The Role of Dispersion in Radionuclide Transport - Data and Modeling Requirements

Revision No.: 1

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List of Acronyms and Abbreviations

ADE	Advective dispersion equation
CAIP	Corrective Action Investigation Plan
CAU	Corrective Action Unit
CTRW	Continuous-time random walk
DOE	U.S. Department of Energy
fBm	Fractional Brownian motion
FGE	Forced-Gradient Experiment
fGn	Fractional Gaussian noise
FPTD	First passage time distribution
HSU	Hydrostratigraphic Unit
lnK	Natural logarithm of hydraulic conductivity
K	Hydraulic conductivity
K_d	Distribution coefficient
KH	Hydraulic conductivity at land surface
km	Kilometer
ld	Depth decay
m	Meter
m^2/day	Square meters per day
m^2/yr	Square meters per year
m^2/s	Square meters per second
NDEP	Nevada Division of Environmental Protection
NTS	Nevada Test Site
PDF	Probability density function
1-D	One-dimensional
2-D	Two-dimensional

1.0 Introduction

This document is the collaborative effort of the members of an *ad hoc* subcommittee of the Underground Test Area Project Technical Working Group. The subcommittee members are Keith Halford, U.S. Geological Survey; Ahmed Hassan, Desert Research Institute; Ken Rehfeldt, GeoTrans Inc.; Paul Reimus, Los Alamos National Laboratory; and Andrew Thompson, Lawrence Livermore National Laboratory. Additional comments were provided by H.J. Turin, Los Alamos National Laboratory. Each subcommittee member provided valuable insights into the role of dispersion in radionuclide transport data and modeling. The objective of this document is to synthesize all of these insights.

Dispersion is one of many processes that control the concentration of radionuclides in groundwater beneath the Nevada Test Site (NTS). The Nevada Division of Environmental Protection (NDEP) has commented in several letters about the need for site-specific data related to transport parameters. In particular, they discuss the need for dispersivity data from the Pahute Mesa Corrective Action Unit (CAU). In a December 20, 1999, letter from Mr. Paul Liebendorfer (NDEP) (Liebendorfer, 1999) to Ms. Runore Wycoff (U.S. Department of Energy [DOE]) in regard to the NDEP review of the *Corrective Action Investigation Plan, Corrective Action Units 101 and 102: Western and Central Pahute Mesa, Nevada Test Site, Nevada*, NDEP presents two comments specific to dispersion:

1. “CAU-Specific Diffusivity/Dispersivity Data – The CAIP-PMR1 does not set forth CAU-specific diffusivity or dispersivity data. (Model input parameters derived from assumed probability distribution functions (pdfs) are not to be equated with actual CAU-specific field or laboratory data. Note also that the term “CAU-specific” means in and on the boundaries of CAUs 101 and 102 as they currently exist). This lack of CAU-specific information is a deficiency to be remedied.”
2. On p. 34 of the document, the statement is made that: “No site-specific investigations of dispersion have previously been conducted at Pahute Mesa, however, longitudinal dispersivity values were estimated from the three tracer tests conducted within or near the NTS (Borg et al., 1976; Neuman, 1990; Daniels and Thompson, 1984).” On p. 109 of the document is a discussion of a study of “...dispersivity observations from 59 different field sites, domestic and abroad.” Attempts to use non-CAU specific data in place of CAU-specific data for a CAU-specific model, particularly when the needed data do not exist for the CAU in question, are not acceptable. Pahute Mesa CAU-specific measured dispersivities, which are likely different for each pollutant and contaminant, are needed.

These comments define NDEP's desire for dispersivity values from experiments conducted within the boundaries of the Pahute Mesa CAU. The Pahute Mesa Corrective Action Investigation Plan (CAIP) did not present results from the BULLION Forced-Gradient Experiment (FGE), but did describe the experiment. NDEP is aware of the BULLION experiment, but apparently considers that data insufficient to address their concerns. To address the NDEP comments, DOE would need to perform a number of field-scale dispersion measurements on Pahute Mesa. Dispersion measurements typically require elaborate and expensive field experiments.

1.1 Purpose of the Technical Basis Document

The purpose of this technical basis document is to: (1) define dispersion and its role in contaminant transport, (2) present a synopsis of field-scale dispersion measurements, (3) provide a literature review of theories to explain field-scale dispersion, (4) suggest approaches to account for dispersion in CAU-scale radionuclide modeling, and (5) to determine if additional dispersion measurements should be made at this time.

1.2 Organization of the Document

The document is organized into six sections.

- [Section 1.0](#) presents this introduction.
- [Section 2.0](#) defines dispersion and presents some simple examples. The intent of [Section 2.0](#) is to provide the basic terms and concepts needed to understand later sections.
- [Section 3.0](#) is a literature review. Data are presented that document the apparent scale dependence of dispersion. Theoretical approaches to explain the scale effect are also presented. The theoretical approaches contain some highly technical topics without a great deal of explanation. The intent of the theoretical section is merely to provide the reader with a survey of the wide range of approaches available and to highlight similar concepts. The interested reader is encouraged to consult the references for further information.
- [Section 4.0](#) discusses application of scale-dependent dispersion to the NTS work. Results of previous modeling studies are presented along with some recommendations for handling scale-dependent dispersion.
- [Section 5.0](#) is the summary, conclusions, and recommendations for future measurements.
- [Section 6.0](#) is the reference list.

2.0 Definition of Dispersion

The general concepts of dispersion are presented in this section. These concepts lay the ground work for the theories presented in later chapters.

2.1 Classical Description of Dispersion in Homogeneous Porous Media

Early descriptions of dispersion in porous media were presented in terms of groundwater flow and contaminant transport in homogeneous porous media. This is what we will term “classical dispersion” and provides a good way to introduce basic concepts. In the simplest terms, dispersion is the process of spreading a contaminant over a volume that is larger than it would have occupied by advection alone. This simple definition combines two related concepts, pure spreading and mixing.

Pure spreading can be visualized in terms of a contaminant volume being preserved at a small scale, but where the contaminant is spread in a twisted and contorted manner via mechanical means. This is often referred to as “mechanical dispersion.” [Figure 2-1](#) is a schematic diagram of this process.

The perception of mechanical dispersion is related to the scale of observation. Consider the three scales of observation presented in [Figure 2-1](#). At each scale, the concentration of contaminant in water is an average value over the observation interval. At the smallest observation scale (labeled A in [Figure 2-1](#)), the concentration at the downgradient end may be nearly the same as the upgradient end, or may be zero. Observations at this scale will be discontinuous and would describe the spreading process as a complicated mechanical process. Characterization of contaminant movement at observation scale “A” requires a large number of detailed measurements and is typically not feasible in most situations.

The second scale (labeled “B” in [Figure 2-1](#)) is typical of field observations. At this scale, observations near the source will show higher concentrations of contaminant than observations further downgradient. The channels with contaminants are now interspersed with uncontaminated water via mechanical means; thus, a composite water sample will mix contaminated water with uncontaminated water, the result being a decrease in bulk concentration. Observations at this scale will show mechanical dispersion of the contaminant.

The third scale (labeled “C” in [Figure 2-1](#)) is very large. At this scale, upgradient and downgradient average concentrations may be the same (after the leading edge of the plume has passed) and perceived mechanical spreading is negligible. At

Figure 2-1
Schematic Representation of Mechanical Dispersion

this observation scale, the spreading of a developing plume would be evident at the downgradient plane because the breakthrough of contaminant would arrive at different times for each small channel. It is important to recognize that at typical scales of observation, mechanical dispersion is the result of averaging a smaller scale mechanical process.

Mixing is the process of dilution and volumetric growth caused, for example, by molecular diffusion. Dispersion, defined as spreading, is the combined process of mixing and volumetric (or cross-sectional) averaging of pure spreading at a downgradient location.

Mathematically, dispersion is represented by a dispersion coefficient, D , with units of length squared per time (L^2/T) and is taken as the sum of mechanical dispersion and effective diffusion:

$$D = D' + D_d^* \quad (2-1)$$

where

D' = The mechanical dispersion
 D_d^* = The effective diffusion coefficient.

In multidimensional systems, the mechanical dispersion coefficient and the dispersion coefficient (using the relationship in Equation 2-1), are defined with respect to the direction of flow. Longitudinal dispersion (D_L) is in the direction of flow and transverse dispersion is perpendicular to the direction of flow. The transverse dispersion is further subdivided into a horizontal transverse dispersion coefficient (D_T) and a vertical transverse dispersion coefficient (D_V). The mechanical dispersion coefficients are often represented as the product of a dispersivity (α) and mean groundwater velocity in the x -direction (v).

In multidimensional systems, it is common to align the x -coordinate with the direction of flow and to represent the dispersion coefficient as a tensor, with the form: (2-2)

$$D = \begin{bmatrix} \alpha_L v + D_d^* & 0 & 0 \\ 0 & \alpha_T v + D_d^* & 0 \\ 0 & 0 & \alpha_V v + D_d^* \end{bmatrix}$$

The effective diffusion component (D_d^*) is the product of the diffusion of the contaminant in water (D_o) times an empirical coefficient to account for the solid phase that occurs in aquifers. The empirical coefficient is meant to account for tortuosity and porosity in the porous medium. Freeze and Cherry (1979) give a typical range of values for the empirical coefficient of 0.01 to 0.5. Therefore, pure diffusion in an aquifer is from 2 to 100 times less efficient than in water alone. A reasonable range of the effective diffusion coefficient is 1×10^{-11} to 1×10^{-9} square meters per second (m^2/s) (Freeze and Cherry, 1979). The other component of the dispersion coefficient is the mechanical dispersion coefficient.

Mechanical dispersion is caused by velocity variations at scales less than the scale of observation. In homogeneous porous media, the velocity profile in pores, and the varied small-scale paths around grains leads to velocity variations. Citing earlier work on laboratory columns, Marsily (1986) defines a relationship between D' and D_d^* that depends on the mean grain diameter and the mean groundwater velocity. Defining the Peclet number as vd_m/D_d , where v is the mean groundwater velocity, d_m is the mean grain diameter, and D_d is the free water diffusion coefficient, the relative importance of dispersion and diffusion is approximated by the curve in Figure 2-2. In Region I, the Peclet number is so small that diffusion dominates over mechanical dispersion. Region II is a transition region where both processes are important. In Regions III and IV, mechanical dispersion dominates. In Region V, Darcy's Law may no longer be valid according to Marsily (1986). The Peclet number for most groundwater problems lies in Regions III and IV, thus mechanical dispersion is the dominant component of the dispersion coefficient for most groundwater problems.

Figure 2-2
Ratio of Mechanical Dispersion to Effective Diffusion as a Function of Peclet Number

2.2 Dispersion in Flowing Groundwater

The physical processes that control the flux of a contaminant are advection and dispersion. The equation governing the migration of a nonreactive contaminant in saturated, homogeneous, isotropic porous media under steady uniform flow in the x -direction is given by:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - v_L \frac{\partial C}{\partial x} \quad (2-3)$$

where:

- C = The concentration
- D_L = The longitudinal dispersion coefficient
- v_L = The average linear groundwater velocity in the x -direction

In many applications, the mechanical dispersion coefficient in [Equation 2-1](#) is much larger than the effective diffusion coefficient. In these cases, the dispersion coefficient and the mechanical dispersion coefficient are equivalent.

The time rate of change in concentration (left-hand side of the equation) is a function of the dispersive term (first term on the right-hand side) and the advective term. Written in this form, the dispersive flux has been represented as the product of the longitudinal dispersion coefficient and the concentration gradient in the x -direction. This representation of the dispersive flux is analogous to Fick's second law of diffusion (Bear, 1988) and is commonly referred to as Fickian dispersion. For two-dimensional transport with steady uniform flow in the x -direction, an additional term would be added to [Equation 2-3](#), which is the product of the transverse dispersion coefficient and the second derivative of concentration in the transverse (y) direction.

2.3 Examples of Dispersive Transport

Domenico and Schwartz (1990) provide several clear examples of dispersion at typical observation scales. Consider a one-dimensional (1-D) column with water flowing through it at a steady rate ([Figure 2-3a](#)). If a contaminant of concentration C_0 is introduced at one end ([Figure 2-3b](#)), it will travel through the column. In the absence of dispersion and diffusion, the contaminant will travel as a plug, or piston, at the velocity of the water. At the exit boundary ([Figure 2-3c](#)), the concentration will be zero until the instant the plug arrives, then the concentration will jump to $C/C_0 = 1$. In reality, as demonstrated by numerous column experiments, the leading edge of the contaminant does not remain sharp, rather it begins to spread. This zone of spreading is small at small distances of travel, and grows as the distance increases. At the exit boundary, the concentration will be

Figure 2-3
Example of a Dispersion Experiment in a One-Dimensional Column
 (Modified from Domenico and Schwartz, 1990)

zero until the zone of spreading begins to arrive. Concentration will increase as the zone of spreading passes, eventually reaching the value of C_0 ($C/C_0 = 1$).

At the exit boundary of this 1-D column experiment, the contaminant concentration is the averaged concentration over the cross-sectional area of the column. Recalling the concept of pure spreading, one could envision the contaminant transport as a large number of small cross-sectional stream tubes, each with a contaminant concentration nearly equal to C_0 (diffusion prevents the concentration from being exactly equal to C_0). The contaminant in each of these stream tubes does not travel at the same velocity; therefore, at the exit boundary, the contaminant in the stream tubes arrive at different times. As the first contaminant arrives, it is averaged over the entire cross-sectional area and the average concentration appears to be small. As the contaminant in more stream tubes arrive, the average concentration increases.

In this simple 1-D example, the contaminant can spread only in the direction of flow. The size of the zone of spreading in the direction of flow is a function of the dispersion coefficient. The zone of spreading can be identified as the region where $C/C_0 < 1$ and $C/C_0 > 0$. In practice, the breakthrough curve approaches both $C/C_0 = 0$ and $= 1$ asymptotically. Therefore, the zone of spreading is typically defined by fixed endpoints such as $C/C_0 > 0.05$ and $C/C_0 < 0.95$. The concentration behind the zone of spreading is constant at $C/C_0 = 1$ (i.e., at steady state) because no lateral spreading is allowed.

Consider this same 1-D column, but with a finite pulse of mass injected into the upstream end (Figure 2-4a). At selected times after the injection (times t_1 and t_2), cross sectional average concentrations would yield the displayed distributions of average concentration as a function of distance from the injection end of the column. As that pulse moves through the column, it spreads forward and backward. At time t_1 , the pulse is wider than when it started and the peak concentration is decreased. At a later time, t_2 , the pulse is wider still and the peak concentration is further reduced. The spreading of the pulse is due primarily to mechanical dispersion and averaging of observations across the cross section of the column.

When transverse spreading is allowed to occur (multidimensional transport), which is the case in nearly all natural systems, the concentration behind the longitudinal zone of spreading also decreases because mass spreads laterally. Examples of two-dimensional (2-D) dispersion are presented in Figure 2-4b for instantaneous and continuous source functions. In this case, the contaminant can be viewed as having been introduced at one location in the 2-D domain. For the instantaneous source, a pulse of finite concentration over a small volume of the aquifer is introduced at time $t = 0$. As the contaminant moves ($t = t_1$ or $t = t_2$), it spreads symmetrically about the center of mass, and the peak concentration decreases in magnitude. The pulse spreads more in the direction of flow than in the direction perpendicular to it, indicating that the longitudinal dispersive flux is larger than transverse dispersive flux. Therefore, dispersion is greater in the direction of flow than perpendicular to flow. The center of mass moves at the

a) Variation in Contaminant Concentration in One Dimension

Instantaneous Source

Continuous Source

b) Variation in Contaminant Concentration in Two Dimensions

Figure 2-4
Example of Dispersion of a Pulse of Contamination in One and Two Dimensions

average linear velocity of the groundwater. The distance traveled by the center of mass is given by:

$$d = vt \quad (2-4)$$

where:

- d is the distance
- v is the average linear velocity of groundwater
- and t is the time since contaminant was introduced

For the continuous source, contaminant is introduced at a constant rate in a steady, uniform flow system resulting in constant concentration with time at the injection location. At time $t = t_1$, given by the darker shaded plume, the leading edge of the plume has traveled as far as in the pulse injection case. Behind the leading edge, concentrations remain elevated back to the source along the center line of the plume. At time $t = t_2$, the plume has traveled farther downgradient, and is now longer and wider than at earlier times.

In this continuous source case, concentration gradients in the longitudinal direction are small except near the leading edge of the plume. Thus, longitudinal dispersion is occurring primarily at the leading edge of the plume. In the transverse direction, the transverse concentration gradient is large along the entire length of the plume. The transverse concentration gradient, coupled with the large surface area of the plume, suggests that a significant dispersive flux occurs transverse to the direction of flow despite the fact that transverse dispersion coefficients are typically smaller than longitudinal dispersion coefficients.

Domenico and Schwartz (1990) state that transverse dispersion leads to decreased concentrations ($C/C_0 < 1$) everywhere away from the source of the plume, whereas longitudinal dispersion will only cause spreading at the frontal portions of the plume as in the 1-D column example. A continuous source does not need to be of a constant concentration, but rather could vary with time. An example of a situation on the NTS where a continuous source of contaminant might be appropriate is the dissolution of melt glass, which will introduce radionuclides into the flow system for a long period of time (although not necessarily at a constant rate).

The spread of contaminant about the center of mass is a function of both mechanical dispersion and effective diffusion, but is dominated by mechanical dispersion in most situations. In the discussion below, it is assumed that the dispersion coefficient and the mechanical dispersion coefficient are essentially the same. For simplicity, the discussion is in terms of the dispersion coefficient. The spreading can be described by a variance in space (see the standard deviation, σ_L , in [Figure 2-4a](#)). In 1-D, the variance (σ_L^2) characterizes the longitudinal

dispersion and the ratio of one half the variance to time is a constant termed the dispersion coefficient:

$$D_L = \frac{\sigma_L^2}{2t} \quad (2-5)$$

If the velocity is uniform and constant (steady flow), the dispersion coefficient, D_L , can be represented by:

$$D_L = \frac{\sigma_L^2}{2x} v \quad (2-6)$$

Typically, D_L is represented by the product of longitudinal dispersivity (α_L) and velocity, then dispersivity is represented by:

$$\alpha_L = \frac{\sigma_L^2}{2x} \quad (2-7)$$

As noted by Domenico and Schwartz (1990), the spatial variance can be transformed into a temporal variance (σ_t^2) which can be determined from a breakthrough curve. In this case, the longitudinal dispersivity is defined as:

$$\alpha_L = \frac{v\sigma_t^2}{2t} \quad (2-8)$$

Dispersion in directions transverse to the direction of flow can also be defined in a manner similar to [Equation 2-5](#):

$$D_T = \frac{\sigma_T^2}{2t} \quad (2-9)$$

In [Equation 2-9](#), the transverse direction could be either horizontal or vertical. In contrast to the longitudinal dispersion, there is no simple conversion to eliminate the transverse spatial variance and replace it with the temporal variance because the mean velocity in the transverse direction is zero. Additionally, some caution may be necessary when representing transverse dispersion as a purely mechanical process. Transverse dispersion, particularly in the vertical direction and in slowly flowing groundwater, may be of a similar magnitude as effective diffusion.

2.4 Other Factors Influencing Observed Dispersion

To this point, the discussion of dispersion has been limited to nonreactive contaminants being transported under uniform flow conditions in homogeneous porous media. In real aquifer systems, many contaminants decay or react with the aquifer material, the flow conditions may not be uniform, other physical processes such as matrix diffusion may be occurring, the aquifers are composed of fractured rock, and may be very heterogeneous. The impact of each of these factors on the spreading of contaminants, if unrecognized or not included in the analysis, will often be lumped into dispersion. This complicates the assessment of dispersion and will be discussed in more detail in [Section 3.0](#).

2.5 Concluding Remarks Related to Classical Dispersion

Classical dispersion, typically viewed as the spreading of contaminants in relatively uniform porous media, can be summarized by:

- Dispersive flux in flowing groundwater is characterized by a Fickian process where the flux is a product of a dispersion coefficient and the concentration gradient.
- The dispersion coefficient is the sum of a mechanical dispersion coefficient and a diffusion coefficient.
- Mechanical dispersion dominates at larger Peclet numbers, but diffusion is more important at very small Peclet numbers. In most groundwater systems, mechanical dispersion dominates.
- Mechanical dispersion can be viewed as the averaging of processes and variations that occur at scales smaller than the current scale of observation. This subscale velocity variation is present regardless of the scale of observation. Thus one could expect that the magnitude of the mechanical dispersion would increase with increases in observation scale because larger and larger mechanical processes are being averaged.

3.0 Literature Review

The literature review provides a sample of the work to date and provides guidance for application of dispersion to the NTS and the Pahute Mesa CAU modeling task.

3.1 Measured Dispersivities

Several summaries of measured dispersivities have been published in the literature. The most recent summaries of measured dispersivity data are presented by Gelhar et al. (1985 and 1992) and Neuman (1990). Figure 3-1 (Shaw, 2003) is a plot of the longitudinal dispersivity from Gelhar et al. (1992) with new data added from studies conducted since the publication of the original plot in 1992. Gelhar et al. (1992) examined the data and noted the following observations:

- Each data point represents the apparent dispersivity that has evolved to that particular scale, with each data point being one interpretation. Scale represents the distance between the source and point of observation.

Figure 3-1
Longitudinal Dispersivity Versus Tracer Test Scale Classified by Porous or Fractured Media

- With few exceptions, the data do not represent snapshots of dispersivity as a function of scale of an evolving plume at a single site. The instantaneous dispersivity of an evolving plume at a particular location will not be the same as the apparent dispersivity applied uniformly over the entire distance of travel. The reader is directed to Freyberg (1986) or Garabedian et al. (1991) for examples of multiple snapshots of an evolving plume at a single site.
- There is not a clear difference in dispersivities measured in fractured versus porous media.

Gelhar et al. (1992) also ranked the reliability of the dispersivity data based on how the test was conducted, the adequacy of data collection, and the method of analysis. Figure 3-2 is a plot of the longitudinal dispersivity with reliability indicated. Gelhar et al. (1992) concluded:

Figure 3-2
Longitudinal Dispersivity Versus Tracer Test Scale
(Modified from Gelhar et al., 1992)

- If reliability of the values is ignored, the data appear to increase indefinitely with scale.
- Many of the large-scale, low reliability results come from application of numerical models. Numerical dispersion is often undocumented in many modeling applications. If numerical dispersion is present, it may lead to underestimates of the dispersivity (for calibrated models) because only a portion of the spreading is due to the dispersivity (the remainder is undocumented numerical dispersion). In other cases, large dispersivities

were used for numerical stability reasons unrelated to actual observations. Thus, the reliability of dispersivities from numerical models is low.

- When only the most reliable data are used, the trend is still present, but it is not clear how to extrapolate it to large scales. The largest high reliability, longitudinal dispersivity is about 7 meters (m) at a distance of near 300 m.
- At any scale, the range of values is about 2 to 3 orders of magnitude wide. A portion of the range may be due to errors in the data caused by any number of factors such as poor data and inappropriate method of analysis (Gelhar et al., 1992). The remainder of the range can be explained by existing stochastic theory in which dispersivity is proportional to the product of variance and correlation scale of the natural logarithm of hydraulic conductivity. The range of values may simply represent differences in heterogeneity from one site to another.

An analogous plot from Neuman (1990) for longitudinal dispersivity is similar to [Figure 3-1](#) because it is based on similar, but not identical datasets, and has the same basic trend of values that increase with increasing scale. Neuman (1990) did not assess reliability of the data, but did attempt to show how universal scaling hypotheses could be used to explain the data. The universal scale will be discussed in more detail later in this report.

[Figure 3-3](#) is a plot of horizontal transverse dispersivity. A similar plot of vertical transverse dispersivity is provided in [Figure 3-4](#). As with longitudinal dispersivity, these plots present apparent dispersivity for plumes that have evolved to a particular scale. There are far fewer transverse dispersivity values for several reasons. First, field-scale measurements of transverse dispersivities usually require a natural gradient experiment which are very costly to perform. Second, in the vertical direction, most numerical modeling studies do not treat vertical transverse dispersivity as independent of horizontal transverse dispersivity. It is clear from these plots that transverse dispersivities are smaller than longitudinal values. In addition, the transverse dispersivities also appear to be scale dependent. However, the large-scale behavior is quite different for high reliability data versus other data. The high reliability data are all relatively small scale (up to a few hundred m); therefore, extrapolation to large-scale behavior of transverse dispersivity is difficult based on observed data.

The transverse dispersivities for porous and fractured media may be different. The four largest transverse horizontal dispersivities in [Figure 3-3](#) are from fractured rock formations as is the largest transverse vertical dispersivity in [Figure 3-4](#). This may suggest the transverse dispersivity is larger in fractured formations than in porous formations. However, the data from fractured formations are ranked as either low or intermediate reliability. Thus, a firm conclusion regarding transverse dispersivity in fractured formations cannot be drawn.

The summary plots represent a composite of results from many different field experiments and display apparent dispersivity of an evolving plume as a function of scale, with one problem represented by one data point. Some field tests have

Figure 3-3
Transverse Horizontal Dispersivity Versus Tracer Test Scale
(Modified from Gelhar et al., 1992)

provided multiple “snapshot” observations of the evolving dispersion process (see below) that suggest dispersivities may grow with an increasing scale of displacement up to a particular asymptotic dispersivity value. It is probably not reasonable to assume that the data in [Figure 3-2](#), [Figure 3-3](#), and [Figure 3-4](#) at scale “x” are indicative or representative of “snapshot” observations. However, these plots are useful and provide a general confirmation that large-scale, longitudinal, dispersivity values appear to be appropriate for larger scale problems. The large-scale behavior of transverse dispersivity is unclear based on the observed data.

However, as noted by Gelhar et al. (1992), these plots do not define how, or if, longitudinal dispersivity grows with distance at any particular field site. To address this question, several detailed natural gradient field experiments were conducted. Two such experiments, one at the Borden site (Freyberg, 1986; Sudicky, 1986) and another at the Cape Cod site (Garabedian et al., 1991), demonstrated that dispersivity grew with distance at the beginning of the test, then reached asymptotic values as stochastic theories at the time had predicted. At the Borden site, Freyberg (1986) noted that at the largest distance, a large-scale heterogeneity was encountered and the dispersivity again began to increase. A counter example is presented by Moltyaner and Killey (1988a and b). They did not observe scale-dependent dispersion at their Chalk River site over distances of 20 to 40 m and found field-scale values comparable to laboratory-obtained values. The reason for the apparent lack of scale dependence of dispersivity at the Chalk River site is not clear, but this observation appears to be atypical.

Figure 3-4
Transverse Vertical Dispersivity Versus Tracer Test Scale
 (Modified from Gelhar et al., 1992)

These field studies suggested that longitudinal dispersivity does reach an asymptotic value after a short travel distance. However, this conclusion is not easily transferable to other sites. The Borden, Cape Cod, and Chalk River sites are all relatively clean sand and gravel aquifers with small degrees of heterogeneity compared with other locations. In fact, as shown by Garabedian et al. (1991), the dispersivities from the Borden and Cape Cod sites are the smallest measured for their respective scales.

At the MADE site in Columbus, Mississippi, a different situation was observed. The MADE site is very heterogeneous compared with the Borden and Cape Cod sites. As a result, much more spreading was observed. Adams and Gelhar (1992) interpreted the asymmetric spreading of the plume as being caused by advection and dispersion in a converging nonuniform flow field. They concluded that a dispersivity on the order of 5 to 10 m was appropriate if the nonuniform flow effects were modeled directly. If nonuniform flow is ignored, a dispersivity of nearly 70 m is obtained. Two important observations can be drawn from the MADE site. First, dispersivity appears to increase with increasing heterogeneity as stochastic theory predicts; and, second, ignoring nonuniform flow caused by the larger scale heterogeneity leads to much larger dispersivities.

To appreciate the impact of nonuniform flow on the calculation of dispersivities, consider a simple 2-D example. Figure 3-5 is a schematic cross section of a confined aquifer with heterogeneity described by two distinct zones, one of high

Figure 3-5
Schematic Cross Section of an Aquifer with Multi-Scale Heterogeneity

velocity (Region 2) and one of lower velocity (Region 1). This difference in velocity creates a nonuniform flow field. Within each region, there is similar small-scale heterogeneity. Consider injection of tracer in an upgradient well and migration to a downgradient observation well. The observation well is constructed such that it can sample Regions 1 and 2 independently, but can also sample the whole aquifer. The breakthrough curves at the bottom of the figure present the result. If the nonuniform flow is recognized, the transport in each region can be analyzed separately. The breakthrough curves from Regions 1 and 2 are similar in shape, but offset in time because of the different velocities. Each curve would produce a dispersivity value representative of the small-scale variability in each region. If the nonuniform flow is not recognized and a composite sample of the observation well is used, the composite breakthrough curve will show greater spreading with time than either of the curves from either region alone. The interpreted dispersivity from the composite breakthrough curve will be based on an average uniform velocity and will be larger than the dispersivity from either region alone.

This nonuniform flow example highlights the link between observation (or application) scale and dispersivity. Two predictive models of contaminant transport at the observation well could be developed. One model would have a single mean uniform velocity and a larger dispersivity, while the alternative model would have a separate mean velocity in each region and two smaller dispersivities values. In both cases, the integrated concentration breakthrough curve at the observation well would be similar. Incorrect results would be obtained if the region-specific dispersivities were applied with a single uniform velocity or if the larger dispersivity from the composite breakthrough analysis were used in region-specific predictions.

Another aspect of the MADE site is noteworthy. It was observed that at early time, the estimates of mass in the aquifer were up to 3.5 times the injected mass. At later time, the total mass was calculated to be 50 percent of the injected mass. In addition, although the center of mass moved slowly downgradient, the peak concentrations lagged well behind the center of mass. Harvey and Gorelick (2000) have reinterpreted the MADE data with a model that uses the nonuniform flow field proposed by Adams and Gelhar (1992), but allows rate-limited diffusion into low permeability regions. As a result, they did not need to invoke large-scale dispersion to account for the observed shape of the plume. This raises an interesting possibility. If the magnitude of heterogeneity gets very large, as at MADE, then perhaps the classic single-porosity, large dispersivity model is no longer valid. In the case of MADE, Harvey and Gorelick (2000) developed what amounts to a dual-porosity approach. They did not attempt to estimate a dispersivity to use with their model, but presumably it would be smaller than the value of 5 to 10 m estimated by Adams and Gelhar (1992). The issue of highly heterogeneous sites is addressed later in this report.

The ability of the uniform flow, nonuniform flow, and dual-porosity models to reproduce field-scale transport at the MADE site highlights the fact that different model conceptualizations and parameter sets may each produce acceptable representations of the behavior of the system. It is important to recognize that identification of a single optimal model will not be possible in data-limited

situations, and multiple conceptual models should be considered. Although each conceptual model will acceptably reproduce observed data, the predictions of each model may be quite different. Uncertainty analyses will need to consider a broad range of possibilities, especially if data to constrain the models are sparse.

3.1.1 Features of Observed Field-Scale Dispersivity

Longitudinal and transverse dispersivity have been shown to vary with scale. In all cases, the transverse dispersivities are smaller than the longitudinal dispersivities. At mildly heterogeneous sites (Cape Cod, Borden, Chalk River), the dispersivities appear to reach relatively small magnitude asymptotic values. At more heterogeneous sites (MADE), the magnitude of the longitudinal dispersivity is larger, but the experiments were too small to determine large-scale behavior. Carefully planned and conducted tracer experiments are not available for scales greater than 300 m or so. Dispersivity data at larger scales (greater than 300 m) are not as reliable; therefore, there is considerable uncertainty regarding the appropriate dispersivity values for large scales. The appropriate dispersivity at large scales cannot be definitively determined from current data.

3.1.2 Data Transferability

Figure 3-6 is a plot of the longitudinal dispersivities with the data from NTS highlighted. This indicates that the NTS-specific data (Shaw, 2003) fall within the range of other data, suggesting that there is nothing unusual about the aquifers in and around the NTS with respect to dispersive behavior.

3.2 Theoretical Studies Addressing Scale-Dependent Dispersion

This subsection presents a sampling of the theoretical studies that have addressed scale-dependent dispersion. The general concepts are presented followed by specific issues.

3.2.1 General Concepts

Over the past 20 years, a great many theoretical studies have been undertaken to explain the observation that dispersivities obtained from field measurements are larger than for experiments in laboratory columns, even for similar porous media. The theoretical studies address the observation that field-scale dispersivities appear to increase with the scale of the measurement as presented in [Section 3.1](#).

The intent of the theoretical section is merely to provide the reader with a survey of the wide range of approaches available. Much of the theory is based on stochastic analyses, the detailed development of which is beyond the scope of this report. The interested reader is encouraged to consult Dagan (1989) or Gelhar (1993) for in-depth presentations of the application of stochastic methods to

Figure 3-6
Longitudinal Dispersivity Data with NTS Data Highlighted

subsurface contaminant transport problems. Nonetheless, a brief definition of some general concepts will aid the reader.

As we noted in [Section 2.0](#), dispersion results from observations that are averages of complex small-scale flow paths. This sub-observational variability begins with Brownian motion at the molecular level, is evident in the velocity profile in pipes that leads to the classic Fickian dispersion, and is present in laboratory cores where complex flow through pores produces dispersion when cross-sectional averaged concentrations are examined. The theoretical analyses below all begin with the premise that heterogeneity in the groundwater velocity field leads to observed field-scale dispersion. This heterogeneity is observed in nature and occurs at many scales. Some researchers work directly with the velocity variability, while others relate the velocity to the controlling parameters of hydraulic conductivity (K), porosity, and hydraulic gradient. Typically, most studies find that the most important parameter is the hydraulic conductivity and treat the porosity and hydraulic gradient as constants.

If K could be measured everywhere in the flow system, the dispersion process would be modeled directly as mechanical dispersion based on the detailed velocity field. In reality, the K is observed at few locations. Stochastic analyses are utilized because the heterogeneity of K is described as a spatial random process that can be described by a few parameters representing the variability statistically. Observations of K variability indicated that it can be well described by a lognormal probability distribution. This means that $\ln K$ is represented by a

normal distribution which is fully described by its mean and standard deviation. If the ensemble statistics describing the variability of $\ln K$ do not vary spatially, the variability is defined as stationary. Generally, nonstationarity in the ensemble mean can be removed by subtracting the mean, resulting in a zero-mean random process that is stationary in the variance, often called second-order stationarity. Further relaxation of the stationarity assumption occurs if the variance of the difference of two values depends only on the separation distance, not on the specific locations of the two points. This is referred to as the intrinsic hypothesis.

Many analyses are based on linearizations of key governing equations. The linearizations are often based on assumptions of small variability ($\ln K$ variance much less than 1 for example). In addition, other key parameters such as porosity are often assumed constant and the mean groundwater velocity field is assumed uniform and time invariant (steady). Many of these assumptions are quite restrictive, suggesting that theory based on these assumptions will apply to only a few locations.

At the vast majority of sites, one or more of these assumptions is violated. Variability of $\ln K$ is highly nonstationary; the flow is nonuniform (generally related to large nonstationarity, but could be introduced by a well for example); other processes such as decay, solute/solid reactions, or matrix diffusion are present and active. Each of these nonidealities will be discussed below. First, however, the results of idealized cases are presented because they provide insights in the dispersive process.

3.2.2 Analyses Based Upon Idealized Assumptions

Most theoretical studies begin with a description of contaminant dispersion analogous to Taylor/Aris advection-diffusion mechanisms (Bear, 1988), where dispersion is modeled as the interaction of two processes: advection along streamlines with different velocities, and diffusion between streamlines. The original Taylor/Aris work was designed to explain dispersion in capillary tubes where under steady laminar flow, a tracer moves at different velocities depending on where it occurs in the cross section of the tube due to the parabolic velocity distribution in the tube. In the absence of diffusion, the tracer will continue to spread longitudinally, indefinitely. When lateral diffusion from one streamline to another is included, the radial concentration differences are reduced. The tracer mass flux per unit time per unit cross-sectional area can be written as the product of a dispersion coefficient and the cross-sectional averaged concentration gradient in the direction of flow. Thus, the tracer is dispersed by both longitudinal convection and radial molecular diffusion relative to a plane moving with a constant-mean velocity. This process is describable by Fick's Law of molecular diffusion, where the diffusion coefficient has been replaced by the dispersion

coefficient. This leads to the familiar 1-D advective - dispersion equation given as:

$$\frac{\partial \bar{C}}{\partial t} = D' \frac{\partial^2 \bar{C}}{\partial x^2} - \bar{V} \frac{\partial \bar{C}}{\partial x} \quad (3-1)$$

where:

$\bar{C}$ = The cross-sectional averaged concentration
 $\bar{V}$ = The cross-sectional average velocity
 x = Distance
 t = Time
 D' = The effective dispersion coefficient

Often, the dispersion coefficient is represented as:

$$D' = \bar{V} \alpha_L + D_d \quad (3-2)$$

where:

α_L = The longitudinal dispersivity
 D_d = The effective diffusion coefficient

In most applications, the effective diffusion coefficient (in the x -direction) is much smaller than the dispersion coefficient and is ignored. Diffusion across streamlines (transverse to flow) is already embodied in the dispersion equation. Bear (1988) notes that this form of the transport equation leads to a solution with an average concentration distribution in the form of a normal (Gaussian) distribution about the center of mass as portrayed in [Figure 2-4](#).

Researchers recognized the importance of heterogeneity in the advective velocities of different streamlines in porous media and began to develop theories to represent this phenomenon. Gelhar (1986), Dagan (1987), and Neuman et al. (1987) related spatial variability in the natural logarithm of hydraulic conductivity to the field-scale dispersion process. They represented hydraulic conductivity heterogeneity as a stationary spatial random process (i.e., one in which the statistics of the variability are uniform in space) represented by a covariance function of the natural log of hydraulic conductivity. The field-scale dispersion is

parameterized by a macrodispersivity (Rajaram and Gelhar, 1993) derived from a Fickian-based approximation of the form:

$$A_{ij}(t) = \frac{n}{2q_1} \frac{dM_{ij}}{dt} = \frac{1}{2} \frac{dM_{ij}}{dX_1} \quad (3-3)$$

where:

- q_1 = The mean-specific discharge (assumed uniform and in the x_1 direction)
- n = The effective porosity
- X_1 = The location of the center of mass
- M_{ij} = The second spatial moment of the ensemble average concentration field

Many researchers then relate M_{ij} to properties of the log hydraulic conductivity heterogeneity or properties of the velocity field. This leads to a tensorial form of the macrodispersivity that is analogous to the tensorial form presented in [Section 2.0](#).

For example, in the case of isotropic heterogeneity with 1-D uniform mean flow, Gelhar (1986) gives the following expression for the longitudinal macrodispersivity:

$$A_{11} = \frac{\sigma_f^2 \lambda}{\gamma^2} \quad (3-4)$$

where:

- σ and λ = The standard deviation and correlation length, respectively, of log hydraulic conductivity (f) covariance function and
- γ = A flow factor that may or may not equal one, depending on the form of the lnK covariance function and the geometry of the flow system.

Any number of equations of a form similar to [Equation 3-3](#) and [Equation 3-4](#) have been generated which account for anisotropy in the hydraulic conductivity covariance, different flow directions, or averaging in one or more dimensions. All of these equations have similar characteristics:

- The rate of change of the second moment reaches a constant, or asymptotic value.

- The derivations rely on the assumption of mild heterogeneity ($\sigma < 1$).
- The log hydraulic conductivity is assumed to be a stationary, spatial, random process.

Hess et al. (1992) summarize the results of measured and calculated longitudinal macrodispersivity values from natural gradient tracer experiments at Cape Cod (Garabedian et al., 1991), Borden (Freyberg, 1986), and Aefligen, Switzerland (Hufschmeid, 1986). The predicted longitudinal macrodispersivities, A_{11} , are similar to measured values in each case (Table 3-1). In addition, as predicted by theory, the sites at which the product of variance and correlation scale is larger (Equation 3-4) showed larger measured and predicted values of A_{11} . At each site, the measured transverse dispersivity was larger than predicted by theory. In general, the predicted transverse dispersivities are very small.

Table 3-1
Comparison of Measured and Predicted Longitudinal
Macrodispersivities
 (Modified from Hess et al., 1992)

Parameter	Cape Cod	Borden	Aefligen
lnK variance	0.24	0.29	2.15
lnK correlation scale (m)	2.9 - 8	2.8	15 - 20
Predicted A_{11} (m)	0.35 - 0.78	0.61	1.3 - 3.8
Measured A_{11} (m)	0.96	0.36	2.2 - 22

These early studies were conducted at geologically simple sites in porous media, where idealized theoretical models were appropriate. Extensive data collection efforts allowed the calculation of the covariance function of the natural logarithm of hydraulic conductivity (lnK). It has been observed that the logarithm of hydraulic conductivity follows a normal distribution (Gelhar, 1993); therefore, working with lnK is statistically advantageous. The lnK field is assumed to be stationary (the mean and variance do not vary spatially) and the porosity was assumed to be constant. The mean groundwater flow was considered uniform. Each of these sites was mildly heterogeneous; therefore, small variability assumptions inherent in the early theoretical studies were valid.

The success of the early stochastic-based theories of solute transport in naturally heterogeneous porous media to explain field-scale macrodispersivity was encouraging. However, the results were limited in the following ways:

- The experiment sites were primarily clean sand and gravel aquifers with small to modest variability.
- The attainment of asymptotic longitudinal macrodispersivities at scales less than about 200 m does not explain the much larger observed values in Gelhar et al. (1992).

- Nonuniform flow, nonstationary heterogeneity, chemical processes were not addressed in these studies but are present at other sites.
- Predicted transverse macrodispersivities (horizontal and vertical) are very small, much smaller than observed values. Several researchers (Rehfeldt and Gelhar, 1992; Goode and Konikow, 1990; Dagan et al., 1996) identified slowly varying, unsteady, uniform flow characterized by variation in the direction of the hydraulic gradient as a possible explanation for the observed transverse macrodispersivities being larger than predicted by the steady-state theory. This mechanism allows the plume to slowly shift from side to side. Each time the plume shifts, it leaves some contaminant mass behind. This appears as enhanced lateral spreading and leads to larger transverse dispersivities.

The early applications of stochastic methods to address dispersion at the field scale were encouraging, and suggested that analysis of the scale dependence of dispersivity was amenable to stochastic methods. However, significant challenges remained for application to non-ideal sites.

Neuman (1990) examined the macrodispersivity data presented by several researchers including Gelhar et al. (1985), and observed, as did Gelhar et al. (1985), that the dispersivity values increase with increases in the scale of measurement, apparently without bound. This is in sharp contrast to the Fickian-based results, which suggest constant or asymptotic macrodispersivities are obtained. Neuman (1990) proposed a fractal scaling relationship for the dispersivity data that could be explained by assuming a corresponding fractal structure to the log hydraulic conductivity heterogeneity.

Neuman (1990) proposed a self-similar random field with homogeneous increments characterized by a semi-variogram that increases indefinitely as the square root of the distance. This semi-variogram is based on a notion that the heterogeneity is represented by a continuous hierarchy of scales. In this case, the variance of the natural logarithm of hydraulic conductivity ($\ln K$) fluctuations and the corresponding correlation scales increase as the scale of measurement, or area of investigation, increases. Neuman (1990) cautions that this universal scaling does not necessarily describe conditions at any particular locality. He suggested a comparable scale rule, but with locally derived parameters, is one explanation of the scatter in the observed macrodispersivity data about the universal scaling relationship. Other explanations include errors in data collection and interpretations. One conceptual difficulty of the self-similar description of $\ln K$ heterogeneity is that it leads to the development of exploding plumes (i.e., plumes that continue to disperse at an ever-increasing rate as they travel downgradient). The Cape Cod sewage plume, which extends over 2 miles in length but maintains a narrow width (LeBlanc, 1984), clearly shows that this is not the case.

3.2.3 Impact of Plume Size on the Dispersion Process

The theoretical results of Gelhar and Axness (1983) and Dagan (1987), among others, do not account for plume size in the calculation of dispersion coefficients.

Rajaram and Gelhar (1993) showed that for stationary random fields analogous to the work in Gelhar and Axness (1983), the predicted longitudinal macrodispersivity is slightly smaller when the size of the plume is taken into account. This smaller dispersivity was termed the “relative dispersivity” in Rajaram and Gelhar (1995), and accounts for the fact that an individual plume will be smaller than the ensemble of all plumes. For the Borden and Cape Cod site-tracer sites, Rajaram and Gelhar (1993) estimated that the dimensionless reduction factor for the longitudinal macrodispersivity ranged from 0.64 to 0.865.

Subsequent work by Rajaram and Gelhar (1995) extended their analysis to include hydraulic conductivity heterogeneity that incorporates large-range correlations. A fractional Gaussian model of variability, characterized by fractional Gaussian noise (fGn), is a stationary process with an infinite variance and an infinite correlation scale. Rajaram and Gelhar (1995) note that a fGn model is appropriate for processes with variograms that exhibit a slow approach to a sill, and cite the work of Robin et al. (1991) where the fGn model was fit to horizontal hydraulic conductivity data from the Borden site.

A self-similar random field, or fractional Brownian motion (fBm), was also examined. A fBm field is one in which the variability is statistically similar at all scales and is of the type suggested by Neuman (1990) in his paper on Universal Scaling of Dispersivity. Robin et al. (1991) found that the fBm model was a good fit to the vertical variations in the hydraulic conductivity data from the Borden site.

For the fGn description of hydraulic conductivity heterogeneity, Rajaram and Gelhar (1995) demonstrated that the longitudinal macrodispersivity will reach an asymptotic value, the magnitude of which depends on the initial size of the plume. The larger the plume, the larger the asymptotic longitudinal macrodispersivity. The transverse macrodispersivities increase for short displacements, then decrease. The larger the initial plume size, the larger the transverse dispersivity values.

When a self-similar, fBm, description of heterogeneity is used, a slightly different result was obtained. Both the longitudinal and transverse dispersivity show an increase at small distances, then both reach approximate asymptotic values for a range of scales. At large displacement, the dispersivities again begin to grow. For the example in Rajaram and Gelhar (1995), the early growth phase extended out about 10 m, then an approximate asymptotic value is valid to distances up to about 2,000 m. By 10,000 m, the dispersivity is growing again. These results assume a self-similar model of heterogeneity out to large scales, while a uniform mean velocity is assumed to apply. Di Federico and Neuman (1998) found that if a low frequency filter is applied, an asymptotic dispersivity results even for self-similar media. They define their low frequency cutoff as “The integral scale λ_i of the lowest frequency model (cutoff) is related to the length scale of a sampling window defined by the domain under investigation...” (Di Federico and Neuman, 1998).

3.2.4 Impact of Local Dispersion

Analogous to Equation 3-2, macrodispersion has been defined as the sum of a term caused by velocity variations and a term that accounts for local-scale dispersion (similar to pore-scale diffusion in classical dispersion, Equation 2-1). Most of the theoretical studies of macrodispersivity caused by spatial variability of hydraulic conductivity usually dismiss the local dispersion term as of second-order importance. Recent work has begun to recognize the importance of local dispersion as a mechanism to disperse solute mass across streamlines.

The role of local-scale dispersion has been examined recently. Several early papers, Kapoor and Gelhar (1994a and b), point out that theories that account only for advective spreading of plumes do not include a mechanism to destroy concentration fluctuations. In this case, advection may distort a plume, but it does not create dilution. Based on numerical experiments, Zhang and Neuman (1996) conclude local dispersion causes a reduction in longitudinal macrodispersion and an increase in transverse macrodispersion. In contrast to Kapoor and Gelhar (1994a and b), Zhang and Neuman (1996) believe that as local dispersion tends to zero, so does its impact on macrodispersion.

Dagan and Fiori (1997) also examined the impact of local-scale dispersion by formulating the questions in terms of a Peclet number defined as:

$$Pe = \frac{V\lambda}{D_d} = \frac{\lambda}{\alpha_d} \quad (3-5)$$

where:

- V = The mean velocity
- λ = The hydraulic conductivity correlation scale
- D_d = The local scale dispersion coefficient
- α_d = The local scale dispersivity

In the case of zero local dispersion, the Peclet number is infinite. Dagan and Fiori (1997) found that local dispersion has a minor influence on the predicted mean concentration, but has a significant impact on the concentration variance. In other words, the ability of existing theories to predict actual concentration is enhanced by including the effect of local dispersion. This conclusion had previously been reached by Kapoor and Gelhar (1994a, 1994b).

Andricevic (1998) extended the previous results to include the impact of sample volume. He finds, as did previous work, that local dispersion and the sample volume have a relatively minor impact on the predicted mean concentration, but have a significant influence on the concentration fluctuations about the mean. The reduction in concentration fluctuations caused by local dispersion generally increases with travel distance because advection has distorted the plume such that there is a large enough surface area with concentration gradients for the local dispersion to become important.

Recent work by Fiori (2001) contradicts the results of Rajaram and Gelhar (1995) and suggests that even for finite size plumes in self-similar media, the longitudinal

dispersivity will grow without bound when local-scale dispersion is present. He argues that local dispersion, primarily the transverse component, allows the plume to occupy adjacent stream tubes, thus sampling a greater portion of the heterogeneity. He cautions, however, that his results apply at large time scales of $t \gg l^2/D_d$ where l is the initial transverse dimension of the plume. Using the NTS as an example, where l may be on the order of two times the cavity radius (150 m) and local dispersion is on the order of 0.5 to 18 square meters per year (m^2/yr) (based on $D=V\alpha$ with a velocity estimate using minimum travel times of 11 to 27 years [no radionuclides in Oasis Valley yet]), distances of 24 to 40 km, and local dispersivities of 0.005 to 0.0005 m (Kapoor and Gelhar, 1994b), the times must be much greater than 1,200 to 50,000 years before the results of Fiori apply. This would suggest that work of Fiori (2001) will not apply at the NTS over the 1,000-year time scale of interest.

At the present time, there does not appear to be a consensus in the scientific literature about the effect of local dispersion and it appears to be undecided at this time. On one hand, it leads to true dilution and reduction in the variance of concentration. It may also enhance plume spreading and contribute to increases of macrodispersivity with travel distance. In contrast, other studies found that finite plume size may limit spreading. The interaction of these two mechanisms is not yet clear.

3.2.5 Observations and Theory of Dispersion in Highly Heterogeneous Aquifers

Many of the field experiments, such as at Cape Cod and Borden, were carried out at mildly heterogeneous sites. Additionally, many theoretical calculations are performed under the assumption of small heterogeneity to justify linearizing assumptions. However, many sites are highly heterogeneous and it is necessary to understand dispersion in those situations. Adams and Gelhar (1992) present the results of spatial moments analysis of transport at the MADE site in Columbus, Mississippi. Rehfeldt et al. (1992) analyzed hydraulic conductivity and determined the $\ln K$ variance to be more than 10 times larger than for the Borden or Cape Cod sites. This large variability led to a nonuniform flow field that developed near the tracer injection wells. Adams and Gelhar (1992) examined the tracer plume and found it to be non-Gaussian in shape with a long leading edge, but most of the mass remained near the injection area. A Gaussian fit to the data yielded large longitudinal dispersivities of 50 to 75 m, but it was a very poor fit to the overall plume shape. When a simple, nonuniform, flow-field model was applied, the apparent longitudinal macrodispersivities dropped to the range of 5 to 10 m. It may safely be concluded that if significant flow variability is ignored, the dispersivity will be overestimated. The danger of this situation is that predictions made with the larger dispersivity in a uniform flow field will overestimate dilution. Later analysis by Harvey and Gorelick (2000) of the MADE data used a rate-limited mass transfer model (similar to a dual-porosity model) to explain the behavior of the MADE plume. Their comparison of the mass transfer model to the macrodispersion model of Adams and Gelhar (1992) suggested that a macrodispersion model provided a poor fit to the data compared with the mass transfer model. One may conclude from Harvey and Gorelick (2000) that it may be inappropriate to treat heterogeneous systems as macrodispersion-dominated

flow systems with large dispersivity values, at least at small distances. Doing so will result in overestimation of dilution and underprediction of concentration. It is important to note that both Adams and Gelhar (1992) and Harvey and Gorelick (2000) used the same nonuniform flow field as their starting point. The majority of flow in these highly heterogeneous systems is controlled by the relatively few highly permeable pathways. Further, this may suggest that using the heterogeneity of the whole aquifer system may not be appropriate if dual porosity is assumed to be a viable mechanism. In these cases, description of the variability of the more permeable portion may be more representative. The appropriate value for dispersivity will be a function of how well the velocity field is simulated, and how well other transport processes are represented.

Becker and Shapiro (2000) conducted tracer experiments in fractured crystalline rocks at the Mirror Lake site. They observed late-time tailing of the breakthrough curves for a variety of tracers and injection design configurations. They concluded that the tailing was not the result of dual-porosity matrix diffusion effects because they observed no differences in tailing behavior for tracers of differing diffusion coefficients. Rather, they conclude the tailing is the result of a dispersive behavior. The breakthrough curves exhibit the same shape regardless of the pumping rate, indicating that the dispersive behavior is also proportional to advection. Becker and Shapiro postulate that in the highly heterogeneous crystalline rock, the non-Fickian behavior may be related to a relatively short distance of travel that has not been sufficiently long for ensemble mean behavior to take effect.

3.2.6 Anomalous Transport and Alternative Approaches

Anomalous transport is a term that has crept into the literature in recent years to describe scale-dependent behavior. It has been applied to transport that has also been called preasymptotic, non-Gaussian, or non-Fickian. In general, it represents departures from the classical Gaussian-shaped plume describable by Fick's law with a constant dispersivity. Berkowitz et al. (2000), among others (Tompson, 1988), go as far as to suggest that anomalous behavior may be the norm rather than the exception. The Fickian behavior is a special case that is useful when the conditions are appropriate. Anomalous behavior is unfortunate terminology for conditions that are more common than uncommon. Anomalous dispersion, or departures from Fickian representations, become more pronounced when (1) the degree of heterogeneity is large and (2) the scale of the plume is small in comparison to the scale of heterogeneity, or (3) when a plume continuously encounters a larger scale of heterogeneity as it moves.

Some researchers have suggested that one way to approximate anomalous transport is to use a dispersion coefficient that is a function of time $D(t)$. Berkowitz and Scher (1995) argue that the conventional advective dispersion equation with $D(t)$ leads to untenable physical results and is, thus, an inappropriate approach to the problem of anomalous dispersion. They suggest an alternative approach, based on the continuous-time random walk (CTRW) method. The

CTRW is a generalization of the traditional random walk (where the continuation of the walk occurs at discrete time steps) on a lattice:

$$R(s, t) = \sum_{s'} \int_0^t \psi(s - s', t - \tau) R(s', \tau) d\tau \quad (3-6)$$

where:

$R(s, t)$ = The probability for a particle to just arrive at a site s at time t
 $\psi(s, t)$ = The probability per unit time for a transition between sites separated by s and arrival times t

Berkowitz et al. (2000) point out that the above equation combines advective, dispersive, and diffusive transport and is fundamentally different from the traditional random walk where particles follow a streamline and are then randomly perturbed to simulate diffusion (or local dispersion). Berkowitz et al. (2000, Figure 1) present a diagram of anomalous transport (Figure 3-7) with most of the mass near the source, but with a long leading edge that is very similar to the plume from the MADE site. They apply the CTRW technique to laboratory transport data and show that the CTRW provides a better fit to the data. They also mention that other recent and complementary formalisms, such as Levy flights and fractional derivative transport equations, are simply special cases of the more general CTRW.

Berkowitz et al. (2001) again apply the CTRW via a first-passage time distribution (FPTD) solution to two rather small tracer experiments: one for data 1.37 m from the inlet of a lab column, and the other for 2.5 and 4 m of vertical transport in a fractured till. The FPTD solution fit the observed data very well with a minimum number of parameters. This is in contrast to Fickian-based solutions which did not fit the data as well. The extension of these results to larger scales has the same difficulties as previous work, namely that the character of the heterogeneity may change and the model parameters determined from small-scale experiments may not be valid at large scale. In addition, the currently available CTRW solutions do not account for retardation, decay, or production processes.

Berkowitz et al. (2002) expand their analysis of the CTRW method to highly heterogeneous systems. They show that their results reduce to the advective dispersion equation if a smooth particle distribution representing the plume is assumed and if the first and second temporal moments of ψ are assumed finite. When ψ is represented by a power law function with dependence on time at large time, a non-Fickian or anomalous transport results. They demonstrate that fractional derivative equations are asymptotic limit cases of their more general CTRW theory.

It is worth noting that many features of anomalous behavior, such as those portrayed in Figure 3-7, may be modeled with Fickian-based approaches in some cases. For example, a Fickian model with an extremely large dispersivity and low velocity, basically a diffusion problem with a large diffusion coefficient, could produce curves similar to those in Figure 3-7. Generally, this approach does not

Figure 3-7
Example of Anomalous Transport
 (Modified from Berkowitz et al., 2000)

capture the appropriate dispersive mechanisms and would be considered a less desirable alternative.

3.2.7 Nonlocal Models of Transport

Another suite of approaches that looked to explain the non-Fickian field observations relied on nonlocal models of transport (i.e., constitutive models that involve either integrals or higher-order derivatives). Such theories have been derived from both Lagrangian (e.g., Cushman, 1991; Cushman and Ginn, 1993; Cushman et al., 1994) and Eulerian (e.g., Koch and Brady, 1988; Deng et al., 1993; Cushman et al., 1995; Hu et. al., 1995, 1997a, b; Huang and Hu, 2000) frameworks. Cushman et al. (1995) argue that media which are either nonperiodic (e.g. media with evolving heterogeneity) or periodic media, viewed on a scale wherein a unit cell is discernible, must display nonlocality in the mean. They state that nonlocality is a manifestation of the lack of use of boundary data in the upscaling process. They suggest that owing to the scarcity of information on natural scales of heterogeneity and on scales of observation associated with an instrument window, constitutive theories for the mean concentration should at the outset of any modeling effort be nonlocal. If the scale of observation turns out to be large relative to the heterogeneity scale, the process can be considered local. However, nothing will be lost in using the nonlocal constitutive theory since it will reduce to its correct local counterpart. Nonlocality can appear in both the

dispersive flux and the advective flux as well as in sources and sinks of mean concentration. The fully nonlocal theory can be localized in space or time alone, or it can be localized in both space and time resulting in a fully localized theory.

3.2.8 Scaling Considerations

As is clear from the discussion of recent literature, much of the theoretical effort directed at the problem of dispersion in aquifers is focused on the question of how dispersivity changes with distance traveled, which is primarily a question of scaling.

McKenna and Rautman (1996) completed a literature review and numerical experiments to assess the scaling of material properties at Yucca Mountain. They emphasized hydraulic conductivity scaling, but interpreted particle-tracking results in terms of dispersion. They determined the amount of increase in the dispersivity required to keep the same amount of dispersion as the block size in a model was increased. For isotropic hydraulic conductivity fields, they found that dispersivity increased by more than an order of magnitude as the dimensionless ratio of grid length to $\ln K$ correlation length increased from 0.1 to 10. When examining anisotropic conductivity fields, the authors tried to fit scaling relationships to power law functions. They were successful for all parameters except the dispersivity. They concluded that dispersion must be modeled using a dispersivity parameter that takes into account the dispersion occurring at scales below that of the flow model element size. In short, McKenna and Rautman (1996) found that a grid-scale dispersion term is required, even if simulations are performed with random fields.

Pawloski et al. (2001) showed that the random field-based simulation breakthrough curves obtained at a plane 305 m from the CHESHIRE source (in the absence of heat) can be reasonably approximated by an effective 1-D representation with A_{11} lying between 100 and 200 m. However, the simulations at CHESHIRE may be more representative of anomalous dispersion than by Fickian-based results, at least at the scale of their simulations. Thus, their results cannot be readily extended to larger scales. One approach would be to choose one of the previously mentioned theoretical approaches, then essentially calibrate that approach to the apparent dispersivity at 305 m, then use that relationship to predict larger scale values.

Gomez-Hernandez and Wen (1997) used 2-D numerical simulation to examine longitudinal and vertical dispersion in four random fields: one is a multi-lognormal field, the second displayed high connectivity of high hydraulic conductivity values, the third displayed high connectivity of low hydraulic conductivity values, and the fourth displayed high connectivity of both high and low hydraulic conductivity values. Each model had the same log-normal histogram with zero mean and variance of 2.0. All models had the same low-conductivity covariance and differed only in their indicator variograms at extreme thresholds. They computed longitudinal and transverse dispersivities at various correlation lengths from the source. In all cases, the longitudinal and transverse dispersivities developed according to patterns predicted by first-order

theory. The differences in longitudinal dispersivity were as much as a factor of three, with the fields having high connectivity of high conductivity layers having the largest dispersivity. One conclusion from this work is that scaling, which underestimates the impact of high hydraulic conductivity pathways, may underestimate the true dispersion.

Additional work to address the scaling of dispersivity has been presented by Russell et al. (1995) and Dean and Russell (1998). The latter paper uses a Lagrangian numerical approach in an attempt to avoid assumptions such as small variance, ergodicity, and single correlation scale that are commonly made in theoretical and many numerical studies. Their method is based on particle tracking and is designed to specify the dispersion coefficient on a numerical finite element grid. Their method does require knowledge of the covariance function of the hydraulic conductivity, which is used to generate random fields following a spectral turning bands method.

Berkowitz et al. (2002) note that one of two approaches is generally taken to model field-scale transport: (1) treat the region as one domain with heterogeneities characterized by random fields (with or without drift), and (2) explicit description of certain heterogeneities such as hydrostratigraphic units (HSUs) that produce nonstationary domains when viewed as a whole. Ensemble-averaged (stationary) descriptions do not provide much insight into real field-scale problems. When explicitly describing large-scale heterogeneities, the question of how to model smaller scale heterogeneity comes into play, and how to link the various scales of heterogeneity. Citing numerical studies with random fields within deterministic structures, Berkowitz et al. (2002) argue that even highly discretized models fail to adequately capture plume patterns because of unresolved heterogeneity at small scales. They propose a CTRW model define the unresolved heterogeneity at the sub-grid block scales.

3.2.9 Dispersion of Reactive Solutes

The discussion up to this point has focused on conservative solutes that do not react with the aquifer material and do not alter the flow system. Dagan (1989) and Gelhar (1993) describe preliminary studies addressing features such as radioactive decay and solute sorption as described by distribution coefficients (K_d). Dagan (1989) shows that simple radioactive decay does not change the movement of the center of mass, nor the second moment dispersive characteristics. A solute plume with a decaying solute is similar to a plume of a non-decaying solute, except for a scale down of the concentration with time in the decaying plume.

Transport of reactive solutes is more complicated. If one assumes the reactivity, as parameterized by the K_d which is also spatially variable, then there is a complex interaction between K and K_d . Dagan (1989) showed that if retardation and $\ln K$ are positively correlated, dispersion is reduced relative to the reactive case. Gelhar (1993) presents a case of negatively correlated $\ln K$ and K_d . In this case, the dispersion is enhanced.

Further evidence of the interaction of contaminant reactivity and dispersion is provided by Thompson (1993) and Pawloski et al. (2001). The correlation between velocity heterogeneity and reactivity is important to determining if reactivity will increase or decrease apparent dispersion.

3.2.10 Dispersion in Dual-Porosity Media

Gelhar (1993) presents analyses of dispersion in dual porosity or dead-end pore systems. These flow systems are representations of extreme heterogeneity, with some regions of large velocity and others of zero velocity. As some of the solute mass diffuses into the matrix, then later back out, the plumes tend to show a steeply rising initial breakthrough followed by a long tail. The dual porosity can be modeled by a single-porosity system with a larger dispersivity. However, failure to account for this important physical mechanism will result in an overestimate of dispersivity. It is not clear at this time how important matrix diffusion may be on the estimation of transverse dispersion.

3.2.11 Parameter Estimation - A Difficult Problem

Dagan (1989) and Gelhar (1993) discuss the issue of parameter estimation. The theories presented to predict the large-scale dispersive behavior assume the necessary parameters are known. In reality, this is not the case. Dagan evaluates the impact of estimation errors of the mean velocity and its impact on predictions. Mean velocity is calculated from the relationship $V = K_{eff}J/n_e$ where each parameter has estimation error. Dagan (1989) concludes that uncertainty in the position of the center of mass may result to a greater extent from estimation error in the mean velocity than from spatial variability in $\ln K$. He also finds that the second moment, characterized by the dispersion, is less susceptible to estimation error in the mean. For overall predictions of the location of contamination (mean displacement and dispersion), Dagan concludes that refined models of $\ln K$ variability are of little predictive use if the estimation errors associated with the mean velocity are large.

Gelhar (1993) devotes an entire chapter of his book to parameter estimation issues. Several key observations are: (1) dispersion is usually some function of the product of $\ln K$ variance and the correlation scale, so uncertainty in both terms is important; (2) it is generally easier to assess uncertainty in the variance than in the correlation scale, but care must be taken to account for correlated samples in the variance uncertainty calculations; (3) even with rather large datasets, it is difficult to identify the exact form of the covariance function; therefore, choosing a simple form such as the exponential is usually justified; (4) large-scale measurements are generally superior to scattered small-scale measurements for assessing covariance parameters because of the greater information content of the larger scale measurement; and (5) heterogeneities larger than the scale of the plume should be treated as component of the mean flow, whereas heterogeneity smaller than the plume contribute to dispersion.

It is important to recognize that the parameters describing heterogeneity, even in a stochastic framework, are uncertain. Parameter uncertainty will translate into prediction uncertainty.

3.3 *Synthesis of Theoretical and Field Studies*

A large number of studies have been examined to chronicle the research over the past 25 years or so into field-scale dispersion. Much of this work has provided valuable insights into the process of dispersion in heterogeneous media, while others, as noted by Dagan (2002), “address esoteric topics.” Limited high quality data from tracer experiments over large scales are not, nor will they ever be, available. The times and distances are simply too great to undertake such experiments. A large number of approaches have been developed to extend our detailed knowledge of transport on the scale of several 100 m (with time frames of several years) to field-scale problems extending out tens of kilometers with time frames of 1,000 years or more. Due to the practical impossibility to collect relevant data, none of these theoretical approaches can be shown to be “correct.” However, a number of conclusions or observations can be made that will help guide our approach to modeling dispersion at the field scale:

- Longitudinal dispersion, as typically observed at the field scale, will be much larger than measured in the laboratory.
- Longitudinal dispersion will be small for small distances, but grow for some period of time, or some distance. At large distances, there is considerable debate about what happens; it may reach an asymptotic value or may continue to grow indefinitely. In addition, the magnitude of dispersion tends to be smaller for smaller plumes or plumes that have not moved great distances because: (1) a plume encounters larger scales of heterogeneity as it moves, (2) an anomalous dispersion effect, (3) measurement scales, or (4) all of the above.
- Stationary random field assumptions, self-similar fields with low wave number cutoffs, or plume-scale averaging all lead to situations where the longitudinal dispersivity reaches an asymptotic value.
- Self-similar random fields or strongly heterogeneous fields that exhibit channeling or other “non-ergodic” behavior tend to lead to dispersion coefficients that grow large at large distances.
- Ensemble plume variability, or some similar measure of the expected error between mean plume predictions and reality, may be quite large, but appear to be reduced by the effects of local-scale dispersion.
- As the velocity field is better defined (for example, by deterministically modeling large scale, observable features), the smaller the effective longitudinal dispersion needs to be to account for the unmodelled, small-scale heterogeneity. The heterogeneity of importance might be as large as a plume if uniform properties are used, or as small as a model

grid cell if spatially variable parameters are used. Heterogeneity at scales larger than the size of the plume impact the mean displacement and should be treated as part of the (potentially uncertain) mean and not part of the dispersive term. The better the velocity field is defined, the less important longitudinal dispersion parameters become.

- Transverse dispersion is significantly smaller than longitudinal dispersion, both observed, and predicted by theory.
- Transverse dispersion is an important parameter because several studies contend that true dilution of a plume comes from the small transverse dispersion terms that become important as the plumes get large.
- The source-release function governs, in part, the relative importance of longitudinal versus transverse dispersion. Downgradient dilution of continuous sources will be governed by the transverse dispersion. Pulse-source releases are influenced by both longitudinal and transverse dispersion.
- The leading edge of a plume, which may be most important for defining first arrivals and maximum extent, is primarily governed by the longitudinal dispersion. As a first approximation, it appears reasonable to address leading edge or maximum extent questions with 1-D particle-tracking methods. These methods, however, may not be adequate to address questions of concentration distribution between the source and the leading edge.
- Dispersivities measured with tracer test-scale experiments (up a few hundred meters) are almost certainly not applicable to large-scale simulations of thousands to tens of thousands of meters.
- The prediction of the future location and distribution of a plume depends on the mean movement and the dispersion about that mean, both of which are uncertain.
- All currently available scaling methods rely on knowledge of the hydraulic conductivity covariance function and treat the covariance function as known. In fact, the form and parameters of the covariance function will be uncertain. This translates into predictions of dispersivity that are also uncertain. This uncertainty needs to be taken into account when using the theory to predict large-scale dispersivity values.

4.0 *Application to the Nevada Test Site*

The dispersion of radionuclides while being transported in groundwaters beneath the NTS needs to be simulated as part of the CAU-scale modeling. The CAU-scale modeling may include multiple models at various scales from the near-field scale of Pawloski et al. (2001) to the CAU scale which may be as large as 40 km. The treatment of dispersion may differ depending on the scale of the model. In this section, dispersivity refers to the parameter governing spreading appropriate to the scale of the model. We discard the artificial distinctions of effective, macro, or anomalous dispersivity. Review of the recent scientific literature indicates that dispersion, and its associated parameters, need to account for the following observations:

- Dispersion is the result of sub-plume scale variability that is averaged via an observation process.
- The modeling needs to differentiate between uncertainty in the mean (variability at scales larger than the plume) and sub-plume scale variability that leads to dispersion. The topic of sub-plume variability is the focus of this Technical Basis Document.
- Longitudinal dispersion will grow with the scale of transport because the plume encounters a larger portion of the variability as it moves. The rate and form of the growth depends on the nature of the heterogeneity at large scales.
- Transverse dispersion, both horizontal and vertical, must be smaller than the longitudinal, but not zero. The appropriate large-scale dispersive behavior in the transverse directions depends on the nature of heterogeneity at large scales, but also on large-scale temporal variability.
- The observed dispersivity values (longitudinal and transverse) from around the world show apparent trends with scale of observation, but there is considerable uncertainty (two or more orders of magnitude) about the appropriate value to use. Low reliability data at large scales increase the uncertainty of representative values at large scales.

There is no widely accepted comprehensive theory to predict the dispersivity values to use for any particular field situation. Even if one theory was accepted, the data requirements necessary to characterize the heterogeneity are large. Therefore, longitudinal and transverse dispersivities applied to CAU and sub-CAU models will need to be treated as uncertain parameters regardless of how the dispersive process is simulated.

4.1 Experience from Previous NTS Modeling

Four simulation studies related to radionuclide transport in groundwater at the NTS provide some insights into the role of dispersion. One-dimensional finite element simulations were performed to assess the transport of tritium from the TYBO underground test to the discharge area in Oasis Valley during the regional model simulations (IT, 1996). As part of the simulations, sensitivity analyses were conducted where one parameter was varied within a specified range of values using a Latin Hypercube Monte Carlo approach. The maximum concentration of tritium at downgradient distances of 1, 10, and 30 km were compared to the case of all parameters held at their mean value. Nine parameters were examined:

- Source Concentration: the initial source concentration at the cavity location. It was allowed to vary over two orders of magnitude.
- Longitudinal Dispersivity: the longitudinal dispersivity was varied from 100 to 500 m. The distances of travel were up to 35 km.
- Effective Porosity: the entire domain was assumed to be fractured volcanic rocks with effective porosity (dimensionless) that ranged from 5×10^{-4} to 4×10^{-3} .
- Matrix Porosity: the process of matrix diffusion was modeled explicitly with matrix porosity values (dimensionless) that varied from about 0.08 to 0.50. This range was based on the observed range in measured values.
- Block Width: the spacing between fractures was allowed to vary from 0.9 to 2.5 m. This range was obtained from studies of the distribution of open fractures in core.
- Matrix Diffusion Coefficient: the parameter that governs the diffusion of mass from the fractures to and from the matrix was assumed to range from 2.6×10^{-4} to 7.9×10^{-3} m²/yr.
- Hydraulic Conductivity (K): two parameters define the hydraulic conductivity at depth, a hydraulic conductivity value at land surface (KH) and a depth decay parameter (ld). These values were defined for each HSU. The transport model does not use K directly, rather the uncertainty in groundwater flow due to uncertainty in K was quantified via sensitivity analyses. Then a factor of 10 range in K was translated into the equivalent effect on groundwater flux.
- Recharge: a dimensionless multiplier on the total flux to account for the impact of unknown recharge. It was allowed to vary between 0.17 and 5.92, with 90 percent of the values between 0.4 and 2.6.

A cumulative frequency distribution plot for the 1 km distance is presented in [Figure 4-1](#). The parameter with the largest influence near the source was the source concentration itself. The longitudinal dispersivity also had a small effect, particularly when it led to increased concentrations. [Figure 4-2](#) shows the results

Figure 4-1
Regional Model Uncertainty Analysis
Impact of Parameter Uncertainty 1.0 km from the Source (IT, 1996)

Figure 4-2
Regional Model Uncertainty Analysis
Impact of Parameter Uncertainty 10 km from the Source (IT, 1996)

at a distance of 10 km. In this case, source concentration is still important, but now several other parameters are equally important: recharge and the parameters related to matrix diffusion (i.e., block width, matrix porosity, and diffusion coefficient). At a distance of 30 km (Figure 4-3), the recharge (total flux) and matrix diffusion parameters dominate. At any distance, longitudinal dispersion variability had only a minor impact on the results and was much less important than other parameters.

Two recent modeling studies, Wolfsberg et al. (2002) and Pawloski et al. (2001), addressed transport of radionuclides on Pahute Mesa. In both studies, the macrodispersion was simulated by modeling the hydraulic conductivity as a random field and applying particle-tracking methods. Pawloski et al. (2001) looked at the sensitivity of including a local-scale (sub-grid block) dispersivity in their calculations. They found no noticeable difference except in the case where the local dispersivities were $\alpha_L=100\text{m}$ and $\alpha_L=10\text{ m}$. These local-scale values are quite large given the 10 m grid dimension used in the simulations. A conclusion that may be reached is that the random field was sufficient to account for dispersion in the near-field model. An initial analysis of the simulated radionuclide flux through the system was scaled up to represent a model of steady uniform flow with a constant dispersivity via application of a more classical advective dispersion equation (ADE). In this case, a longitudinal dispersivity on the order of 100 to 200 m was determined to provide an approximate fit to the breakthrough data at a plane 305 m downgradient of the test (Figure 4-4). That magnitude of dispersivity is quite large compared with the data from other sites around the world and is reflective of the degree of averaging necessary to account for the heterogeneity and the nonuniform flow field created by heat-driven convection in the cavity and chimney.

The different curves in Figure 4-4 represent two approaches to simulating the impact of sub-plume variability on the spreading of contaminants. The large-scale dispersivity ADE approach accounts for the sub-plume heterogeneity and non-uniform flow with a large magnitude dispersivity. The random field approach generates realizations of heterogeneity and simulates flow and transport through that field. It utilizes small local-scale dispersivity values, but requires significant computing power to perform. Figure 4-5 from Pawloski et al. (2001) highlights the differences in the approaches as a function of observation scale. If small-scale observations are available and important, the random field approach with its 2,400 grid blocks in the observed plane alone provides a detailed picture of possible radionuclide breakthrough. Each realization is a possible view of reality and provides the observer with a broad range of possible small-scale concentration values. On the other hand, averaged ADE approaches will spread the mass evenly over a large value and obtain average concentrations similar to mean concentrations that would be obtained from the random field approach if they were averaged over all realizations. Detail is lost in the averaged ADE approach, but it does represent mean behavior. If the scale of observation is large, then the averaged approach may be sufficient.

The simulations of Wolfsberg et al. (2002) also utilized particle tracking through a random field. They did not calculate an equivalent dispersivity for their simulations but showed that significantly different transport realizations were

Figure 4-3
Regional Model Uncertainty Analysis
Impact of Parameter Uncertainty 30 km from the Source (IT, 1996)

Figure 4-4
Comparison of Simulated Radionuclide Flux with an
Effective Dispersion Coefficient Solution at the CHESHIRE Site (Pawloski et al., 2001)

Figure 4-5
Conceptual Representation of the Dilution Effect Created by Mapping the Integrated Flux Coming
out of the Finely Discretized Near-Field Model into a Coarsely Gridded CAU Model

possible. In a deterministic simulation without a random field, they showed that the addition of a transverse dispersivity term of 3 m led to increased lateral spreading of a plume from TYBO. These two approaches were designed to assess the impact of sub-plume scale variability on the spreading of radionuclides.

The fourth study was the interpretation of the BULLION FGE using a numerical model (IT, 1998). Interpretations using a semianalytical model were presented by Reimus and Haga (1999). The BULLION FGE was a radial flow FGE where tracers were injected in observation wells located about 100 m away from the production well. The calibrated fit to the observed breakthrough curve using an ADE was quite sensitive to even a factor of two change in the dispersivity (longitudinal and transverse) values. Alternative calibrations where multiple parameters were simultaneously adjusted to obtain calibration suggests that the dispersivity values could vary by about a factor of 5 and yield calibration to the observed data as long as other parameters were also varied.

4.2 Conclusions from Previous Modeling Studies

Two different approaches have been used in previous NTS modeling studies to simulate the dispersion of radionuclides; one based on effective parameters coupled with an ADE approach, and a second approach based on highly resolved random fields and small local dispersion coefficients. Both approaches aim to account for the sub-plume scale variability that leads to dispersion. In the case of the BULLION FGE, the effective parameter ADE approach is justified because the observation is the breakthrough curve at a discharge well that effectively integrates all the pathlines as they enter the well. The scale of observation matched the approach.

The near-field and intermediate-scale models of Pawloski et al. (2001) and Wolfsberg et al. (2002), respectively, utilized both the highly resolved random fields and effective average parameter approaches. It is clear that representation of radionuclide concentration and breakthrough history (in the near field [up to several km]) is enhanced with highly resolved realizations of random fields. Although both Pawloski et al. (2001) and Wolfsberg et al. (2002) found that general features of the concentration could be obtained by deterministic simulations, the details cannot be simulated. Based on stochastic theory, the ergodic assumption, and laws of spatial averaging, one might expect that deterministic ADE models will work best when predicting transport at large time and distance where the scale of observation is also expected to be large. However, that is an expectation based on theoretical arguments and cannot be proven at this time. A disadvantage of the ADE approach is the uncertainty in measured values at large scale as presented in [Section 3.0](#), and the difficulty of parameterizing large-scale heterogeneity necessary to predict large-scale dispersivity using theoretical approaches.

The random field approach would appear to offer significant advantages in the near field and perhaps intermediate scale where smaller scale observations may be available or desirable. Both approaches have an important role to play in CAU-scale simulations. The random field approach aids in sensitivity and uncertainty

analyses which help to establish uncertainty bounds and parameter distributions for ADE methods. The ADE methods are generally computationally less demanding and likely provide a good measure of mean behavior at large scales. What is not clear, however, is whether uncertainty analyses using the ADE approach with uncertain dispersivity parameters provides an equivalent assessment of uncertainty compared with realizations of highly-resolved random fields.

Disadvantages of the random field approach are related to lack of data. The random field approach (as well as theoretical approaches for ADE parameters) requires the definition of a statistical description of the variability. In the simplest case of a stationary random function, it requires a variance and three correlation scales. As Pawloski et al. (2001) and Wolfsberg et al. (2002) have shown, credible estimates of variance and vertical correlation scale can be obtained from existing data. The horizontal scales, however, are now (and will likely remain) educated guesses at best. This limitation makes the random field approach and the theoretically predicted ADE approach questionable for CAU-scale prediction.

What is not clear at this time is which approach (random field, ADE with uncertain parameters based theoretical predictions, or ADE with uncertain parameters based on historic observations) provides the most defensible predictive capability for large-time, CAU-scale simulations. All approaches have substantial uncertainty, and neither is clearly superior for long-term prediction.

4.3 Proposed Handling of Dispersivity in CAU Models

A top priority will be to develop techniques that guard against numerical dispersion. The best approach is to simulate transport via some form of particle tracking. This approach will allow for dispersion to be simulated without the typical numerical dispersion associated with the solution to the advective dispersion equation. This is particularly important for transverse dispersion. Excessive simulated transverse dispersion will lead to underestimation of radionuclide concentrations. Conversely, it is not appropriate to ignore transverse dispersion because that will overestimate radionuclide concentrations.

Radionuclide migration will continue to be simulated with advective dispersion equation formulations. Although some researchers have recently proposed modified governing equations based on fractional partial derivatives or continuous-time, random-walk methods, these have not been accepted as standard methodology. In addition, these new formulations require new data and parameters to be estimated. This does not appear to be a viable approach at this time. At a later time, the simulations may need to be modified for new governing equations, but for now the standard advection dispersion formulation will be used.

The CAU-scale models have been planned to include significant geologic features such as major HSUs and structural features such as faults. In general, the dispersivity is a parameter that accounts for spatial variability at scales smaller than the scale of the plume in the model. The CAU models will be calibrated by assigning constant parameter values to large portions of, if not entire, HSUs. The

existing calibration target data are not sufficient to allow calibration of local-scale parameters on the scale of the mesh spacing. Therefore, the appropriate scale for the dispersivity is the scale of the HSU or fault blocks. Within the Silent Canyon Caldera complex, structural blocks are as small as 1.5 km on a side to as large as about 7 km on a side. Closer to the discharge area, the structural blocks are larger, on the order of 10 km or so. In the range of 1 to 10 km, Gelhar et al. (1992) show no data of moderate to high reliability. The range of low reliability dispersivity are: longitudinal (L) 6 to 1000 m, transverse 0.01 to 90 m, and vertical 0.001 to 1 m. Gelhar et al. (1992) show that the ratios of longitudinal/transverse dispersivity are 3 to 50 and for longitudinal/vertical dispersivity 10 to 700.

Some of the theoretical studies indicate that if scale of heterogeneity increase over the flow domain, the dispersivity values may also increase without bound. Other studies, however, appear to offer the prospect that finite dispersivities are expected to apply. Large-scale features such as major HSUs and other structures that are present at scales of km are modeled deterministically in the CAU-scale models. Coupling plume-scale averaging from Rajaram and Gelhar (1995) with the cutoff scale (several km based on deterministic structure) concept of Di Federico and Neuman (1998) suggests that finite, but uncertain, dispersivities will be appropriate for CAU-scale radionuclide transport modeling. In addition, the scale of these dispersivities would be on the order of the large-scale features in the geologic models.

The dispersivity will need to be treated as an uncertain parameter. The longitudinal and horizontal transverse values will range over about two orders of magnitude, while maintaining a ratio of longitudinal to transverse of at least 3 and no more than 50. It will be difficult to reduce the uncertainty in CAU-scale dispersion parameters until many years into the future. Reductions in dispersion parameter uncertainty will occur only after observed radionuclide migration can be observed over large travel distances and used to constrain model predictions.

The random field approach would define the hydraulic conductivity of each node or element in the model based on generated random fields. In this case, the dispersivity would need to account for sub-grid scale variability at scales on the order of 100 m. This would reduce the lower bound of the longitudinal dispersivity to less than 1 m, and will decrease the upper bound based on Gelhar et al. (1992) to about 100 m. The random field approach may not be practical at the CAU scale because it requires definition of the hydraulic conductivity three-dimensional covariance function, potentially for each HSU. Whether this limitation is any worse than the uncertainty in the ADE approaches remains to be investigated.

At smaller scales, it is clearly advantageous to use random fields because there are typically fewer HSUs to model, and more importantly, there are radionuclide observational data with which to constrain the results. In other words, realizations that fail to reproduce observed data would be excluded from further analysis. Without radionuclide observations at large time and distance, the random field approach does not offer a clear advantage in making defensible predictions at the CAU scale. However, as noted earlier, the random field approach may be useful

to assess the sensitivity and uncertainty of the model predictions to sub-plume scale heterogeneity.

For the CAU-scale simulations, the initial approach will be to use an ADE approach with dispersivity parameter values chosen from the range of observed values as presented in [Section 3.0](#) and Gelhar et al. (1992). To provide confidence in the outcome of those simulations, random field-based simulations will also be required for comparison.

5.0 Summary and Conclusions

In recent reviews of the Pahute Mesa CAIP, NDEP has commented that site-specific, and potentially CAU-specific, dispersion measurements will be needed.

We have shown via literature review of theoretical, measurement, and modeling studies that CAU-scale dispersion is a scale-dependent parameter. Field experiment scale (300 m) measurements of dispersivity are not expected to directly provide CAU-scale longitudinal or transverse dispersivity values unless the entire model area were simulated with a random field approach with grid cells on the order of 300 m. The difficulties of generating random fields over the entire CAU model area have already been presented. The impracticality of measuring CAU-scale dispersion via tracer experiments, or predicting CAU-scale dispersion via stochastic theory (due to an inability to define the covariance at the appropriate scale) suggests that dispersion be treated as an uncertain variable in CAU modeling using an ADE approach. Additional comparisons between the ADE approach and the random field approach will be required to provide confidence in the ADE-based predictions. These additional comparisons will not replicate site conditions, rather they are designed to demonstrate that for a given assumed form of heterogeneity, an ADE equivalent can be defined. The initial choice of the ADE approach is a pragmatic one, it is simply easier to implement and is expected to be no more uncertain than approaches that require quantification of the heterogeneity at large scales.

Recent modeling studies at the NTS suggest that longitudinal dispersion may not be a very important parameter, compared with other parameters at the CAU scale. However, transverse dispersion is expected to be important at the CAU scale. At smaller scales, modeling dispersion via random field representation of hydraulic conductivity variability appears to be a better approach than the classical advection dispersion equation. However, at the CAU scale, the advection dispersion equation with an uncertain dispersion coefficient is probably the most reasonable way to predict large scale and large-time transport.

In conclusion, there is little or no benefit to performing additional tracer experiments at scales up to a few hundred meters for the sole purpose of measuring dispersion. Of course, if tracer tests are conducted for other reasons (for example to investigate matrix diffusion), then dispersion parameters should be obtained as well.

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