somewhat more complicated than saturated media. Not only the speed but the trajectory of tracer particles could change with time as a result of a change in boundary conditions or flow parameters in the unsaturated case. For example, in a fractured porous medium, conditions of high infiltration could cause certain fractures to fill with water and establish paths not present during periods of lower infiltration.

A.2 Mathematical Representation of the Repository and its Environment

Analysis of the GWTT for any real repository must depend on methods of indirect inference from observations of hydrogeologic data at the site. Artificial tracers are useful in some cases, but the time and distance scales are too great for direct characterization of a HLW repository by such methods. Naturally-ocurring isotopes and those produced from atmospheric weapons testing and nuclear reactors can be used for ground water dating to support estimates of travel time distributions for real sites. Such techniques should be used whenever possible, although investigations must usually resort to mathematical models of the repository for predictions of performance.

Values of travel time from the disturbed zone to the accessible environment are usually obtained from mathematical models consisting of the equations governing the hydraulic potential, flow of ground water, and transport of a tracer. There are many models for ground water flow in various media which are based on the equations at steady state or transient conditions in one, two or three dimensions. A major issue in modeling strategies for determining the GWTT distribution is whether to use deterministic or stochastic models. This is discussed below.

A.2.1 Deterministic Models

Deterministic models consist of equations whose solution is based on the assumption that the parameters, e.g., hydrogeologic properties, initial conditions and system geometries, are known. Uncertainty and variability of the data are usually taken into account by obtaining many solutions, each one based on a different statistical realization of the parameter set. such simulations are generally known as "Monte Carlo" simulations. The results obtained by applying many random realizations of the parameter sets to the mathematical model can then be statistically analysed in order to estimate the travel time distribution (Smith and Schwartz, 1980, Smith and Schwartz, 1981, Clifton, 1984). Alternatively, the model may be used with conservative values of the input parameters in order to obtain conservative estimates of the GWTT.

A.2.2 Stochastic Models

Stochastic models deal with the variability and uncertainty of the data in a more direct way. The coefficients and variables of the equations are treated as random processes rather than deterministic quantities. The PDE's are solved indirectly in terms of the moments of the dependent variables (e.g., mean and variance). This technique has the advantage of requiring only one solution rather than the numerous Monte-Carlo solutions required for the deterministic approach. Direct stochastic approaches to modeling are at a much less developed state than Monte Carlo techniques, although it is an area of rapid development. The stochastic approaches have been used to estimate means and variances of fields such as head (Mizell et.al.,1982), pore velocity (Devary and Doctor, 1982), and concentration (Gelhar and Axness, 1983). They have apparently not yet been used to calculate directly such spatially integrated properties as GWTT. It might be possible to determine the GWTT distribution directly from concentration estimates by the approach discussed in Section A.4.1.

Both the deterministic and stochastic approaches have their strengths and weaknesses. Either approach is acceptable, so long as it is well justified. The use of a deterministic model in a Monte Carlo approach is outlined in Section A.4.

A.3 Site Characterization from Field Data

Four levels of parameter quantification for site characterization can be stated (ONWI, 1983):

- Bounding value estimates - the range of possible values of the parameter. This is usually an extreme values of a range of parameters which does not take into account the correlation of the parameter with other parameters.

- Best estimate values - a single value of the parameter which is based on field measurements, laws of physics, expert opinion, or combinations of the above.

- Interval estimates - a bounding estimate which has been tempered by field data, laws of physics, expert opinion or combination of the above. Correlations of the parameter may be taken into account (e.g., relationships between porosity and hydraulic conductivity).

- Probability density functions (PDF's). A function in which the probability that the parameter exceeds a certain value is known.

The PDF is of course the most informative quantification of the parameter, but requires the most knowledge of the site. In those cases where the data are too sparse for direct inference, rough estimates of the variability of parameters in the field may be inferred during early phases of the site characterization from expert opinion and observations of the distributions of the parameter in similar rock masses. For example, parameters such as hydraulic conductivity are often observed to follow a log-normal distribution, and conform to certain models of the spatial covarience function (Neuman, 1982). Expert opinion is not a substitute for field data, however.

Both data gathering and modeling depend on the establishment of a good conceptual model for the site. The conventional quantification of aquifer hydrogeologic parameters (i.e., transmissivity, storativity, hydraulic conductivity, effective thickness, etc.) is based on a framework of established assumptions. Significant departures from this ideal case will yield nonrepresentative values of the quantities sought.

Errors may be introduced because the collected data are misinterpreted. For example, water levels determined by a steel tape may be interpreted incorrectly because of temperature or salinity differences in the wells (ONWI, 1983). Another example might be the misinterpretation of transmissivities (hydraulic conductivities) from a drawdown test caused by phenomena such as leakage from another aquifer or a boundary of low permeability (e.g., fault or dike) within the cone of depression. In these cases, the principal cause of error is once again, the inadequacy of the conceptual model. The degree of sophistication for the model will frequently be limited by the availability of data.

Overall discussions of parameter estimation should include discussions of the reasonableness, within the known hydrogeologic regime, of all key assumptions. The likely effects of erroneous assumptions on parameter estimation and GWTT calculations should be discussed. The NRC recognizes the importance of expert opinion in providing defensible interpretations of all types of aquifer field testing.

A.3.1 Treatment of Uncertainties in Site Characterization

There are many possible sources of uncertainty in the estimation of the characterization of the site for determining GWTT. Among the most likely sources are:

- Measurement Errors in Data. These errors may be procedural (e.g. human) errors or systematic errors caused by faulty or improperly calibrated instruments. The staff recommends that these types of errors be minimized and quantified by standard techniques such as calibration, redundancy, and by using several independent ways of obtaining the same data (e.g., using both a neutron probe and tensiometer for moisture content).

- Validity of Analytical Assumptions (Conceptual Model) for Site Simulation The simulation of flow and transport may not be representative of the physical system because of a poor understanding of the basic physical phenomena or oversimplification because of computational expediency. For example, the equivalent porous media (EPM) approach is often used to represent a fractured medium as a porous medium. The EPM approximation may be useful only for large scale transport, and not valid at scales in which the effects of individual fractures are important (Long et.al., 1982). Some investigators question the validity of the EPM approximation for properly modeling transport along the direction of fracture orientation regardless of scale (Endo,et.al., 1984). The validity of the conceptual model for simulating the site is closely coupled to the conceptual model used for interpreting site data.

  The staff recommends that alternative conceptual models be proposed and tested in order to determine the sensitivity of the results to the choice of the conceptual models which can reasonably be constructed from the available data.

- Interpretation of Sparse Data. The temporal and spatial distribution of hydrogeologic field data are always less dense than desired. Conditions between field measurements must be inferred, either by interpolation, fitting of a surface through the data points, or using a physically-realistic model to infer the data. Sophisticated interpolation methods such as Kriging (e.g., Matheron, 1971) yield an estimate of the variance as well as the mean of spatially varying data. Mathematical models may be adjusted manually in order to produce a best fit to the available data (e.g., Fogg, 1978, Mercer and Faust, 1980). In some cases, the fitted parameter may be determined automatically without the need for manual adjustment. Statistical inverse methods are available for fitting the hydraulic conductivity to head data in saturated media, and also calculate the variance of the hydraulic conductivity (e.g., Neuman and Yakowitz, 1979, Hoeksema and Kitanidis, 1984).

- Computational Errors. Since computer codes must be used extensively, errors may be introduced because of mathematic approximations (e.g., element size, step size) and intrinsic errors such as round-off and truncation. Computer codes should be verified with analytical solutions, validated with real field data, and compared or benchmarked with other similar computer codes (Silling, 1983). The sensitivity of the results to node size, time steps, grid orientation, or other parameters and assumptions should be tested by computational experiments.

A.3.2 Determination of the Input Data for the Model.

Once the conceptual model has been coded into a computer program, the computations must be performed with parameters inferred from the available data in order to generate the GWTT distribution. The types and quality of data available will determine how the computations are to be performed. For example, if only a few data points are available for a particular parameter, a conservative estimate of that parameter may have to be made and carried through the calculations. With more data, a mean and variance of the parameters can be calculated and used with a simple sampling approach (ONWI, 1983). If the site is well-characterized, spatially varying properties of the parameters can be generated, permitting conditional simulations or stochastic models to be applied.

The GWTT computed using this general guidance will be sensitive to the degree of characterization of the site. That is, investigators of poorly-characterized sites will be forced to use conservative or at least overly-wide estimates to represent the distribution of the input parameters. Sites that have been tested with valid drill and test programs based on defensible conceptual models will facilitate the development of a more defensible GWTT distribution function. The GWTT distribution with smaller variance is preferable for the reasons stated in Section 2.4 of the Position.

A.4 Estimating GWTT from Deterministic Models with Randomly-Generated Input

The GWTT distribution can be calculated from multiple runs of deterministic models, with each run made for a realization of the data which can be inferred for the site. In the steady-state saturated flow example, each realization of the data requires the solution of the hydraulic head and velocity field. This is generally accomplished by solving the PDE's using techniques such as finite differences or finite elements. Once the velocity field is known, travel time distributions can be calculated by simulating the release of tracer particles from single or multiple locations along the Disturbed Zone and count their arrival times as they reach the accessible environment (Nelson, 1978).

Alternatively, the tracer could be represented as a continuum by solving the time-dependent PDE for solute transport of a tracer. Flux or concentration boundary conditions for the PDE could be specified at the disturbed zone in order to simulate equally-weighted or preferential points of release. The travel time distribution would be extracted from the knowledge of input of tracer to the model and the concentration calculated at the accessible environment (see Section A.4.1).

A.4.1 Treatment of Spatial Variability

A large part of the variability of GWTT is caused by spatial non-uniformity of the parameters which determine ground water movement, particularly hydraulic conductivity and effective porosity. The motion of hypothetical tracer particles leaving the disturbed zone will be determined by the gradient, hydraulic conductivity and effective porosity encountered along the path. This variability alone will cause the paths of the particle leaving different parts of the disturbed zone to diverge. Added to this phenomenon is the incompleteness of the data which determine flow paths within the hydrological regime and uncertainty due to measurement errors in field data.

If the site is fairly-well characterized, it is generally worthwhile to take the spatial variability of the parameters into account, since the analyses will yield a smaller variance of the GWTT distribution. This will give a higher estimate of the (small) percentile criterion for GWTT than a distribution with a higher variance.

At least one method, conditional (or unconditional) simulation, has been applied to account for the spatial distribution and uncertainty of field data in the determination of GWTT. This method has been applied to 2-dimensional steady state, saturated flow models for equivalent porous media (e.g., Delhomme, 1979, Clifton and Neuman, 1982), but could be adapted to three dimensions (Mantoglou and Gelhar, 1985). The procedure is outlined below for the 2-dimensional, steady state case (Clifton, 1984):

a. Determine Spatial Variability and Uncertainty of Data

Field data for hydraulic conductivity and porosity are collected, and evaluated by methods of statistical inference in order to determine their spatial covariance and drift, which are measures of the variability of the property in space, and the "nugget effect," which is an indication of the measurement error or uncertainty. Expert judgement based on prior knowledge of the properties of rocks in similar formations may be useful in estimating the proper covarience models to apply to these data in this step (Mantoglou and Gelhar, 1985).

b. Generate Realizations of Data

Random fields of the model parameters are re-generated from the spatial covariances, drift, and uncertainties determined in Step a, so that the spatial covariances and auto-covariances of the new field or "realization" are identical to those determined for the original data. It is usually necessary to treat the random variable and boundary conditions as "ergodic", for which the principles of first and second order stationarity apply. Cross correlation of the data, e.g., correlation between effective porosity and hydraulic conductivity, may be taken into account in this step. Two widely-used procedures for generating these random fields are the "nearest neighbor" method (Smith and Freeze, 1979) and the "turning band" method (Mantoglou and Gelhar, 1985). The random fields can be forced to comply with the original data by a process known as "conditioning;" otherwise, the parameter fields are "unconditional". Conditional simulations reduce the variance considerably, but are generally worthwhile only if there are sufficient high-quality data (Clifton, 1984).

c. Run Deterministic Model for Heads

The random fields are used with a finite difference or finite element model to generate a steady state head and ground water flow field under the influence of either fixed or random boundary conditions.

d. Calculate Travel Times of Particles

The trajectory of tracer particles is tracked from one or multiple locations on the disturbed zone along the postulated paths, to the plane representing the accessible environment. The travel time of the particles from their starting position to the accessible environment is recorded.

e. Generate Multiple Realizations

Steps b through d are repeated numerous times in order to generate a large number of travel times for multiple tracer particles so that their cumulative distribution can be drawn. The probability of each realization is taken to be equal to any other realization for the purpose of constructing the CDF.

A continuum model of tracer transport, as discussed in Section A.4 could be used for the calculation in Step d of the above procedure. An impulse or step function input of an inert tracer would be simulated to travel from the disturbed zone to the accessible environment along the path. These models may be more suited to investigating the phenomena of unsaturated flow and matrix diffusion. The response of the mathematical model to an impulse forcing function will yield the residence time density function, E(t) (Seinfeld and Lapidus, 1974), which is defined:

$$E(t) = C(t) \, / \int_0^\infty C(z)\, dz$$

where C(t) is the observed concentration at time t.

The integral of E(t) over time would be the CDF of the GWTT distribution for the system and the particular realization of the data. Travel time distributions could also be obtained directly by using a step forcing function and observing the normalized "breakthrough" concentration at the accessible environment. The GWTT distribution would be averaged with those for other realizations of the Monte Carlo simulation.

The above example was for a two-dimensional steady state case. It would not necessarily be suitable for determining GWTT in transient cases or for those calculations where three dimensional phenomena are overwhelmingly important.

A.5 Simplified Analysis

The user is not required to generate a detailed CDF of the GWTT distribution. A simplified approach would be acceptable, provided that the 1000 year GWTT objective could be met and the results could be demonstrated to be conservative. Alternatively, it has been shown that in the (conditional or unconditional) simulations outlined in Section A.4.1, high spatial covariance of hydraulic conductivity correlates with wider travel time distributions (Clifton, 1984). If the medium is assumed to be spatially uniform (i.e., infinite spatial covariance), then it must be assumed that all variations of the parameters are caused by measurement error. The GWTT distribution is widest under these circumstances, which gives a conservative indication of the T_x estimate of the CDF (but not necessarily T_{50}).

Appendix B - Choosing paths of radionuclide travel

B.0 Introduction

The paths which radionuclides will follow from the disturbed zone to the accessible environment are to be described in a macroscopic sense. In crystalline rocks, paths may consist of fractured, weathered or brecciated zones. In porous media, paths will generally consist of layers of porous, permeable sediments. Paths may also consist of fractured zones in consolidated porous media. In a uniform medium, a distinct conduit for radionuclide transport may not be evident, in which case the path could be defined by the direction of the gradient.

There may be several alternative conceptual models for the repository, each of which might determine a different path for radionuclide transport. The analysis of GWTT therefore should consider all paths for radionuclide transport defined by alternative conceptual models, unless they can clearly be demonstrated to be unlikely. Collection of data at the site must be directed to identifying these paths, establishing the validity of the conceptual models for interpreting and simulating the hydrogeology, and making a reasoned determination that potentially faster paths have not been overlooked.

Examples for several generic types of repository media are given in the sections below.

B.1 Repositories in saturated media

High Level Waste underground facilities located in saturated media will usually be emplaced in a rock unit of low permeability. More permeable units may underlie and overlie the repository horizon, however, as shown in Fig. B.1. Some of these horizons may intersect the disturbed zone. While there may be little movement of ground water in the host rock, there may be factors which could cause the movement of radionuclides from the disturbed zone to these more permeable horizons. Transport between horizons could be by fracture or porous flow under the driving force of natural hydraulic gradients. The fastest paths should therefore follow the horizons which have the highest ground water velocities.

The choice of the path need not be mechanistic; e.g., it is not necessary to propose or calculate the mechanisms by which transport from the horizons intersected by the disturbed zone to the faster horizons can occur (unless credit will be taken for the travel time from the disturbed zone to the horizon). It may be necessary, however, to determine whether such paths are "likely", or can be excluded from consideration. For example, an analysis could determine that the driving force would be inadequate to allow transport to other horizons above a certain level, even if the necessary interconnections existed. Therefore, these horizons would not be on "likely" paths and could be ignored. Even for "likely" paths, such analyses might allow quantification of travel times along the portion of the path from the disturbed zone to the assumed horizon.

B.2 Unsaturated media

Definition of paths for repository sites in unsaturated media will differ from those in saturated media. The direction of flow is likely to be vertically downward until the water table is reached. In some cases, the path may be defined in terms of the direction of the gradient, unless there are barriers to flow such as contrasts in hydraulic conductivity leading to perched water tables. The possibility of perched water under reasonably conceivable conditions (e.g., a series of wet years which are not a major climatic change, but could occur under present climatic conditions) should be explored, even if such conditions currently do not exist at the site. Paths should also consider the possible connections of perched water to fractures or other structural features of the site which would allow short-circuiting of the unsaturated material in which the repository would be placed. Phenomena peculiar to unsaturated flow such as "fingering" should also be considered. Examples of such paths are illustrated in Fig. B.2.

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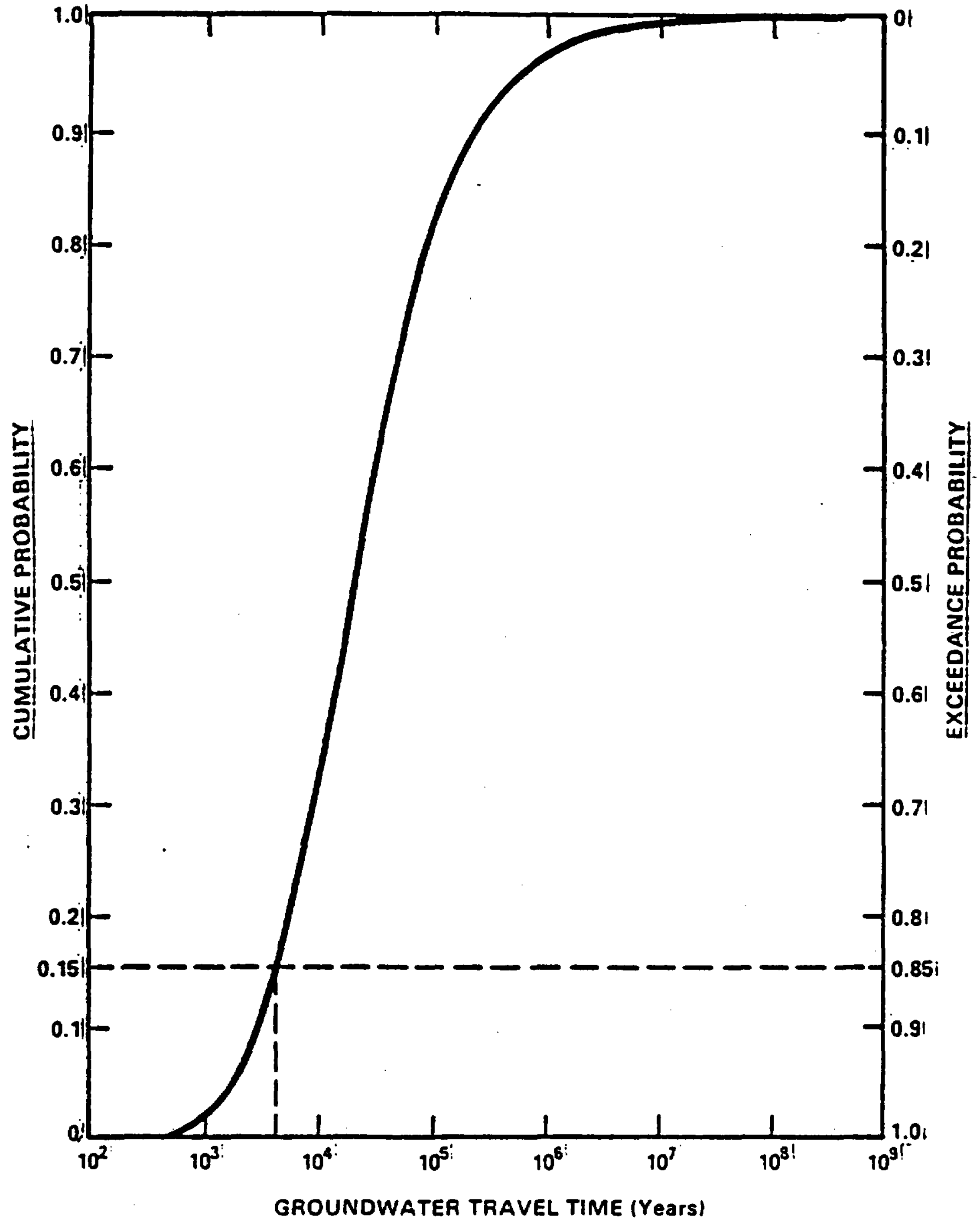

Figure 1 - Ground Water Travel Time Distribution

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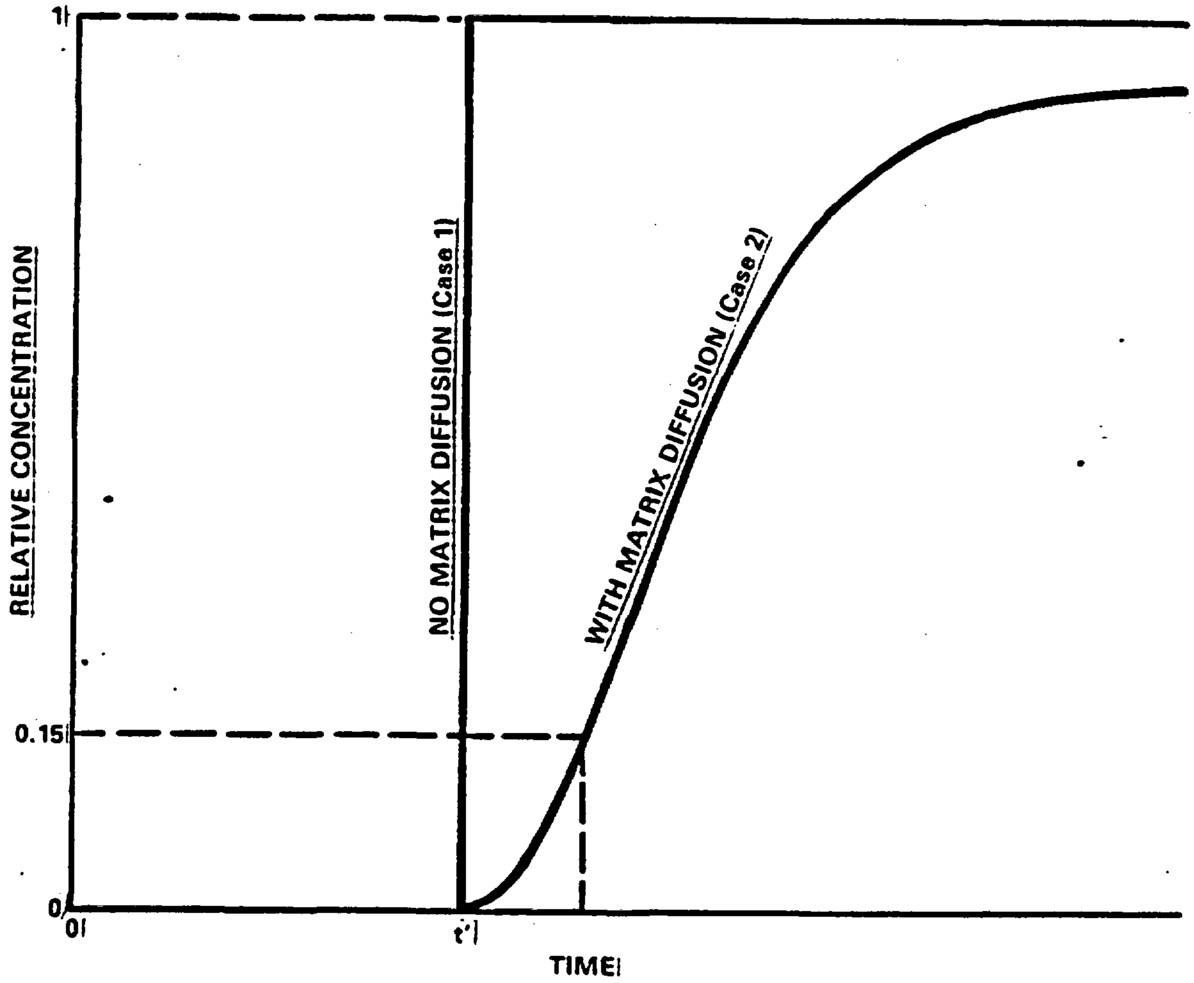

Figure 2 - Breakthrough Curve for Fracture
With and Without Matrix Diffusion

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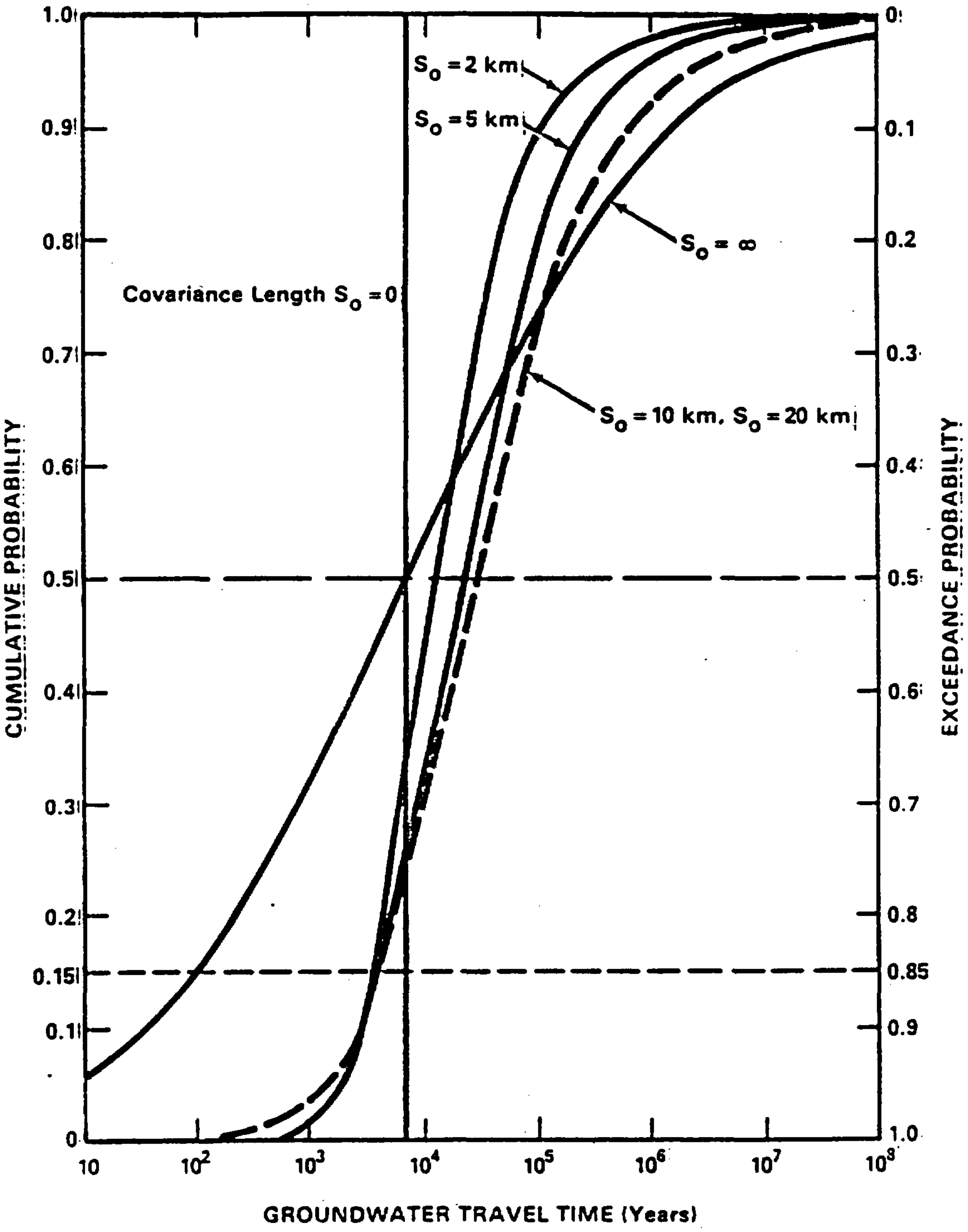

Figure 3 - Effect of Spatial Covariance Length for Hydraulic Conductivity (Clifton, 1984)

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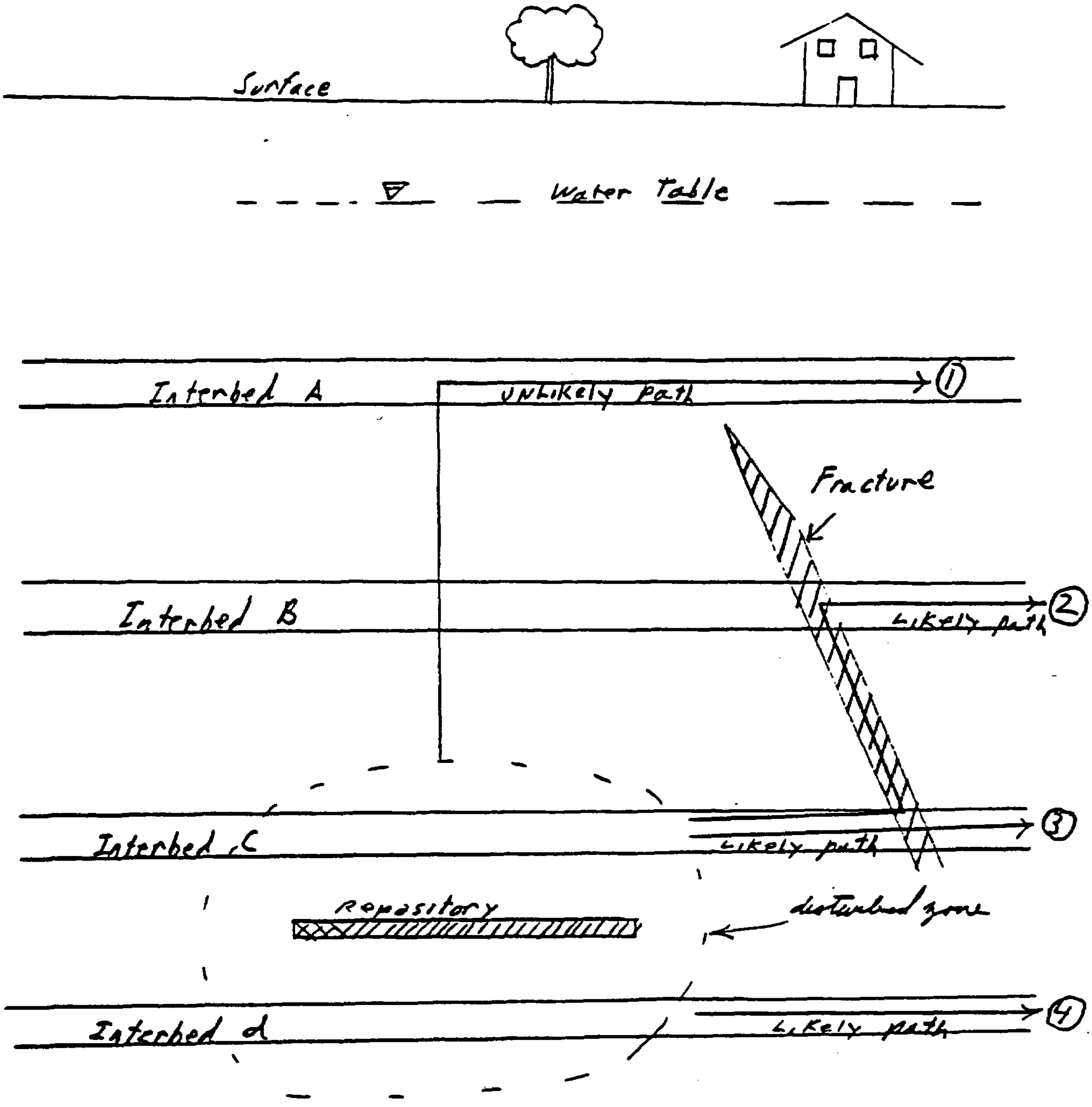

Figure B.1 - Definition of Paths in Saturated Media

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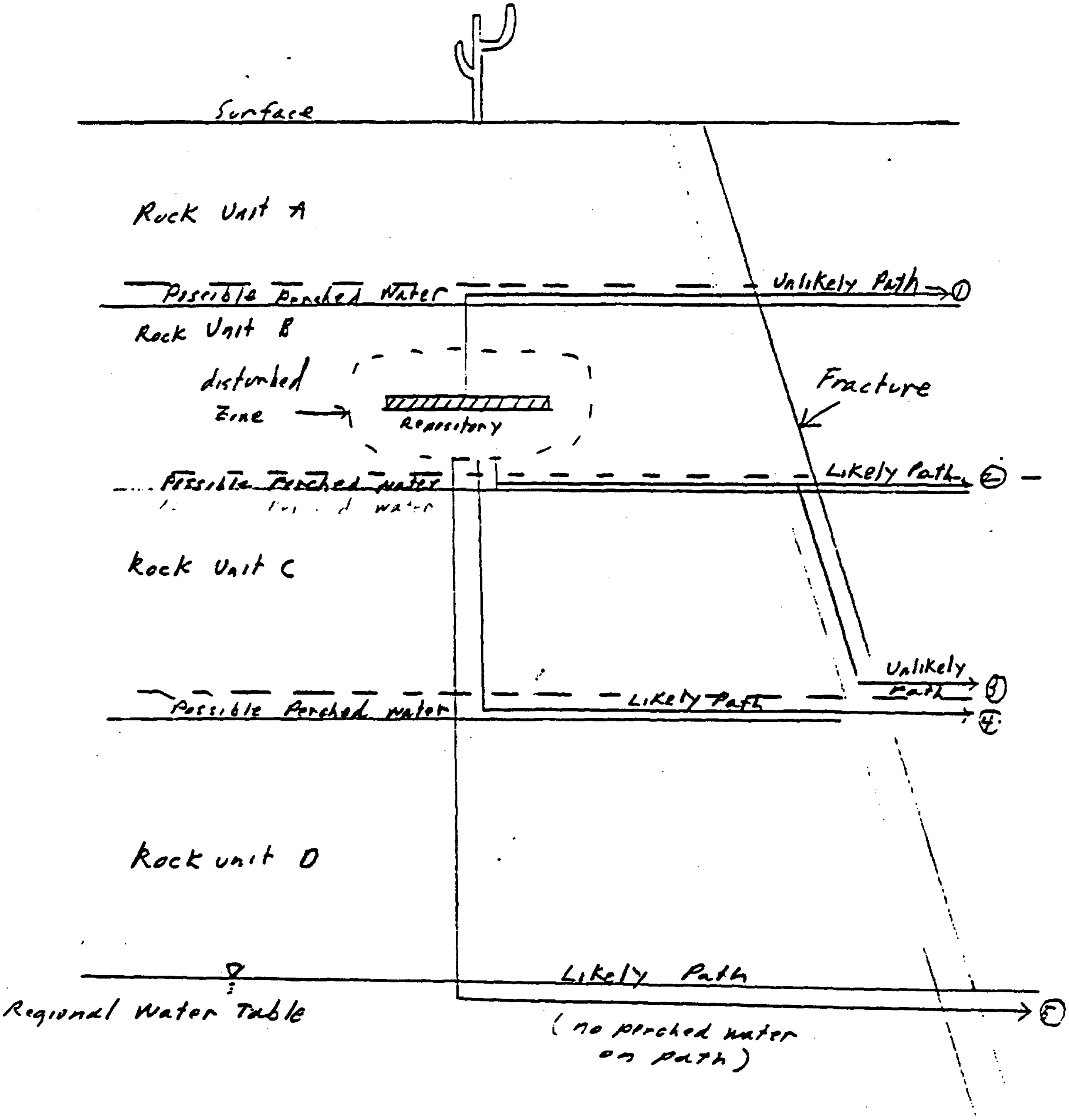

Figure B.2 - Definition of Paths in Unsaturated Media