DISPERSIVE PROCESSES IN MODELS
OF REGIONAL RADIONUCLIDE MIGRATION

A TECHNICAL MEMORANDUM

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For

University of California
Lawrence Livermore Laboratory

By

Donald E. Evenson
Michael D. Dettinger

Camp Dresser & McKee Inc.

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FOREWORD

This technical memorandum will be incorporated with other research efforts sponsored by Lawrence Livermore Laboratory this year to produce the Task 2--Fiscal Year 1979 Annual Report. This annual report will describe site suitability criteria for the disposal of high level radioactive wastes in a deep geological formation. The annual report will be disseminated nationally to provide part of the technical information necessary to make policy decisions about radioactive waste disposal.

The scope of work undertaken by Camp Dresser & McKee, Inc. under purchase order number 569609 covers three basic tasks. The tasks are described as follows:

TASK 1. EVALUATE 2-D VERSUS 3-D GROUNDWATER MODELS

This task shall include an evaluation of the extent a lower order model can adequately simulate the regional flow of radionuclides, and a comparison between two- and three-dimensional flow and quality problems. Consideration shall be given to such conditions as heterogeneity, anisotropy, boundary geometry, and various sources and sinks as they relate to predictive accuracy. A literature search shall be conducted and a reference list assembled to the extent that it supports the evaluation and comparison.

This task shall also include studies of two- and three-dimensional analytical solutions for homogeneous/isotropic cases to show, in the absence of any modeling approximations, where there is a real need for three-dimensional models.

Although there are conceivable regional flow cases where a three-dimensional model may be necessary, an evaluation of modeling techniques (finite difference versus finite element) shall also be included to study model approximating procedures still remaining that may cause additional problems in the needs evaluations process.

A selected number of idealized computer simulations shall be carried out for those areas of particular interest as illustrations of higher dimensional models.

TASK II. EVALUATE PROBLEMS ASSOCIATED WITH DISPERSION PROCESSES IN GROUNDWATER MODELS

The purpose of this task is to evaluate problems associated with representing dispersion processes in groundwater models. For purposes of this task, "dispersion processes" refer to those conditions, assumptions or processes that cause mixing to take place or to appear to take place in either the prototype or the model. CDM's recent Technical Memorandum titled "Processes and Parameters Involved in Modeling Radionuclide Transport in Bedded Salt Repositories" pointed out that values of dispersivity from model calibrations were 100 to 1000 times greater than those measured in the laboratory. This task shall investigate the reasons for these differences and recommend methods of dealing with them.

Factors that shall be considered are: 1) model assumptions concerning anisotropy and homogeneity; 2) level of detail in modeling local changes in stratigraphy, solute stratification and sampling errors; 3) numerical errors inherent in the mathematical solution techniques; and 4) variability in grain size distribution. In addition, CDM shall review alternative formulations for estimating dispersivity values and shall test the sensitivity of the dispersion transport process as compared to advective transport.

TASK 111. PREPARE SPECIFICATION FOR DEVELOPMENT OF 3-D MODEL

This task shall include a complete definition of the three-dimensional problem that would be in need of solution. An outline of all equations to be modeled, a list of parameters needed for input, definition of boundary conditions, and output requirements shall be assembled. A specifications list shall also be assembled that addresses techniques used and numerical accuracy, stability, and conveyance concerns. A set of known theoretical solutions shall be chosen and outlined to provide comparative tests of the integrity of the developed code.

At the conclusion of this task, CDM shall prepare a technical memorandum for the University discussing and providing a checklist of the specifications. The form of the memorandum shall be such that it could be given directly to the model code developers.

TECHNICAL MEMORANDUM

This technical memorandum covers the work conducted under Task 11.

PROJECT ORGANIZATION

Preparation of this technical memorandum was accomplished through the direction and efforts of the project's co-Principal Investigators, Donald E. Evenson and Thomas A. Prickett. The major portion of this memorandum was prepared by Michael D. Dettinger. Becky Wilson, Connie Morris, David Prior and Henry Evans provided technical and editorial support in the preparation of the memorandum.

Terry Steinborn, Tom Naymik and Willard Murray of the Lawrence Livermore Laboratory provided valuable assistance and guidance in preparing this memorandum.

ABSTRACT

Camp Dresser & McKee Inc. was contracted by the Lawrence Livermore Laboratory of the University of California to evaluate problems associated with dispersion processes in regional groundwater models. This technical memorandum is the product of our research.

Three broad areas of concern in the development of aquifer scale transport models will be local scale diffusion and dispersion processes, regional scale dispersion processes, and numerical problems associated with the advection-dispersion equation. Local scale dispersion processes are fairly well understood and accessible to observation. These processes will generally be dominated in large scale systems by regional processes, or macro-dispersion. Macro-dispersion is primarily the result of large scale heterogeneities in aquifer properties. In addition, the effects of many modeling approximations are often included in the process. Because difficulties arise in parameterization of this large scale phenomenon, parameterization should be based on field measurements made at the same scale as the transport process of interest or else partially circumvented through the application of a probabilistic advection model. Other problems associated with numerical transport models include difficulties with conservation of mass, stability, numerical dissipation, overshoot, flexibility, and efficiency. We recommend the random-walk model formulation for Lawrence Livermore Laboratory's purposes as the most flexible, accurate and relatively efficient modeling approach that overcomes these difficulties.

1. INTRODUCTION

SCOPE OF REPORT

This technical memorandum presents the results of an evaluation of problems associated with the representation of dispersion processes in regional groundwater models. For the purposes of this report, "dispersion processes" refer to the conditions, assumptions, or processes that cause mixing to take place or to appear to take place either in the physical system or in a model. The purpose of the evaluation was to investigate and recommend methods for dealing with these processes.

During the course of this investigation, it became clear that two primary problem areas exist in regional groundwater models. These are:

1. Macro-dispersion phenomena, and
2. numerical errors inherent in most transport models.

These two considerations tend to dictate, to a large extent, the methods which can be meaningfully applied to represent dispersion processes numerically. In recognition of their importance, this report concentrates on the investigation and development of recommendations for handling these primary problem areas.

Our recent technical memorandum on "Processes and Parameters Involved in Modeling Radionuclide Transport in Bedded Salt Repositories" pointed out that laboratory measurements of dispersion processes result in dispersivities that are 100 to 1000 times smaller than those required to adequately calibrate numerical models of mass transport in aquifers. In this report we will investigate the processes that are represented in regional models, and we will investigate means of determining meaningful coefficient values for use in transport models of regions near radionuclide waste repositories.

In the past, it was almost routinely assumed that dispersion processes represent a secondary correction to the effect of advection processes (often referred to as "convection processes" in groundwater literature). With the realization that laboratory measurements represent very different mechanisms than are active in regional models, it has become clear that dispersion processes can have much larger effects. These effects are referred to as "macro-dispersion." The zone in which contamination from repository failures can be detected or is potentially dangerous can be expected to be significantly increased by macro-dispersion. This process may, on the other hand, decrease the potential for dangerous levels of contamination through the aquifer's ability to dilute by increased mixing. Thus, it is important that the macro-dispersion process be adequately and realistically accounted for in model simulations applied to investigations of repository siting.

This report also reviews available methods and strategies for modeling mass transport in aquifers. Because we expect dispersion to be an important component of mass transport in aquifers, our review is restricted to problems associated with models of the advection-dispersion equation of mass transport. Because numerical errors can be difficult to detect and differentiate from "valid" dispersion processes, considerable effort should be employed to reduce or at least anticipate the onset of these errors. These numerical problems in transport models tend to arise suddenly and model results tend to degenerate quickly following their onset. Therefore, an understanding of the behavior of available numerical modeling techniques is crucial to decisions of which model types are best applied in a given model application. With this understanding, a model type can be chosen advantageously and strategies for its accurate application can be developed. These strategies are at least as important as the initial choice of models. Because of the great uncertainties currently associated with dispersion processes in aquifers, two very important strategic decisions in model applications will be discussed: the choice of the level of model detail, and the choice between deterministic and probabilistic modeling approaches.

These decisions are related to the general problem of modeling a system for which some parameters are uncertain or unknown.

REPORT CONTENTS

This report consists of five additional chapters and two appendices. Chapter II presents a brief review of local dispersion and diffusion processes. A basic understanding of the processes is important because it provides a basis for the analogies used in discussions and theories concerning macro-dispersion. Chapter III contains an extensive discussion of the macro-dispersion phenomenon. Chapter IV reviews numerical modeling techniques used for mass transport in aquifers and, in particular, the numerical errors that arise in applications of the various techniques. Chapter V is a discussion of methods for determining dispersion coefficients for regional transport models. A summary of the report is presented in Chapter VI. The first appendix presents a description of a simple numerical mass transport model based on the random-walk solution method. The second appendix presents the results of a series of simulations investigating the parameters affecting macro-dispersion in a simple layered porous medium.

II. LOCAL DISPERSION AND DIFFUSION PROCESSES IN POROUS MEDIA

INTRODUCTION

Diffusion and dispersion are two processes that irreversibly distribute dissolved constituents within porous media. In this chapter, these processes will be discussed as they are manifested over distance scales ranging from microns to a few meters. This scale is the one at which these processes are best understood and is the scale at which all laboratory studies of these phenomena have been conducted. Although the next section will show that extrapolation of results from this small scale to larger scale regional aquifer transport models is impossible, it is important to understand local dispersion processes because all larger scale models and measurements are based on analogies to laboratory results and Fickian diffusion.

MOLECULAR DIFFUSION

The term diffusion is often used in reference to the physiochemical mixing process referred to as molecular diffusion; it results from the existence of chemical potential gradients wherever constituent concentrations are variable within a medium. Alternatively, the driving mechanism may be temperature gradients, pressure gradients, or certain external forces which selectively affect the various constituents (Fried and Combarnous, 1971). Diffusion within fluids appears to be dependent on such fluid properties as temperature, concentration, and viscosity as well as temperature and concentration gradients. Within a porous medium, the diffusive process is also a function of the pore structure or tortuosity of the solid matrix, which tends to inhibit the free diffusion of the constituents by providing a complex set of barriers to mass transport. For one dimensional geometries the diffusion process is generally described mathematically according to Fick's Law:

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

where C is the concentration of a constituent in the fluid, t is time [T], x is the spatial dimension [L], and D' [L²/T] is the diffusion coefficient. In a porous medium, D' might be defined as T·D_m, with T equal to a matrix tortuosity correction factor and D_m the free fluid diffusion coefficient [L²/T]. The coefficient D' may be a function of position or direction since both the matrix tortuosity and fluid properties, particularly viscosity, may be variable. In practice, however, the variation of D' is unknown and Fick's Law is usually simplified to:

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

with D' equal here to an average or effective diffusion coefficient ranging from 10⁻⁵ to 10⁻⁸ cm²/sec. (Lerman, 1971).

DISPERSION PROCESSES

Dispersion in porous media is a general term describing mixing of constituents brought about by the vast number of complex flow paths along which constituents are carried as the fluid moves through the solid matrix. Variability of path length, flow velocity, and the resulting travel times result in longitudinal and lateral spreading or dispersion of constituents. At a very local or microscopic level, this spreading of constituents is the result of the variations of fluid velocity within pores, variation of pore diameter along the flow lines, and variations of flow and pore axis directions. However, since porous media are not observed at this microscopic level, the media are modeled as equivalent continua and averaged parameters, such as porosities, permeabilities, and specific discharges are used to describe fluid flow. To describe the effect of microscopic variations on the transport of constituents in the fluid at a larger, continuum scale, an averaged parameter, often referred to as

the local dispersion coefficient, is used. At the scale of a single pore volume, the transport of a constituent carried along with an incompressible fluid flow can be described, in one dimension, by

$$\frac{\partial C}{\partial t} + \frac{\partial (vC)}{\partial x} = \frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = 0 \quad (2-3)$$

where v is the flow velocity in the pore, and $\frac{\partial v}{\partial x} = 0$ due to the assumption of fluid incompressibility. When a volume containing many of these pores is averaged, the flow velocity may be considered

$$v = u + v' \quad (2-4)$$

where u is the average flow velocity (or seepage velocity), v' is the variation of flow velocities within the pores, and the concentration can be expressed by

$$C = c + c' \quad (2-5)$$

where c is the average concentration within the fluid in many pores and c' is the variation from pore to pore. The transport equation can then be expressed as

$$\frac{\partial C}{\partial t} + \frac{\partial C'}{\partial t} + u \frac{\partial C}{\partial x} + v' \frac{\partial C}{\partial x} + u \frac{\partial C'}{\partial x} + v' \frac{\partial C'}{\partial x} = 0 \quad (2-6)$$

which may be averaged to obtain

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + \langle v' \frac{\partial C'}{\partial x} \rangle = 0 \quad (2-7)$$

(with $\langle \rangle$ signifying "the average value of") since the average value of v' , c' and their derivatives equal zero. By analogy to Fick's Law, a dispersion coefficient can be defined so that the transport equation becomes:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} D_L \frac{\partial c}{\partial x} = 0 \quad (2-9)$$

where D_L is defined as the longitudinal mechanical dispersion coefficient. When molecular diffusion is included and the analysis is expanded to an isotropic two-dimensional medium, the advection-dispersion equation becomes

$$\frac{\partial c}{\partial t} \quad (1)$$

$$+ U_x \frac{\partial c}{\partial x} + U_y \frac{\partial c}{\partial y} \quad (2) \quad (2-10)$$

$$= \frac{\partial}{\partial x} \left[D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} \right] + \frac{\partial}{\partial y} \left[D_{yy} \frac{\partial c}{\partial y} + D_{yx} \frac{\partial c}{\partial x} \right] \quad (3)$$

with U_x , U_y equal to the seepage velocities in x and y directions respectively, with

$$D_{xx} = D_L \frac{U_x^2}{U^2} + D_T \frac{U_y^2}{U^2} + D' \quad (2-11a)$$

$$D_{yy} = D_L \frac{U_y^2}{U^2} + D_T \frac{U_x^2}{U^2} + D' \quad (2-11b)$$

$$D_{xy} = D_{yx} = (D_L - D_T) \frac{U_x U_y}{U^2} \quad (2-11c)$$

where D_L is equal to the longitudinal dispersion coefficient, which is the coefficient describing the component of the mechanical mixing along the flow and D_T is equal to the tranverse (perpendicular to the flow) mechanical dispersion coefficient (Borg, et al, 1976). It has been assumed that the molecular diffusion coefficient (D') is a scalar in the definitions of D_{xx} and D_{yy} given above. In theory, D' may be tensor valued. The terms of this equation represent respectively,

1. The time rate of change of the concentration at some point,
2. plus the rate at which the constituent is advected to or away from that point, and
3. equals the rate at which dispersion to or from surrounding areas changes the concentration.

Much time and effort has been spent on estimating appropriate values of the coefficients of the above equation. Laboratory investigations have generally shown that the longitudinal dispersion coefficient is related to the seepage velocity u according to the equation:

$$D_L = \alpha u^m$$

where α and m are constants with respect to velocity (see for example Rumer [1962], Banks and Jerasate [1962]). D_L is also functionally related to fluid properties such as viscosity and matrix properties such as grain diameter and specific permeability. For example, Harleman et al (1963) observed that

$$\frac{D_L}{v} = \alpha_0 \left[\frac{\sqrt{k}}{\sqrt{c_0}} \cdot \frac{u}{v} \right]^n \quad (2-12)$$

where

$$\begin{aligned} \nu &= \text{kinematic viscosity [stokes]} \\ c_0 &= 6.15 \times 10^{-4} \text{ (for their medium)} \\ k &= \text{specific permeability [cm}^2\text{]} \\ n &= 1.06 \\ \alpha_0 &= 1.92 \end{aligned}$$

Lateral dispersion has been studied as well; Li and Lai (1966) reported the relationships

$$\frac{D_T}{\nu} = \beta \left[\frac{u d_{50}}{\nu} \right]^{3/4} \quad 0.3 < R_e < 10$$

and

(2-13)

$$\frac{D_T}{\nu} = \gamma \left[\frac{u d_{50}}{\nu} \right]^{4/3} \quad 10 < R_e < 380$$

where β , γ are constants (which vary with the medium from 0.03 to 0.12 and 0.03 to 0.02 respectively), d_{50} is the median grain diameter (cm) and R_e is the Reynolds number, $u d_{50} / \nu$.

Such results are of little use in practice since they depend on parameters which are difficult to estimate and are highly dependent on the geometry and materials used in the measurements. For these reasons the dispersion coefficients are generally treated in a simpler manner. New constants, α_L and α_T , which represent longitudinal and lateral dispersivities, are generally defined according to the equations:

$$D_L = \alpha_L u \quad (2-14a)$$

$$D_T = \alpha_T u \quad (2-15b)$$

These constants generally are found to be on the order of a median grain diameter in laboratory porous media, i.e., typically on the order of millimeters or less ($<10^{-3}\text{m}$).

Dispersion processes are usually assumed to dominate diffusion processes even though it is clear that dispersion is very dependent on the average flow velocity through a porous medium as opposed to diffusion that is apparently independent of flow. This domination occurs even though flow rates in aquifers show a tremendous range of variation. In a moderately permeable system a reasonable regional flow rate might be 10^{-5}m/s so that

$$D_L = \alpha_L u = (10^{-3}\text{m}) (10^{-5}\text{m/s}) = 10^{-8}\text{m}^2/\text{s} = 10^{-4}\text{cm}^2/\text{s}.$$

Even higher velocities occur in some aquifers and are prevalent in laboratory situations. Diffusion coefficients are normally several orders of magnitude smaller than this value and therefore can be neglected.

However, when the flow rate is extremely small, molecular diffusion can dominate the transport process. For example, Goodall and Quigley (no date, referred to in Anderson, 1978) considered transport of contaminants situated in a low permeability medium with hydraulic conductivities ranging from 10^{-6} to 10^{-8} cm/s . In this medium, advection was reduced to about 0.5 cm per year; after six years the plume of contaminant was 30 cm long. The difference was found to be adequately explained by assuming a molecular diffusion coefficient for the porous medium of approximately $10^{-6}\text{cm}^2/\text{s}$. Although the rate of transport due to diffusion is slow, it is potentially a very important mechanism for carrying radionuclides from a repository site to more permeable geologic units in which advection and dispersion processes can become large. Because criteria for choosing repository sites include media with low permeabilities and seepage velocities, it is important that diffusion processes be fully accounted for in the region near the repository itself.

Another common assumption regarding dispersivity constants is that the ratio of longitudinal to lateral dispersivities is constant and that the lateral coefficient can be defined very simply in terms of the longitudinal coefficient. In our recent technical memorandum, "Processes and Parameters Involved in Modeling Radionuclide Transport from Bedded Salt Repositories," it was noted that a comparison of several experimental results suggests that this assumption is an oversimplification. Generally, no alternative is available, the lateral coefficient is not known, and, in order to get any results at all, an almost arbitrary choice of the ratio D_L/D_T is used.

Two very simple but important relationships relate dispersion coefficients and thus dispersivities to the spread of the dispersive mixing zone. The amount of spreading that a constituent experiences due to dispersion may be described in terms of a spatial variance σ^2 according to the relationships

$$\frac{\partial \sigma^2_L}{\partial t} = 2\alpha_L u = 2D_L \quad (2-15a)$$

and

$$\frac{\partial \sigma^2_T}{\partial t} = 2\alpha_T u = 2D_T \quad (2-15b)$$

These relationships arise because solutions to the advection-dispersion equation tend to be related to Gaussian (or normal) distribution functions. In a one dimensional transport situation, for instance, a fixed concentration level C_0 at $x = 0$ will be transported into the medium according to

$$C = C_0 \left\{ 1 - \frac{1}{\sqrt{2\pi\sigma}} \exp \left[-\frac{1}{2} \left(\frac{x - ut}{\sigma} \right)^2 \right] \right\} \quad (2-16)$$

with expected value ut and variance $\sigma^2 = 2D_L t$ (Fried and Combarnous, 1971). This relationship is often used to calculate coefficient values based on observations of mixing processes. This relationship will be discussed in more detail at the end of this section.

The relative importance of dispersion and advection in transporting constituents can be compared in a very general sense using the variance relationships presented in the previous paragraph. If we assume that α_L is constant, then

$$\sigma_L^2 = 2\alpha_L ut \quad (2-17a)$$

or the standard deviation of the mixing zone, a measure of the extent of the dispersion process, is

$$\sigma_L = \sqrt{2\alpha_L ut} \quad (2-17b)$$

Advection, on the other hand, transports material a distance

$$d = ut \quad (2-18)$$

Therefore, the ratio of the distances that each process transports mass is

$$\frac{\sigma_L}{d} = \frac{\sqrt{2\alpha_L d}}{d} = \sqrt{\frac{2\alpha_L}{d}} \quad (2-19a)$$

or

$$\frac{\sigma_L}{d} = \sqrt{\frac{2\alpha_L}{ut}}, \text{ is proportional to } \frac{1}{\sqrt{t}} \quad (2-19b)$$

Using the first of these equations, it is easy to see that advection is dominant for transport over distances much greater than the dispersivity. The second form of the equation suggests that dispersion becomes decreasingly important with time. It should be recalled, however, that for large times, the mixing zone can be quite large and important even if it is small compared to advection.

MEASUREMENT OF DISPERSION COEFFICIENTS IN THE LABORATORY

Most common methods of estimating the dispersion coefficient, D_L , in flow through a porous medium (especially in the laboratory) are based on the analysis of breakthrough concentration curves. The procedure may be described as follows: A sudden but permanent change is imposed in the concentration of some easily and/or accurately observable constituent (a tracer) in a fluid flowing into a carefully constructed column of a porous medium. If no dispersive processes were active, the fluid entering the medium would simply flow along the medium carrying the abrupt concentration front imposed on the fluid with it. At any observation point along the medium, the effects of the imposed concentration front would not be detected until the front arrived intact and would be observed as a step change in concentration. In the presence of dispersive mixing, the concentration front is smeared and will be observed at any point to grow to the imposed concentration level in a smooth curve. If, for example, the flow is one-dimensional and the fluid entering the medium receives a perfect step change in tracer concentration from 0 at time 0 to ΔC at all subsequent times, the observed concentrations at some point x_0 along the flow will theoretically be described by (Bear, 1979):

$$c(t, x_0) = \frac{\Delta C}{2} \operatorname{erfc} \left\{ \frac{x_0 - ut}{\sqrt{4D_L t}} \right\} \quad (2-20)$$

where

t = time, and

u = seepage velocity.

Based on this result, the dispersion coefficient can be estimated to be (Greenkorn, 1970):

$$D_L = \frac{1}{4\pi} \frac{x_o u}{S} \quad (2-21)$$

where

$$S = \left. \frac{x_o}{u \Delta C} \frac{\partial C}{\partial t} \right|_{t = x_o/u}$$

Alternatively, assuming a Gaussian model, D_L can be estimated to be (Fried and Combarous, 1971):

$$D_L = \frac{u^2 \Delta t_o}{8 \left(\frac{x_o}{u} \right)} \quad (2-22)$$

where

$$\Delta t_o = t_{.84} - t_{.16}$$

and $t_{.84}$ is the time when a concentration of $0.84\Delta C$ is obtained.

Also employed in determining D_L and D_T are pulse input methods. The strategy in these experiments is to introduce a tracer into the flow over a short time interval. Once again, assuming that dispersion is a Gaussian process, it can be shown that the mixing zone should spread with a spatial variance,

$$\sigma_L^2 = \int_{-\infty}^{\infty} c (x-ut)^2 dx = 2 D_L t \quad (2-23a)$$

and

$$\sigma_T^2 = \int_{-\infty}^{\infty} c y^2 dy = 2 D_T t \quad (2-23b)$$

This approach to estimating these coefficients requires spatially distributed observations and thus can be difficult and expensive to apply to porous media. Therefore, this method has seen more use in measuring transport phenomena in other systems such as the atmosphere and surface water.

Measurement techniques analogous to these laboratory experiments have been carried out in numerous aquifers in an effort to understand the dispersive behavior of natural porous media. Because natural systems are not under the careful control of the experimenter and because aquifer materials tend to vary in a different manner than the porous media employed in laboratory tests, measurements in the field have resulted in very different coefficients than found in the laboratory. The nature of the difference and reasons for this difference are discussed at some length in the next chapter.

III. MACRO-DISPERSION PROCESSES

INTRODUCTION

Throughout the course of development of theoretical and analytical models of mass transport in groundwater, a major assumption has been that transport processes in aquifers behave according to theoretical results and results generated in laboratory studies of transport through homogenous porous media. A Fickian formulation of the transport equation has always been assumed and coefficients (e.g. aquifer dispersion coefficients and aquifer dispersivities) equivalent to those measured in the laboratory have served as model parameters. Field measurements, however, have always tended to suggest that, because of the great disparity between the media studied, the time/distance scales and the modes of observation in laboratory and field situations, aquifer scale transport coefficients are not measures of the same processes as laboratory scale coefficients. At the aquifer scale it appears that heterogeneities in permeability and other medium properties, solute stratifications, medium anisotropies, sampling strategies, and even model approximations and errors are considerably more important in producing what appears to be dispersive behavior than mixing at the pore scale. Thus we have no assurance that the Fickian formulation is always valid as applied to aquifers, and may rest assured that laboratory measurements will differ substantially from field experiments.

In this section a summary of recent measurements and theoretical results concerning dispersion processes in aquifers (these processes are commonly referred to as macro-dispersion) is presented. A table of measured and calibrated values of dispersivities in a variety of aquifers is first presented and discussed. Next a simple model of transport in a one-dimensional flow field developed for the purposes of this study is described and simulation results discussed. Two examples of more sophisticated numerical models of macro-dispersion developed by other researchers are also discussed. Finally, the theoretical parameterizations of the macro-dispersion process developed by Gelhar (1979) and deMarsily & Matheron (1979) are reviewed.

OBSERVED AND CALIBRATED VALUES OF MACRO-DISPERSIVITIES

Researchers have been aware of the macro-dispersion phenomenon for a number of years. For instance, large discrepancies between measured values of dispersivities in laboratory experiments and values measured in the field were reported by Lau, et.al. as early as 1957. At that time the discrepancy was explained to be

"caused almost entirely by the variation in lengths of the paths followed by various streamlines."

In 1964, Warren and Skiba reported a series of elaborate Monte Carlo simulations that explored the behavior of macro-dispersion, and, in 1967, Theis (Theis, 1967) attributed the process to local heterogeneities in hydraulic conductivity. Most observations of the phenomenon, however, have been made only in the last ten years; these observations are summarized in Tables 1 and 2. Although Theis' explanation is still the accepted viewpoint, only recently have theories which attempt to quantify and predict macro-dispersivity values been presented.

It is immediately apparent from Tables 1 and 2 that values of dispersivity in the field are 100 to 1000 times greater than those measured in the laboratory. Measured values for aquifers range from 1m to 134m and values arrived at through calibration of numerical models range from 3m to 200m. As noted in the preceding section, laboratory values of dispersivity tend to be on the order of a median grain diameter, ranging generally from millimeters to centimeters.

Results from three different measurement strategies are presented in these tables. In a single well tracer test, a tracer is pumped into an aquifer through a well. Later, pumping is reversed and the tracer is recovered through the same well. While the tracer is being recovered, the effects of

TABLE 1. Dispersivity values obtained directly through measurements of tracer breakthrough curves in groundwater solute transport.

Author	Setting	α_L	α_T	ΔX	$\bar{u}$	Method
Pickens, et al, 1977	Chalk River, Ontario alluvial aquifer	0.034m	na	na	na	Single well tracer test
"	" , strata of high velocity	0.034 - 0.1m	na	na	na	Single well
"	alluvial aquifer	0.5m	na	na	na	Two well
"	" , strata of high velocity	0.1m	na	na	na	Two well
Fried, 1975						
Groundwater Pollution	Lyons, France alluvial aquifer (stratum)	0.1 - 0.5m	nr	nr	nr	Single well
"	" , (full aquifer)	5m	nr	nr	nr	Single well
"	"	12.0m	3.1 - 14m	nr	7.2m/d	Single well test with resistivity
"	"	8m	0.015 - 1m	nr	9.6m/d	"
"	"	5m	0.145 - 14.5m	nr	13m/d	"
"	"	7m	0.009 - 1m	nr	9m/d	"
"	Alsace, France alluvial sediments	12m	4m	nr	nr	Environmental tracer
Grove & Beetem, 1971	Carsbad, NM fractured dolomite	38.1m	nr	38.1m	0.15m/d	Two well tracer
Webster, Proctor, Marine, 1970	Savannah River, SC fractured schistgneiss	134.1m	nr	538m	0.4m/d	Two well
Robson, 1974	Barstow, CA alluvial sediments	15.2m	nr	6.4m	nr	Two well

TABLE 1. Dispersivity values obtained directly through measurements of tracer breakthrough curves in groundwater solute transport (Continued).

Author	Setting	α_L	α_T	ΔX	$\bar{u}$	Method
Ivanovich, Smith 1978	Dorset, England chalk (fractured) (intact)	3.1m 1.0m	na na	8m 8m	na na	Two well "
Lau, et al, 1957	Berkeley, CA sand/gravel	2 - 3m	nr	8m	0.0036 - 0.016m/s	Multiwell tracer test
Fenske, 1973	Mississippi Limestone	11.6m	nr	na	nr	Single well
Claasen & Cordes 1975	NTS, Carbonate aquifer	15m	nr	na	na	Two well tracer
Schwartz, Muehlen- bachs, 1979	SE Alberta, Milk River sandstone	0(50km)	nr	100km	nr	Environmental tracers
Erlich, et al, 1979	Limestone Pensacola, FA	10m	nr	312m	0.6m/d	Two well

na = reference not available for inspection

nr = no reference to the particular quantity in the reference

TABLE 2. Dispersivity values obtained by calibration of numerical transport models against observed groundwater solute transport.

Reference	Setting	α_L	α_T	ΔX	$\bar{u}$	Method
Konikow, 1977	Rocky Mtn. Arsenal alluvial sediments	30.5m	30.5m	305m	nr	Areal model (moc)
Konikow, Bredehoeft 1974	Arkansas River Valley Co, alluvial sediments	30.5m	9.1m	660x1320m	nr	Areal model (moc)
Helweg, Labadie, 1977	California alluvial sediments	30.5m	9.1m	305m	na	Areal
Pinder, 1973	Long Island glacial deposits	21.3m	4.3m	variable (50-300m)	0.4m/d	Areal (fe)
Bredehoft and Pinder 1973	Brunswick, GA limestone	61m	20m	variable	nr	Areal (moc)
Robertson, 1974	Snake River, ID fractured basalt	91m	136.5m	640m	na	Areal
Grove, 1977	Idaho, fractured basalt	91m	91m	640m	na	Areal (fe)
Ahlstrom, et al, 1977	Hanford site, WA fractured basalt	30.5m	18m	nr	na	Areal (rw)
Robson, 1974	Barstow, CA alluvial deposits	61m	18m	305m	nr	Areal (fe)
Rabinowitz and Gross, 1972	Roswell Basin, NM limestone	21.3m	nr	na	nr	Areal
Robertson & Barracough, 1973	Idaho Falls, lava flows and sediments	91m	137m	variable	na	Areal model
Robson, 1978	Barstow, alluvial sediments	61m	0.18m	3x152m	nr	Profile (fe)
Fried, 1975	Alsace, France alluvial sediments	15m	1m	nr	nr	Profile

TABLE 2. Dispersivity values obtained by calibration of numerical transport models against observed groundwater solute transport (Continued).

Reference	Setting	α_L	α_T	ΔX	$\bar{u}$	Method
Segal & Pinder, 1976	Florida (SE) limestone	6.7m	0.7m	variable	nr	Profile
Gupta, et al, 1975	Sutter Basin, CA alluvial sediments	80 -200m (<80 unstable)	8 - 20m	(2 - 20km)	nr	3 - D model (fe)

(fe) indicates use of a finite element model

(moc) indicates method of characteristics

(rw) indicates a random-walk model

na = reference not available for inspection

nr = no reference to the particular quantity in the reference

Note: Many of the values reported in Tables 1 and 2 were found through compilations by Anderson (1978) and Borg, et al (1976).

the irreversible process, dispersion, are observed. In the absence of dispersion, the tracer would be recovered at exactly the input concentration; in the presence of dispersion, mixing occurs as the tracer flows into and out of the medium. Tracer concentration during recovery is smeared, varies more smoothly and is generally decreased. Concentrations of the recovered fluid are used to calculate a dispersion coefficient by computations based on analogy to laboratory step change tracer tests.

A two or multiple-well tracer test involves inputting a tracer at one well and observing its arrival at another well(s) located somewhere downstream from the first. The time history of concentrations of the tracer at the second well are used to calculate the dispersivity of dispersion coefficient in a manner that is directly analogous to the laboratory step change breakthrough curves discussed in Chapter II.

Finally, model calibrations of dispersivities are generally carried out by trial and error experimentation with dispersivity values to obtain numerical model concentration simulations that are similar to observed values. Because errors may exist in other model parameters and because errors and approximations in the model itself may impair the ability of the model to simulate accurately, estimates of dispersivity obtained in this fashion have limited physical meaning. They are "apparent" parameters, applicable only in the model and model configuration for which they were calibrated.

Observations of tracers added to the system for the purposes of experimentation and calibration (as in the single- and two-well tracer tests) can be used to calibrate models and obtain apparent dispersivities. Alternatively, observations of environmental tracers can be used in calibration. Environmental tracers are constituents of groundwater that are present in the aquifer prior to the experiment, and are either present in anomalous concentrations in limited regions of the aquifer or are otherwise distinguishable from the background groundwater constituents. These constituents can be either natural anomalies or caused by man's activities. Environmental tracers are most often used to

calibrate aquifer models because of the large scale at which a model calibration is carried out. The time required for an artificial tracer to spread over a significant part of an aquifer ranges from hundreds of days to hundreds of years, and the mass of tracer and pumping required to create an observable concentration anomaly in a large area are usually prohibitively large.

The dispersivities listed in Table 1, particularly those observed by Pickens, et al. (1977) and Fried (1975), tend to support the hypothesis that macro-dispersion is largely a result of heterogeneities in hydraulic conductivity. When a tracer test is carried out involving observation wells that sample only from a single stratum, the dispersivity measured is very similar to laboratory values. On the other hand, when the tracer test is carried out with observation wells that penetrate the entire depth of the aquifer, dispersivities tend to be significantly larger. To be more precise, this result suggests that one major difference between the aquifer scale dispersivities listed in the Table and laboratory values of dispersivity is that, in the laboratory, concentrations are measured at what is effectively a single point in the three dimensional porous medium, whereas, in the field, measurements are generally made along a line, i.e., over the depth of the well casing. Thus the aquifer is effectively a two dimensional depth averaged horizontal medium for the purposes of the experiment and all of the effects of horizontal stratification are included in the dispersivity constant.

Tables 1 and 2 also indicate that dispersivity increases with the length scale of the experiment. Notice for instance the results reported by Grove and Beetem (1971), Webster, et al. (1970) and Schwartz and Muehlenbachs (1979). Measurements taken at wells separated by approximately 40m yield a dispersivity value that is only 28 percent of the dispersivity found between wells that were 540m apart. Both are dwarfed by the dispersivity suggested by Schwartz's mega-scale observations. Throughout the Tables and particularly among the calibrated values, there is a tendency for large dispersivities to coincide with experiments involving large distances. This observation is somewhat disconcerting since dispersivity is assumed to be constant in most transport models.

The results reported by Ivanovich and Smith (1978) for a chalk in Dorset, England show the importance of the aquifer structure on macro-dispersivity. Notice that fractured chalk displays a 3m dispersivity while an undisturbed chalk has a dispersivity of 1m. Anticipating theoretical conclusions to be discussed later, Ivanovich and Smith's result suggests that although the very small grain size and conductivity variation of the intact chalk is unchanged by fracturing, upon fracturing, the much larger scaled fractures become the dominant heterogeneities in determining the magnitude of the dispersion process. This large scale variability results in a significantly larger coefficient.

There exists another set of field observations that is not presented in Table 1 and 2. These observations, although carried out at the same scale as those appearing in the Tables, resulted in conclusions that no dispersion coefficients or simple dispersion theory could be applied which would explain the concentration profiles present. Two excellent examples are the work of Winograd and Pearson (1976) and Childs, et al. (1974). In both cases, observations of environmental tracers showed very rapid variations of concentration over relatively short distances perpendicular to the general flow field. As a result, the picture of transport that is developed is of plumes of a tracer moving through an aquifer not by general advection and extensive mixing but through advection along "fingers" or channels of material that exhibit considerably higher permeability than the bulk of the aquifer. These fingers of tracer mix only slightly with the water in the surrounding medium. Winograd and Pearson (1976) explain the phenomenon as follows:

"A major assumption common to, but not implicit in, modeling of regional flow of fluids and... constituents through such media is that to a first approximation they can be treated as homogeneous if (1) their heterogeneity is randomly distributed and (2) the heterogeneities are small in comparison to the aquifer area to be modeled."

Winograd and Pearson suggest that what they observe is the breakdown of these assumptions and, furthermore, that "channeling" will be important regardless of scale. Applying a term from the petroleum engineering literature, Winograd and Pearson refer to this "uneven intrusion or fingering of one fluid into another with which it is miscible" as channeling. They note that channeling may be the result of (1) permeability stratification, (2) gravitational segregation of fluid components, i.e., density effects, and (3) segregation of fluid by differences in viscosity.

This breakdown of the simple macro-dispersion model based on analogy to local scale dispersion arises because the effects of individual variations of hydraulic conductivity are of a scale that is readily observable in the measurements. Simple dispersion models depend for their validity on the effects of hundreds of media variations averaged together to produce a smooth mixing zone. This dependence is common at the aquifer scale as well as at the local scale. When, as in the fractured carbonate aquifer observed by Winograd and Pearson, the scale of conductivity variation is so large (or the number of these large scale variations so small) that the observed concentrations are not the average results of the effects of many of these variations, assumption (2) above--heterogeneities are small in comparison to aquifer scale--is not fulfilled and simple models fail. The cases in which channeling is likely to dominate macro-dispersion in observations are:

1. Media in which a few extensive conductivity variations dominate the transport process.
2. Media in which conductivity variations are abrupt, severe and tend to follow well defined paths.
3. Observations that are made on a scale that is small compared to the scale of variation (see Childs, et al., 1974, for example).

4. Media that show variations in conductivity that cannot be modeled as a random field with apparently random values, spatial extents and orientations assumed by the aquifer properties.

The importance of this phenomena should not be underestimated since its existence in an aquifer indicates that simple model predictions are unreliable. Channeling will only, in general, be observed by chance and thus media in which this phenomenon is likely to occur (regionally faulted and fractured systems, solution riddled aquifers and volcanic media with lava tubes) should not be modeled according to Fick's Law without extensive justification. In other aquifers the assumptions listed in the previous paragraph should be reviewed before simple models are applied. As Winograd and Pearson (1976) conclude, "Continued respect for the heterogeneity of such strata appears mandatory."

Table 2 presents a number of dispersivity values that have been obtained by modelers in calibrating transport models. They tend to follow the general trends as discussed with regards to Table 1.

Three characteristics of model calibration values should be discussed in connection with the values reported in Table 2. First, in many numerical modeling efforts, dispersivity can never be calibrated well and is chosen by default to be some convenient value. This appears to be especially true for large scale models. Robson (1974) concluded, for instance, that numerical model predictions are less sensitive to variation of the dispersivity constant as the node spacing of the model increases. This effect is important because the less sensitive the model is to the parameter, the more difficult the parameter is to fit; however, less sensitivity also suggests that the fit of that particular parameter is not as critical to the accuracy of the model. Second, Robson also noted that a much larger dispersivity was required in his numerical models to predict observations than was measured by a two well

test. This observation suggests that the model parameter, dispersivity, includes processes and approximations that are not measured in nature. Finally, the relationship between longitudinal and transverse dispersivities is not clear. There are calibrations that result in transverse dispersivities that are less than, equal to and larger than the corresponding longitudinal dispersivities. Despite this apparent confusion, Robson (1978) has suggested that there is a difference between the calibrated transverse dispersivities found in areal and profile models. Because of horizontal bedding, Robson suggests that transverse dispersivity in profile models is much smaller than in areal models.

In summary, the most important fact to be gleaned from Tables 1 and 2 is that dispersivities in the field tend to be 100 to 1000 times the values measured in the laboratory experiments. A number of other trends are also suggested:

1. The method of measurement or ascertaining dispersivities has a direct bearing on the value that will be obtained. Single well tests tend to yield the lowest dispersivities followed by two well tests and then environmental tracer tests. This conclusion is related in part to the effect that the scale of an experiment or measurement appears to have on the resulting dispersivity. Also, different model structures, such as profile versus areal and detailed nodal grids versus coarse grids, seem to result in variations in calibrated values of the dispersivity. Finally, the coarseness with which measurements are made, for instance the range of depth over which observation wells are open to the aquifer, has a direct bearing on the resulting dispersivity estimates.
2. The length scale of the measurement or model has an effect on the resulting estimate of dispersivity. It appears that the dispersivity increases along with the length between wells in a two well tracer test.

3. The length scale of aquifer property heterogeneities and the magnitude of variation of these properties appear to be important in determining dispersivities.
4. The numerical model parameter, dispersivity, has limited physical meaning and tends to be a fitting parameter which includes calibration errors for other model parameters as well as model structure errors and approximations.
5. Large scale heterogeneities, both deterministic and statistical, should, if possible, be taken into account since they may represent important non-uniformities in the dispersion processes and even a breakdown of the assumptions on which the dispersion model is based.

A SIMPLE MODEL OF A MACRO-DISPERSIVE MEDIUM

In the preceding paragraphs, we noted that the accepted explanation for the macro-dispersion process is that it is the result of aquifer property heterogeneities. In order to investigate the consequences of these heterogeneities, a simple numerical model of mass transport based on a simple conceptual model of a macro-dispersive medium was developed. A number of illustrative simulations were performed. A general description of the conceptual model upon which this simple model is based is presented below followed by a discussion of the simulations performed and the general results obtained. A more detailed discussion of the model and the individual simulations is presented in Appendix A and B, respectively.

Description of a Simple Conceptual Model of a Macro-Dispersive Medium

Perhaps the simplest medium in which one might expect to encounter macro-dispersive transport is a porous medium that is vertically stratified into horizontal layers of different hydraulic conductivities. The simple model developed for this study is based on just such a conceptual model. Figure 1A illustrates a scenario of radionuclide release which might be simulated by the model. The layered shale section is idealized to the simple conceptual model shown in Figure 1B and the simple numerical model is employed to predict the extent of transport of the radionuclides along the medium.

The advecting flow of water through the medium is assumed to be predominantly parallel to the layering and is driven by a regional hydraulic gradient. Transport of the radionuclides or some tracer substance through the medium proceeds through the combined action of advection by the flow field and dispersion at the local scale. We have noted in Chapter II that local dispersion represents a relatively small correction to the advection process. In this case, however, local transverse dispersion may be expected to play an important role in the overall transport because dispersion perpendicular to the flow can move components of the "cloud" of contaminant between layers. Since the different layers have different hydraulic conductivities, and therefore different advection rates, dispersion between layers can be very important in determining the extent of transport and dispersal of the contaminant. If parts of contaminant find their way into layers of very different conductivities the contaminant cloud will be dispersed over a much larger portion of the medium than might be expected as the result of local dispersion processes alone. Finally, if the concentration profiles of the contaminant along the medium are measured by means of a technique that fails to differentiate between layers, such as observing by means of a well that is perforated over the entire depth of the medium, the widely dispersed contaminant cloud will appear to be undergoing extensive mixing in its travels along the medium.

FIGURE 1A. A scenario of radionuclide release into a layered porous medium.

FIGURE 1B. Progress of a tracer point through the layered shale bed as modeled by the simple random-walk model.

NOTE: The radionuclide transport scenario in Figure 1A is idealized to the conceptual model illustrated in Figure 1B and simulated by a simple random-walk model.

A simple numerical mass transport model was employed to test the hypothesis that the heterogeneous hydraulic conductivities in this simple layered medium will lead to macro-dispersive behavior. The simple model employs the random-walk algorithm for solving the advective-dispersion equation and is described in detail in Appendix A. A number of simulations were performed to demonstrate the ability of this simple model to simulate macro-dispersive behavior as well as to test the sensitivity of macro-dispersion to various parameters of the medium.

Simulations of a Simple Macro-Dispersive Medium

Ten simulations were performed in order to investigate the macro-dispersion process in this simple layered medium. A brief description of each of the simulations is presented in Table 3. In the next paragraph, the results of the baseline simulation (F.2) will be described briefly as an example of the results obtained. Following that description, a summary of the general conclusions arrived at through the ten simulations, that is, the effects that certain aquifer and transport model parameters have on macro-dispersion in a heterogeneous medium, will be presented. A more detailed description of the remaining simulations (F.3 - F.11) and their relation to the baseline simulation is presented in Appendix B.

Baseline Simulation Results

The progress of the tracer as it is dispersed through the layered medium under the baseline conditions is illustrated in Figure 2. Under the baseline conditions the tracer is transported along a porous medium made up of 30 horizontal layers. The layers have arbitrarily chosen hydraulic conductivity values ranging between 2 m/yr to 9.2 m/yr with an average of 6.1 m/yr and a standard deviation of 2.22 m/yr. The advecting flow is parallel to the layering. The histograms and parameter values presented in Figure 2 are explained in Appendix A. During the 200 years of simulation, the tracer is advected an average of 484.7 meters and, as a result of differences in

TABLE 3. List of simulations and resulting apparent dispersivities.

Simulation ID	Subject	Apparent Dispersivity
F.2	Transport under baseline conditions	23.8 m
F.3	Transport with no mixing between layers	40.6 m
F.4	Transport with large local dispersivity values.	3.2 m
F.5	Transport in a flow field not exactly parallel to layering	4.7 m
F.6	Transport when the advection rate is halved	19.4 m
F.7	Transport when the conductivities of the layers are uniformly decreased	60.0 m
F.8	Transport when the conductivities are more variable	76.1 m
F.9	Transport from an initial point source	19.6 m
F.10	Transport from a widely spread initial distribution	20.2 m
F.11	Modeling the layered medium as a <u>simple</u> Fickian system	24.7 m

SIMULATION ID : F.2
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

FIGURE 2. Distribution of tracer at 50 year intervals as it is transported along a layered porous medium.

NOTE: This simulation serves as the baseline transport situation for the series of simulations.

advection rates in the various layers, spread over a distance of 600 meters. The varying values of dispersivity reported with each histogram suggests that the dispersal of the tracer from an initial pulse of contaminant to a very broad, dilute "cloud" after 200 years is a continuous, gradual process, and proceeds at a rate that varies with time during the period of simulation. For the first 50 years an apparent dispersivity of 11.5 meters describes the rate of spreading, for the first 100 years the value calculated is 19.1 meters and for the first 150 years the dispersivity calculated is 22.9 meters. During the course of the 200 year simulation the tracer spreads and gradually begins to assume a roughly symmetric profile. The jagged shape of the histogram which detracts from this symmetry is in part due to the statistical approximations inherent in the model, in part due to the discrete spacing of histogram intervals and finally is, in part, the result of the assumed discrete variations in advection rates between layers. Only the last is important in understanding macro-dispersion. It is therefore important to view the profiles illustrated as rough indicators of what the actual concentration profiles would be. The imagination required to arrive at a smooth concentration profile is an input required by many random-walk transport models.

Examination of the results of the baseline simulation as well as most of the other simulations demonstrates that this simple model of tracer transport through a heterogeneous medium tends to reproduce two of the basic trends observed in field studies of dispersive behavior and discussed above in connection with Tables 1 and 2. The two trends are:

- ° The apparent dispersivity in a heterogeneous medium may be several orders of magnitude larger than the local dispersivities measured within a single homogeneous material, and
- ° the dispersivity may be a function of time or distance advected

The first trend is illustrated by the baseline simulation results shown in Figure 2. The apparent dispersivity is 23.8 m in the baseline case while the local longitudinal and transverse dispersivities are assumed to be 1 cm and 3 mm, respectively. Notice in Table 3 that the apparent dispersivities calculated in the simulations range in value from 3.2 meters (Simulation F.4) to 76.1 meters (Simulation F.8). The average value of the apparent dispersivities is 31.3 m. All of the values are considerably larger than the assumed local dispersivities. Another way of viewing the effect of macro-dispersion in the baseline results is to notice that if only local dispersion processes were active, the standard deviation of the tracer distribution for the year 200 would be expected to be

$$\sigma = [2 \alpha d]^{1/2} = [2 \alpha d]^{1/2} \quad (3-1)$$

with α equal to the local longitudinal dispersivity and d equal to the mean distance advected by year 200. The total distance over which the tracer would spread is about four times the standard deviation (two standard deviations on each side of the mean). For Simulation F.2, the baseline simulation, this distance would be

$$\begin{aligned} 4\sigma &= 4[2\alpha d]^{1/2} = 4[2(0.01\text{m})(485\text{m})]^{1/2} \quad (3-2) \\ &\approx 12.5\text{m} \end{aligned}$$

For Simulation F.2, the baseline simulation, four times the standard deviation of the spreading tracer at 200 years is 592m. Thus, it is apparent that the local dispersive effects are being dwarfed by some other dispersive process.

The second trend is evidenced by the considerable variation in the simulation of the dispersivities calculated at times 50, 100, 150 and 200 years. This trend is indicated by the results shown in Figure 3 which presents a graph of the variance of the tracer cloud versus the mean (average) position of the tracer points along the flow path during the baseline simulation. The

dispersivity as defined by Equation (3-3) is equal to half the slope of this curve at any point. It is clear that the slope of the curve in Figure 3 and, therefore, the dispersivity in the baseline simulation varies as the tracer is transported along the medium.

FIGURE 3. Variance, σ^2 , of tracer cloud as a function of average distance advected, d , in the baseline simulation.

Summary of Simulations Results

Comparison of transport under the baseline conditions with the results of the other nine simulations presented in Appendix B suggests that the macro-dispersion process is sensitive to a number of parameters and properties of the layered medium. The general trends may be summarized as follows:

- ° The heterogeneity of the hydraulic conductivities in our layered medium leads to the extensive dispersal of the tracer which, in this simple model, we refer to as "macro-dispersion."

- ° When no mixing between layers in the medium occurs the Fickian description of transport is inadequate to describe the dispersal process. The result is the transport of tracer in a series of pulses which move through the medium at different rates. This behavior is related to the problem of "channeling" discussed by Winograd and Pearson (1976).
- ° Increasing the amount of mixing between layers, whether by increasing the local transverse dispersivity or by adding a vertical component to the flow field, leads to a reduction in the apparent dispersivity.
- ° The macro-dispersion process is a function of the average distance that the tracer is transported.
- ° Macro-dispersion is a function of the mean hydraulic conductivity $\bar{K}$ as well as the variance of the conductivity σ_K^2 . The coefficient of variation of the conductivity, $\sigma_K/\bar{K}$, is a useful parameter of the process.
- ° The initial location of the tracer has a transitory effect on the macro-dispersion process.
- ° Finally, a simple Fickian model of the medium, although it may be calibrated to reproduce the extent and statistics of macro-dispersion at one time, may be expected to project concentration profiles that do not correspond to more detailed models and will not even reproduce the statistics at other times. As noted above, macro-dispersivities may be expected to be time varying.

Before proceeding to a discussion of the results obtained by other researchers applying more complex numerical models and to a discussion of the rigorous analytical results that are available, it is important to place the results listed above in perspective. The model applied above is a very simple representation of highly complex physical mixing processes in natural porous media. The model is simple both conceptually and computationally. The results outlined above, therefore, should not be viewed as having been rigorously tested or proved. Rather, the conclusions listed above have been abstracted and generalized from the simple model results on the basis of qualitative considerations of the processes at work in transport through the medium. The simulation results presented above and in Appendix B were chosen and presented on the basis of their instructional value. On the basis of the intuition developed through this exercise, we believe that the results listed above will prove correct in many modeling situations.

TWO AND THREE-DIMENSIONAL MODELS OF MACRO-DISPERSION

Two extensive attempts to simulate macro-dispersion processes numerically were found in the literature. These models were similar in concept to the simple one-dimensional model discussed previously but have the advantage of multidimensionality. That is, one investigation used a random-walk model of transport through a medium that displayed two-dimensional conductivity variability (Schwartz, 1977) while the other used a finite difference model of flow through a medium with three-dimensional conductivity variations (Warren and Skiba, 1964). These models represent systems that are physically more believable than the one-dimensional model above and thus, add an important verification and extension to the conceptual picture we have formed.

In each case, it was verified that spatial variation of hydraulic conductivity is the likely cause of macro-dispersion. Warren and Skiba (1964) showed that porosity variation is a secondary factor in causing macro-dispersive mixing. They demonstrated that both the magnitude and length scale of conductivity variation are important parameters of macro-dispersion processes.

Schwartz (1977) attempted to parameterize macro-dispersion effects using his two-dimensional model. Perhaps the most important result reported by Schwartz is that unless a sufficiently random medium is simulated, apparent dispersivities never approach constant values but vary erratically or grow without bound. This growth may occur where systems display periodic or nearly deterministic variations of conductivities, or where the scale of variation is large compared to the size of the medium being modeled. Recently, Schwartz, (Smith & Schwartz, 1980) reported that in more extensive studies involving many randomly generated conductivity fields, these limits on the use of constant dispersivities have been verified. This finding has lead Schwartz to suggest that macro-dispersion theory is inadequate to explain transport in real aquifers since 1) current theory based on Fickian analogies assume a statistical averaging of conductivity variations that is not likely to occur until very long distances are transversed, and 2) aquifers are not, he conjectures, particularly statistically homogeneous over such distances. This last point is, of course, purely conjecture and has not been demonstrated. Generally, the question raised is: Is there enough statistical variation within a single aquifer to allow macro-dispersion coefficients to reach a value that is the result of the statistical nature of the variations rather than the result of a single variation? If not, a time varying coefficient will result or, even more problematic, channeling on the aquifer scale will be encountered.

ANALYTICAL PARAMETERIZATIONS OF MACRO-DISPERSION

Currently, two analytical approaches to a parameterization and complete mathematical description of macro-dispersion are available. The approaches are closely related and yield analogous results. Gelhar, et al. (1979) at New Mexico Institute of Mining and Technology have pursued a course of investigation involving a Fourier-Stieltjes integral transform analysis of transport through an infinite porous medium with a one-dimensional stochastic variation of hydraulic conductivity. Meanwhile, Matheron and deMarsily (1979) at Fountainebleau and other researchers in France have conducted parallel investigations through Laplace transform analysis of a Brownian motion transport model, assuming a similar medium. The results obtained by these two research groups suggest that the validity of a Fickian description of transport in a natural porous medium is severely limited; however, specific objections to the basic model that these two schools have assumed have been raised and will be discussed after a presentation of Gelhar and Matheron's work.

Gelhar et al. assume a layered aquifer which is infinite in extent with flow along the horizontal layers. Hydraulic conductivity varies randomly with depth but is uniform at any particular depth. Thus, hydraulic conductivity, $K(z)$, is only a function of depth z . Because of the complexity of real aquifers and the impossibility of determining $K(z)$ at all points in the medium, a stochastic model of the aquifer is assumed; only the mean value, $\langle K \rangle$, and variance-covariance of conductivity are assumed known. With this information and an understanding of the governing equations and boundary condition (constant gradient), Gelhar proceeds to calculate the macro-dispersivity coefficient for the medium.

The procedure for obtaining this coefficient is rather complex; the interested reader is referred to Gelhar's work (1979) or his previous work in stochastic groundwater hydrology. Suffice it to say, Gelhar shows the macro-dispersivity coefficient is closely approximated by

$$\alpha_A = \int_{-\infty}^{\infty} \frac{S_{KK}(z)}{\langle K \rangle^2} \frac{(1 - e^{-\beta t})}{\alpha_T z^2} dz \quad (3-3)$$

where α_A is the longitudinal macro-dispersivity; $\langle K \rangle$, the mean hydraulic conductivity, t is time and

$$\beta = \alpha_T U z^2 \quad (3-4)$$

α_T is the local transverse dispersivity and U is the mean seepage velocity. S_{KK} is the power density spectrum of the conductivity K , a measure of its random variation. It is, more exactly, the inverse Fourier transform of the covariance function of K , $\text{Cov}(z)$.

The resulting dispersion coefficient is generally variable in time, but if a covariance defined as

$$\text{Cov}(z) = \sigma_K^2 \left[1 - \frac{5}{3} \frac{|z|}{\ell} + \frac{1}{3} \frac{z^2}{\ell^2} \right] e^{-|z|/\ell} \quad (3-5)$$

with σ_K^2 equal to the variance of K and ℓ , a length scale of the conductivity variation, is assumed, after a long time, the dispersivity approaches asymptotically the constant value,

$$\alpha_A \rightarrow \frac{1}{3} \frac{\sigma_K^2}{\langle K \rangle^2} \frac{t^2}{\alpha_T} \text{ as } t \rightarrow \infty \quad (3-6)$$

Because the transport process may only be characterized as truly Fickian when the dispersion coefficient is constant, this asymptotic value of D_A is an important assurance that macro-dispersion can be approximated with models based on the simple diffusion analogy within zones of relatively constant U . During the initial stage of the dispersion process, Gelhar finds that the dispersivity behaves quite differently, varying as

$$\alpha_A = Ut \frac{\sigma_K^2}{\langle K \rangle^2} \quad (3-7)$$

growing linearly with time as if only different rates of advection within the medium were causing spreading. Upon choosing "reasonable" values for the various parameters, Gelhar demonstrates that a constant value of α_A of roughly 19m is essentially reached after advection occurs over a distance of about 1000m.

Gelhar also reports that a thesis student, R. Naff (1978), has shown that porosity variations should be unimportant in macro-dispersion in natural materials.

Matheron and deMarsily (1979) have extended Gelhar's results to include several different conductivity covariance structures and to include a small component of flow across, in addition to the predominant flow parallel to the layers. What these researchers realized and Gelhar acknowledges in his work is that the covariance structure that was assumed in Gelhar's work is very special and was chosen explicitly because it leads asymptotically to Fickian results. Gelhar recognized and Matheron and deMarsily demonstrated

that for most possible covariance structures the macro-dispersion coefficient increases to infinity as time proceeds. Thus, in addition to a dependence on the various parameters listed above, the macro-dispersion coefficient seems to depend on the covariance structure chosen to describe the variability of the conductivities.

On a more reassuring note, Matheron and deMarsily show that when a small non-random component of velocity is applied across the layers, i.e. adding a second dimension to the flow field, the dispersion coefficients are more likely to approach asymptotically constant values that are dominated by mixing due to the vertical flow. This behavior is exhibited for most reasonable covariance structures. The effect of including even a small two-dimensional component to the analysis is to produce results that are much more physically pleasing, suggesting that the one-dimensional nature of the analysis may be a severe problem.

A group of "reasonable" values for the parameters were used by Matheron and DeMarsily to show that:

1. environmental tracers will be necessary to measure macro-dispersion coefficients adequately, and
2. measurements will, in many cases, have to be carried out at the same scale as the transport problem of interest.

Environmental tracers are necessary because of the long time and distance scales required to reach the asymptotic value and because the macro-dispersivity measured will be a function of the flow regime including the average horizontal and vertical flow rates. Injecting enough tracer for a large scale experiment may be expected to change flow patterns and flow rates and thus the measured macro-dispersivity will not be indicative of macro-dispersion under natural

conditions. The scale of measurement is important because of the time dependence of macro-dispersivity. Measurements of transport situations with a time scale less than or equal to the time required to approach an asymptotic limit will be applicable only to the particular measurement time scale.

Although the analytical results of Gelhar et al. and Matheron and DeMarsily suggest severe limits on the use of a Fickian model of transport in natural aquifer systems, there are several criticisms to the model assumed in their work which suggest a reason for a more optimistic view of the matter.

First, in these analyses, in order to reach a solution, the medium considered is necessarily assumed to be infinite. During the early stages of transport through very large and thick aquifers, this assumption may be an acceptable approximation. After a sufficient time, however, it should be assumed that boundary conditions will play an important role in determining the extent and time dependence of macro-dispersion processes. In particular, since many transport models are applied to relatively thin, flat aquifer units with complete mixing assumed over the depth of each unit, top and bottom boundary conditions will limit the amount of conductivity variation that can add to the macro-dispersion process.

An even more important criticism has been raised, in anticipation of the analytical work discussed above, by Dagan (1979). Dagan has warned against the results obtained in studies of layer models of dispersive media, ie. one-dimensional investigations. Through a study of simplified models of formation structure, Dagan analyzed the variation of the specific discharge,

$$q = un$$

with n equal to the porosity and u , the seepage or pore velocity, in a random permeability field. Comparison of his results for a model of one-dimensional permeability variation (a layered medium) to results obtained with models of media exhibiting two- and three-dimensional permeability variability showed that

the layered model results did not agree with the more complex results. For instance, when permeability is assumed to be randomly varying according to a log-normal probabilistic distribution and using a physically reasonable variance for the logarithm of permeability

$$\sigma_{\ln K}^2 = 1$$

Dagan calculated that

$$\frac{\sigma_q}{\langle q \rangle} = 14 \quad \text{for the 1-D model} \quad (3-10a)$$

$$\approx 0.8 \quad \text{for the 2-D model} \quad (3-10b)$$

$$\approx 1 \quad \text{for the 3-D model} \quad (3-10c)$$

where σ_q is the standard deviation of q and $\langle q \rangle$ is the mean value of q , the specific discharge. Assuming somewhat more permeability variation (and still not an unbelievable value),

$$\sigma_{\ln K}^2 = 4$$

the disparity between models becomes clearer

$$\frac{\sigma_q}{\langle q \rangle} = 4 \times 10^4 \quad \text{for 1-D variation} \quad (3-11a)$$

$$\approx 1 \quad \text{for 2- and 3-D models.} \quad (3-11b)$$

Since macro-dispersion is very much a function of the variations in discharge rates induced by permeability variations, these comparisons suggest that the 1-D analytical results discussed earlier may yield pessimistically high estimates of dispersivity. This is because the variation of the flow and advection rates from point to point in a layered medium is only dependent on the conductivity in that layer. In a two- or three-dimensional model, on the other hand, flow rates at any point depend on the conductivities at all other connected points. Thus, the average properties become important with variations around the averages tending to cancel each other. Since it is these variations in flow rates that are interpreted as macro-dispersion, as the variations cancel, dispersion coefficients decrease and behave in a more Fickian manner.

Because of these results, the analytical work of Gelhar et al. (1979) and Matheron and deMarsily (1979) should be viewed as a first step in the parameterization and analytical prediction of macro-dispersion coefficients. These results indicate the important parameters and their general functional relationship to macro-dispersion but should not be employed without great caution. Until two- or three-dimensional models of variation are included in the analysis, the applicability of analytical results is dubious.

SUMMARY

In summary, macro-dispersion is a function of the following factors:

1. The length scale of the region of interest, i.e. the distance over which advection is expected to occur in a particular transport situation.
2. Aquifer property variability. Hydraulic conductivity or transmissivity variations are most important with porosity variability of second order importance.

3. The flow field. Macro-dispersion is a function of the tortuosity of large scale flow paths and the general seepage velocity.
4. The degree to which aquifer property and flow variability have been included in the advective terms of a model. If, for example, all flow variabilities were adequately modeled by a very complex, ideal advection model, then the dispersion coefficient required to complete the transport model would be the local scale dispersion and diffusion coefficients.
5. Local dispersion processes. These processes not only serve as a background for larger scale mixing, but play an important role in moderating the effects of aquifer property variations.

Thus, macro-dispersion is parameterized in terms of

- σ_K^2 or $\sigma_{\ln K}^2$, the variance of hydraulic conductivities or transforms of that aquifer property,
- $\langle K \rangle$, mean value of hydraulic conductivities and other medium properties,
- $\bar{v}$, the mean seepage velocity,
- D_T and D_L the local transverse and longitudinal dispersion coefficients,
- t , time or its surrogate, x , distance advected, and

- λ , the correlation length or other length scales of the variations of medium properties.

Finally, it must be recognized that doubts have been raised concerning Fickian models of macro-dispersion and their validity in many situations. In particular, the channeling phenomena reported by Winograd and Pearson (1976) suggest that the assurance with which regional transport models based on Fickian analogy may be applied is extremely limited. Recognition of the unphysical results that models produce for early times when very large coefficients are applied suggests that, at the very least, variable coefficient values should be anticipated.

IV. NUMERICAL MODELING OF REGIONAL TRANSPORT PROCESSES

INTRODUCTION

Numerical models of regional transport through aquifer systems are an accepted tool in water resource planning efforts involving both groundwater quantity and quality. These models are often the only available means of handling complex boundary conditions, multiple inputs and spatially distributed parameters of these systems. With the development of high speed, inexpensive computer facilities regional models have seen extensive application.

Two basic problem areas must be faced before deciding whether a numerical transport model (or any other numerical model) will produce meaningful results in a particular situation. First, decisions must be made regarding the accuracy of the numerical model to be applied. There are a number of ways of increasing accuracy, ranging from choices of the general model structure, to choices of modeling strategy and solution techniques, and to details like choosing particular spatial grids. The second problem area is the question of how well numerical models can be calibrated. A model that is theoretically accurate is of no practical use unless it is structured so that it's parameters can either be measured or otherwise fitted to adequately simulate the behavior of the physical system.

In this section the first of these problem areas will be discussed at some length. The four major available numerical approaches to modeling transport processes will be reviewed and compared in view of a series of accuracy and applicability criteria. This discussion will be followed by a series of suggestions with respect to modeling strategies.

STRUCTURE OF TRANSPORT MODELS

Numerical transport models for aquifers are collections of algebraic equations which yield approximate solutions of the advection-dispersion equation

$$\frac{\partial C}{\partial t} + \sum_i u_i \frac{\partial C}{\partial x_i} = \sum_i \sum_j \frac{\partial}{\partial x_i} D_{ij} \frac{\partial C}{\partial x_j} \quad (4-1)$$

with the summations carried out over the number of spatial dimensions being modeled, u_i equal to the component of seepage velocity in the i direction and x_i the spatial dimension in the i direction. D_{ij} is the ij^{th} element of the dispersion tensor, although in most models the medium is assumed to be isotropic; with that assumption, the dispersion tensor becomes a simple function of the longitudinal and transverse dispersion coefficients.

Before this equation can be solved, values of the seepage velocity must be available. As long as the concentration of the constituents whose transport is being modeled does not effect the flow field, the seepage velocities can be calculated beforehand using another numerical model or field observations. If, on the other hand, the concentration of constituents should effect the density, viscosity or other important physical properties of the transporting fluid or solid matrix, then the flow field has to be solved for concurrently with the concentration fields. This approach is generally accomplished by iterating between flow field solution and transport solution until a solution is achieved that satisfies both models. For the purpose of this investigation it will be assumed that flow patterns are independent of transport. This assumption represents only a slight restriction on the validity of the following discussion of numerical transport models.

Often, the seepage velocities are not input to the transport model because they are not directly measured or calculated by most available techniques. Generally, it is the piezometric head configuration that is simulated or observed. The piezometric head configuration, hydraulic conductivity values and porosities must be used to calculate seepage velocities (Anderson, 1978). This step in initializing the model is a possible source of large errors and should be critically assessed during the design and implementation of models.

Quite often in practice, modelers assume that the advective component of the transport equation dominates the dispersion process completely. Under this assumption, very simple models of groundwater quality can be developed. A simple mass balance approach to the constituent of interest can be applied or advection of hypothetical particle tracers through a system can be simulated (Bear, 1979). This modeling approach has been used extensively with some success. Because laboratory tests have always yielded dispersivities, α , on the order of centimeters and because it has often been assumed that field values should be correspondingly small, the assumption that dispersion is negligible has long seemed to be a valid one. For instance, if the distance that advection carries a tracer in time t is:

$$d = u_i t \quad (4-2)$$

while the distance over which dispersion spreads the constituent is roughly

$$\sigma = \sqrt{2Dt} = \sqrt{2\alpha d} \quad (4-3)$$

If α is 0.01m and the distance advected is 1m then the ratio of mixing distance to advected distance becomes

$$\frac{\sigma}{d} \approx 0.02 \quad (4-4)$$

and dispersion represents a very small correction to advective transport. It has been shown in the last section, however, that when the advection distance is 100 or 1000m in the field, the dispersivities are not on the order of centimeters, rather they are on the order of tens of meters. For instance, using conservative values for α and d , ($\alpha = 30\text{m}$ and $d = 1000\text{m}$)

$$\frac{\sigma}{d} = \frac{\sqrt{2\alpha}}{d} \approx 0.25 \quad (4-5)$$

and if $\alpha = 30\text{m}$ and $d = 10\text{km}$,

$$\frac{\sigma}{d} = 0.11 \quad (4-6)$$

A quick glance at the dispersivity values in Tables 1 and 2 suggests that 30m is a very conservative estimate for this scale. It appears then that dispersion is a very important process and cannot, in regional simulations, be neglected offhand. Unless otherwise demonstrated it should be assumed that the full advection-dispersion equation must be modeled if trustworthy results are to be obtained.

Once the flow field is available, a solution of the full advection-dispersion equation is obtained by applying one of many numerical modeling techniques. In addition to a description of the flow field for each time step to be simulated, the following information is required:

1. constituent boundary conditions, such as where the constituent may enter or leave the system and the existence of any point sources or sinks,
2. constituent initial conditions, where the constituent is initially found, and

3. dispersion coefficients. These coefficients must be specified for each segment of the model and may either be presented in the form of longitudinal and transverse coefficients or x- and y- direction dispersion coefficients.

In addition, a more complete modeling effort generally requires the inclusion of chemical and nuclear processes. When these processes are included both appropriate governing equations and appropriate descriptive parameters must be specified.

NUMERICAL TECHNIQUES FOR THE SOLUTION OF THE ADVECTION-DISPERSION EQUATION

Four principal solution techniques have been applied to numerically simulate the advection-dispersion processes. Computer codes for mathematical models employing each of these four solution techniques exist and are available in the public domain.

Finite difference models solve the governing equations approximately by substituting a series of linear algebraic equations for the differential advection-dispersion equation evaluated at a number of points in space and time. Thus, finite difference models generally solve for concentrations at a series of distinct points in space and time. Taken together, these points may be generated through truncation of Taylor's series representations of the various terms in the governing equation. The procedure by which these equations are generated will become more evident during the discussion of numerical dissipation in finite difference models presented below. Finite difference models are rather simple models to derive, program and understand and this is perhaps their primary advantage. These models can be extended to calculate concentrations which represent average values within the area surrounding each grid point, but this capability is probably handled better by switching to a finite element model.

Finite element models are solutions based on minimization of errors in approximating the governing equation as a series of linear equations. The minimization is accomplished through application of Galerkin methods or variational calculus. The general approach for a one-dimensional geometry is to minimize the integral over the domain of interest of the residual

$$R = \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} \quad (4-7)$$

multiplied by some weighting function, i.e. set

$$\int_A R \cdot \phi \, dx = 0 \quad (4-8)$$

where A is the domain of interest. In the interests of generating a manageable, linear set of equations, a number of weighting functions are chosen to take on some normalized characteristic form (linear, quadratic, Hermite polynomial, etc.) within a "small," finite subdivision of the domain A made up of a number of finite elements; outside its subdivision a weighting function is defined to be identically zero. The regions in which weighting functions are nonzero and smoothly varying are called finite elements. Using this approach, the integration shown in the equation above is carried out numerous times, but each time the integration is limited to a small area. The next step, upon choosing the weighting functions ϕ_j , is to approximate the concentration configuration by a linear combination of the same weighting functions,

$$\hat{C} = \sum_{j=1}^N c_j(t) \phi_j(x), \quad (4-9)$$

with the $c_j(t)$ equal to the set of coefficients which minimize the above integral. Each $c_j(t)$ is associated with one of the weighting functions and is associated in particular with the value of $\hat{C}$ at a point or node. The forms of the weighting functions ϕ_j determine the way $\hat{C}$ varies between node points. The final solution $\hat{C}$, then is a continuous function in

space, although not necessarily continuously differentiable between elements. The numerical model works in terms of the coefficients $c_j(t)$ and N discrete equations are generated, where N is the number of weighting functions or solution node points. Integration is carried out in general analytical terms for each of the weighting functions before the model is coded. The numerical model implements the actual numbers and parameter values and solves the simultaneous equations that are generated. Generally the time derivative in the advection-dispersion equation is approximated by a finite difference scheme quite adequately. Obviously, from this brief and incomplete description of finite element solutions, it is clear that this method is complex and potentially very confusing. A number of good references are available on the subject, including Finite Element Simulation in Surface and Subsurface Hydrology, (Pinder and Gray, 1977); this reference provides much more extensive descriptions of the technique. However, it should be recognized that development of finite element models requires a large initial investment of time in learning the complex theory and application associated with it. An additional consideration is the difficulty involved in explaining the method to interested parties, critical among those are often the management personnel who would use the solutions obtained.

Models based on the method of characteristics solve for concentration using two equations

$$\frac{dx}{dt} = u \quad \text{and} \quad \frac{dc}{dt} = \frac{\partial}{\partial x} D \frac{\partial c}{\partial x} \quad (4-10)$$

Taken together these equations are equivalent to the advection-dispersion equation. This method was first employed by A.O. Garder, D.W. Peaceman, and A.L. Pozzi in 1964 to eliminate numerical dissipation, a problem that will be discussed later in this section. The first equation is solved by applying a moving particle advection model which traces the progress of hypothetical packets of the constituent of interest as they would be carried through the medium by the existing flow patterns. For each time period of simulation, the vector-valued position of packets is calculated

$$\bar{X}(t) = \int \bar{u}(\bar{X}, t) dt \quad (4-11)$$

where $\bar{u}(\bar{X}, t)$ is the vector of velocity. The position $\bar{X}$ is rather easily and accurately estimated by

$$\bar{X}(t + \Delta t) = \bar{X}(t) + u(\bar{X}(t), t) \Delta t \quad (4-12)$$

if $\bar{u}$ is known in sufficient detail and if Δt is chosen to be a sufficiently small time. Next the second characteristic equation is solved.

Traditionally, this is accomplished

1. by calculating the average of the concentrations in the packets present in each model cell after advection. The model cells are the discrete areas into which the numerical transport model is deviated. The cells can be chosen arbitrarily, although quite often they are chosen to coincide with the geometry of the solution scheme used to obtain the velocity configuration,
2. all packets in each cell are assigned a new concentration value equal to the average in the cell in which they are located,
3. the concentration gradients between cells are estimated next, and
4. the concentrations of the packets in each cell are reduced (or increased) to a uniform value according to a finite difference or finite element form of the second characteristic equation above.

An alternative and very efficient scheme for solving the second characteristic equation above is the random-walk model. In this approach, a particle tracing advection model similar to the one employed in the traditional method of characteristics model is used to simulate advection. At the end of each advection time step, the particles, which in this case represent particles of constituent rather than packets of constituent and water, are dispersed by being displaced a random distance in a random direction. Concentrations are calculated by counting the resulting number of elements in each cell and comparing this to the initial conditions. This solution technique is based on the realization that a normal probability distribution is a solution to Fick's Law. This solution method is outlined for a one-dimensional geometry in Appendix I.

CRITERIA FOR ASSESSMENT OF NUMERICAL TRANSPORT MODELS

A comparison of the various modeling approaches discussed above should deal with questions of simulation accuracy first and foremost. It is essential that these questions be faced since numerical error is a large and difficult problem in mass transport models. The structure of the advection-dispersion equation in many situations tends to be first order hyperbolic and, as such, numerous problems arise. A simple example of the problems associated with the hyperbolic structure will be discussed below. Unless the numerical errors are specifically dealt with and controlled, little confidence can be placed in model results. Theoretically, an arbitrary degree of numerical accuracy could be obtained if enough resources were allotted to that purpose; however, this is never the case. Thus, questions of model efficiency and economics must be weighted against the demands of accuracy. Finally, the structure of numerical models should always be chosen to maximize, within the above constraints, such desirable properties as flexibility, ease of implementation, and ease of calibration.

Four criteria for judging the accuracy of numerical mass transport models were suggested by Roberts and Wiess, 1966. The following comparison of modeling techniques will be based on these four criteria plus two criteria related to efficiency and ease of implementation. The six criteria are as follows:

1. Conservation of mass and constituents must be maintained or accounted for in a logical manner.
2. Stability should be assured with no unbridled growth of errors or unreasonable oscillations.
3. Numerical dissipation should be kept at an acceptable level.
4. Overshoot and undershoot should be kept at acceptable levels.
5. The model should be flexible enough to allow experimentation and sensitivity analyses.
6. The model should not be excessively demanding computationally or in terms of implementation.

COMPARISON OF METHODS

Criterion 1: Conservation of Mass

In generating the simultaneous linear equations which approximate an advection-dispersion equation, finite difference and most finite element models use values of seepage velocity which are calculated to apply at discrete nodes or within discrete elements in the solution grid. This amounts, effectively, to an assumption of a discontinuous velocity field.

On a large scale, these discontinuities tend to cancel out, but within each grid spacing these discontinuities become important. These discontinuities can be ignored in most flow models but in advection-dispersion models the advective component of the model can experience serious problems on this small scale. The problems arise where flow patterns are rapidly changing or pressure and concentration gradients are steep and varying (Pinder and Gray, 1977). Thus, unless special and usually expensive measures are taken, at the local level, mass is not necessarily conserved in these models.

Because a moving particle advection model is implemented in the method of characteristics and random-walk models and because this advection model structure can easily handle a continuous velocity function, these methods generally conserve mass within the model boundaries rather well. If the velocity profile available to these models is highly discontinuous and/or erratic, these models may provide results with little meaning; however, it should be expected that mass will be conserved if the implementation is correct.

Boundary conditions, on the other hand, require a great deal of care in the method of characteristics and random-walk models to insure that mass and constituents are conserved. For instance, the existence of an impervious boundary in a random-walk model requires specification of a barrier that particles can not be dispersed randomly across. How this sort of boundary should be handled is not clear. The random movement could be truncated at the boundary as in the simple model presented above; the particle could be modeled as reflecting away from the barrier or it could be left undispersed. Physical arguments for any of these means of maintaining the impervious boundary tend to be unconvincing. Similarly, traditional method of characteristics models take into account the presence of impervious boundaries during the process of simulating the dispersive component of transport and this boundary requires the implementation of averaging and dispersion algorithms that vary from boundary to boundary and are different from the algorithm implemented away from the barrier. Finally, particles

that enter or exit through boundaries either by advection or dispersion must be handled, and the particles must be appropriately initialized or terminated in the accounting system used in the advective component of the models. This requirement imposes an additional burden on the model and a need for very large numbers of advecting particles to be accounted for to maintain large statistical samples and accurate results throughout the period being simulated.

Criterion 2: Model Stability

As noted above, stability implies that there is no unbridled growth of errors or unreasonable oscillations in the model results. Stability does not, however, necessarily imply accuracy, only that the results will not tend to extreme values under the influence of large errors. Stability generally depends on the time integration scheme employed to generate the model equations. A further condition is that the estimator used to estimate or predict flow fields must be stable. If a numerical model is employed to generate flow field estimates, it is generally a finite difference or finite element model and stability is insured by the same considerations as discussed for transport models below.

The stability of finite difference and finite element models depends on the method used to approximate the time derivative and solve the linear model equation. Suppose the advection-dispersion equation is rewritten and a value T is defined:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial c}{\partial x} - u \frac{\partial c}{\partial x} = T \quad (4-13)$$

The time derivative $\frac{\partial c}{\partial t}$ may be approximated using a finite difference formulation as

$$\frac{\partial c}{\partial t} \sim \frac{[c(t + \Delta t) - c(t)]}{\Delta t} \quad (4-14)$$

As noted above, this formulation is usually used in modeling $\frac{\partial c}{\partial t}$ whether in a finite difference or finite element model. At this point a decision must be made whether to approximate the entire equation as

$$\frac{\partial c}{\partial t} = \frac{[c(t + \Delta t) - c(t)]}{\Delta t} = T(t)$$

$$\text{or} = T(t + \Delta t) \quad (4-15)$$

$$\text{or} = \epsilon T(t + \Delta t) + (1 - \epsilon) T(t)$$

with ϵ some weighting factor between 0 and 1.

This is called the choice of time integration scheme and the first option is called an explicit solution ($\epsilon = 0$), the second option is an implicit solution ($\epsilon = 1$), while the third option includes the whole range of solution schemes. Generally, an explicit solution is much less computationally burdensome while the implicit solution requires the direct or indirect inversion of the matrix of the entire set of model linear equations. The implicit formulation is, however, stable over a wider range of model discretization scales with numerical errors tending to be damped out rather than tending to increase in magnitude during the computational process. Since explicit solution predictions are based entirely on initial conditions, there is no adequate check of the reasonableness of predictions, and errors may grow exponentially from time step to time step. The prediction of concentration at a node in the solution grid obtained using an implicit time integration scheme, on the other hand, is based on both initial conditions and the predictions at all other node points. With all predictions based on all other predictions, an essential cross-checking process is effectively carried out and physically reasonable results are obtained. Usually, as ϵ is increased toward unity, the range of stability is increased. Thus, while an implicit solution and even a Crank-Nicholson solution ($\epsilon = .5$) are unconditionally stable, less implicit or explicit solutions are stable

only under certain conditions on the spatial and temporal discretization of the model, Δx and Δt . The criteria vary from solution scheme to solution scheme and are generally presented along with model descriptions in the literature.

Redell and Sunada (1970) implemented and tested a transport model using the method of characteristics which employed a finite difference formulation to calculate the change in concentration due to dispersion. The flow field (actually the pressure field) was calculated using an implicit finite difference model and thus stability of this component was ensured. The finite difference formulation of the dispersive component of the transport model was an explicit solution and a set of criteria for stability of that component had to be developed. These criteria were functions of model parameters such as the dispersion coefficients and the spatial and temporal discretization scales. Their work set something of a precedent stating that if the various components are stable then the entire model is stable. This result hasn't been conclusively shown to our knowledge, but it is a reasonable hypothesis and sees much application.

Redell and Sunada found that the total error in their model behaved erratically. This behavior was blamed on problems with the estimation of average tracer packet concentrations which result from difficulties in maintaining adequate populations of characteristic points in each model cell and on the relative position of the moving points within the cells. Maintaining this adequate population depends on time step length, spatial discretization lengths and flow geometry and velocity. It appears that what is "good" for one area and/or time step may fail in the next; certainly, these problems depend on the particular problem being studied. Method of characteristics models have been used enough so that it appears that in practice oscillations and other problems with errors are not to be expected routinely; the modeler should, however, be conscious that they can appear. In such cases, simple changes in geometry or population of particles are the suggested remedy.

Random-walk models are, generally, stable if the flow predictions are. Errors in these models are generally statistical in nature and are reduced by increasing the number of tracers per unit concentration or area. Error behavior can depend on the method of computing concentrations and the method used to model boundary conditions. These sources of error lead to large oscillations and are probably best handled by implementing physically reasonable analogs to the boundary conditions, substantially reducing the time step length, or increasing the size of the statistical sample being modeled.

Criterion 3: Numerical Dissipation

Numerical dissipation is characterized by rounding (smearing) of sharp concentration fronts resulting in solutions that resemble behavior in the presence of large dispersion coefficients. Figure 4 (a) illustrates the problem in the case of a simple one-dimensional flow field. This arises because of the "hyperbolic" nature of the advective component of the advection-dispersion equation. It is a property of hyperbolic equations that sharply varying components of concentration profiles are often damped in numerical approximations more strongly than smooth variations.

The nature of numerical dissipation and other numerical problems with hyperbolic equations may be shown relatively clearly for simple finite difference formulations. One way of arriving at a finite difference approximation to the transport governing equation is to deal with Taylor's series expansions of the concentration at the node points,

$$c(x = 0) = c_0 \quad (4-16a)$$

$$c(x = \Delta x) = c_0 + \left. \frac{\partial c}{\partial x} \right|_0 \Delta x + \frac{1}{2} \left. \frac{\partial^2 c}{\partial x^2} \right|_0 \Delta x^2 + \dots \quad (4-16b)$$

FIG. 4. Illustrations of numerical dissipation (a) and overshoot (b) in one-dimensional numerical models (from Pinder and Gray, 1977).

NOTE: D is equal to D and Q is equal to U as defined in Equation 4-23. ϵ is the weighting factor used in Equation 4-15.

Based on this expansion,

$$\left. \frac{\partial c}{\partial x} \right|_0 = \frac{c(x = \Delta x) - c_0}{\Delta x} - \frac{1}{2} \left. \frac{\partial^2 c}{\partial x^2} \right|_0 \Delta x - \epsilon' \quad (4-17)$$

with ϵ' equal to higher order error terms.

The advection-dispersion equation, as evaluated at $x = 0$, is

$$\left. \frac{\partial c}{\partial t} \right|_{x=0} + u_0 \left. \frac{\partial c}{\partial x} \right|_0 = D \left. \frac{\partial^2 c}{\partial x^2} \right|_0 \quad (4-18)$$

which may be written

$$\left. \frac{\partial c}{\partial t} \right|_{x=0} + u_0 \left[\frac{c(x = \Delta x) - c_0}{\Delta x} \right] = D \left. \frac{\partial^2 c}{\partial x^2} \right|_0 + \frac{1}{2} u_0 \left. \frac{\partial^2 c}{\partial x^2} \right|_0 \Delta x + \epsilon' u_0 \quad (4-19)$$

but which is generally approximated to be

$$\left. \frac{\partial c}{\partial t} \right|_{x=0} + u_0 \left[\frac{c(x = \Delta x) - c_0}{\Delta x} \right] = D \left. \frac{\partial^2 c}{\partial x^2} \right|_0 \quad (4-20)$$

Thus the first error term in this finite difference approximation to the advective component is similar to the dispersive component so that an apparent numerical dispersion coefficient (or numerical dissipation)

$$D^* = \frac{1}{2} u_0 \Delta x \quad (4-21)$$

is effectively included in the model once the time derivative and dispersive terms have been formulated as finite differences. In addition to this problem, the second error term in the advective component ϵ' , is very often larger than the errors associated with the finite difference dispersive component. Thus, as a result of the error structure of hyperbolic equations, models based on the advective form

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0 \quad (4-22)$$

should be expected to have difficulties in their approximate solutions. This caution extends to the advective-dispersive equation as long as advection is large relative to dispersion.

Pinder and Gray (1977) in a comparison of finite element and finite difference transport models concluded that finite difference models are consistently inferior to finite element and other methods. Because of the different methods by which finite difference and finite element models are derived, a large part of the numerical dissipation that is inherent in finite difference equations has been removed from finite element models. Correction methods to finite difference models have been applied and considerable improvements obtained.

Finite element methods perform fairly well with respect to numerical dissipation, but the problem still exists. Under conditions to be discussed further with respect to the related problem, overshoot, numerical dissipation can mask or distort results so as to render them meaningless. A serious problem is that numerical dissipation is virtually indistinguishable from the results of the dispersion process being modeled. One way of decreasing the effects of numerical dissipation is to implement higher order (Quadratic, Hermite polynomial, etc.) weighting functions in the derivation of model equations. This is generally a valid approach if the higher cost of implementing certain of these model structures is not critical; however, quite often the increase in accuracy is small in light of the added implementation expense. Pinder and Gray (1976)

present an example in which, rather than leading to increased accuracy, the effort proves to be detrimental to the simulation accuracy.

Application of the method of characteristics reduces this source of error by solving the hyperbolic component of the transport equation separately from the dispersive component, and by solving it in a very accurate manner. The effect, according to Garder et al. (1964) and Redell and Sunada (1970) is removed completely by this means. Although numerical dissipation is largely removed in models using the method of characteristics, it is very likely still present in some model formulations. In the examples that were studied by Redell and Sunada (see their page 23), a smearing of a two-dimensional concentration front, which appears very much like numerical dissipation, is presented. This smearing occurred under conditions in which the spatial discretization is chosen to be too large for an accurate solution to be obtained. It will be seen below that the spatial discretization lengths are quite important in determining the extent of numerical dissipation and overshoot. The effect probably enters through the algorithm used to determine the velocity of the individual packets that are traced.

Random-walk models may be subject to the same problems as the more traditional method of characteristics models. A problem which will be more obvious for random-walk models but will also exist in traditional approaches is that numerical dissipation and overshoot will tend to be replaced by statistical errors that resemble the above numerical errors. These errors are effectively dealt with by using large numbers of tracer particles/packets.

Criterion 4: Overshoot

Overshoot is characterized by erroneously large concentration predictions as one approaches a sharp front from the low concentration side (Pinder and Gray, 1977). It generally appears that the initiation of overshoot leads to the sort of oscillation and damping away from the front that is known

as, in electronics, "ringing." The analogous problem on the downhill portion of the concentration is known as "undershoot." Fried (1975) [quotation found in Anderson, 1978], described the phenomena as follows:

"Time steps and spatial dimensions are not well adjusted and the aquifer cannot "absorb" numerically the injected mass of pollutant. The time steps should be chosen carefully and adapted to the problem."

Anderson (1978) goes on to suggest that overshoot can be reduced by including higher order corrections to the time derivative, although this will tend to increase numerical dissipation. Since the time derivative in the transport equation is nearly always solved by a finite difference approximation, regardless of the structure of the spatial derivatives, overshoot is pervasive. It appears even in the method of characteristics as applied by Reddell and Sunada (1970) although only to a small extent. Figure 4 (b) illustrates the effects of overshoot and ringing in a one-dimensional transport model.

Finite difference models are once again inferior to finite elements with respect to overshoot. Correction terms, as noted above, can be included but usually at the cost of increased numerical dissipation. Meanwhile, finite element models show good results under "mild" conditions. The problem is sensitive to the time integration scheme (explicit, implicit) employed as well as to higher order corrections to the time derivative in the initial formulation. "Mild" conditions are those cases in which, using Fried's expression, time and spatial dimensions are reasonably "well adjusted." More will be presented on this subject below. Finally, the method of characteristics and random-walk models perform very well in this regard.

Numerical dissipation and overshoot generally must be traded off against each other in the interests of accuracy and generally are worse when the advection process is large compared to dispersion. Two dimensionless coefficients allow comparison of the two processes in a numerical model application:

$$D = \frac{D\Delta t}{\Delta x^2} \quad \text{and} \quad U = \frac{U\Delta t}{\Delta x} \quad (4-23)$$

Individually, these coefficients are important and the ratio of the coefficients is also very indicative of the potential for numerical problems:

$$\frac{D}{U} = \frac{\alpha}{\Delta x} \quad (4-24)$$

with α equal to the dispersivity. It seems likely that criteria should be developed for the particular model at hand as to when numerical problems will arise since those criteria will probably be unique to that model. Order of magnitude estimates of the criteria can be garnered from a comparison of the results of Smith, et al. (1973), Pinder and Gray (1977), Garder et al. (1964), and Reddell and Sunada (1970). These simple criteria appear to apply to finite difference, finite elements, and method of characteristics models. It seems that large numerical problems (particularly for one-dimensional geometries) begin if, when U , the Courant number, is of the order 0.5, and D approaches and becomes less than 10^{-2} . This result also suggests that, conservatively, the ratio D/U should not drop much less than about 0.1 without special precautions.

Random-walk models, on the other hand, lose the physical analogy on which they are based and can become statistically unstable when the time between random dispersals of the particles becomes large. This effect lowers the number of dispersals and increases the effect of individual random components. This condition is signaled when both U and D become large. This effect lowers the number of dispersals and increases the effect of individual random components of dispersal relative to model discretization.

One advantageous use of these order of magnitude criteria is to check whether or not models of regional transport will encounter numerical difficulties. Notice that for $\alpha = 30\text{m}$ and $\Delta x = 305\text{m}$, $D/U \approx 0.1$ and numerical problems are probably non-negligible. Since this value is the order of magnitude of values presented in Tables 1 and 2, it appears that special precautions will be necessary in modeling transport at this level.

Criterion 5: Model Flexibility

Numerical models are generally designed to be very flexible with respect to parameter, boundary, initial condition values, and time and distance scales. However, the form and nature of boundary conditions, the solution schemes employed, and the governing equations to be solved may range from quite flexible to quite rigid. Given the pioneering nature of regional waste transport mechanism modeling, the time and distance scales required, and given some of the doubts concerning the Fickian formulation of most transport models that have been raised by theoreticians, the models implemented in future regional waste transport studies should be quite flexible, allowing a wide range of experimentation and sensitivity studies.

Finite difference and finite element models are generally very flexible with respect to solution scheme and can be reasonably flexible with respect to the choice of boundary conditions applied. Because of their simplicity, finite difference models are usually easily adaptable to small variations in the differential equations being solved. Derivations that can become quite lengthy are required if new equations are to be solved by finite element techniques. This approach could prove to be quite a hindrance unless a modeler with a thorough understanding of the finite element approach is available. Finally, with respect to cell and boundary geometries, finite element models are extremely flexible. Certain finite difference formulations can be equally flexible, but most are based on either square or rectangular nodal grids. This grid form can be a problem since a solution grid with many cells may be required to model accurately or in detail a restricted portion of the study area. This increase in the number of cells increases the computational burden significantly.

Models based on traditional applications of the method of characteristics are usually fairly flexible as regards model geometry. Model cells can be chosen arbitrarily as long as adequate interpolation formulas for the velocity and concentration gradients at various points can be derived and

as long as adequate averaging algorithms are available for the calculation of the concentrations in model cells. These formulas and algorithms will generally be specific to the particular model structure and, since they will be the largest source of errors, a great deal of attention should be paid to their proper development. Implementation of different kinds of boundary conditions can be tricky and should be programmed with flexibility as well as a good physical model/analog in mind. As with the interpolation formulas above, boundary conditions are a potential source of errors and rigidity, and deserve special attention. Finally, the solution scheme is always based on the two equation form of the transport equation and thus the dispersive component of the model is relatively independent and easily altered.

Models of the forms discussed in the last two paragraphs- finite difference, finite element, and traditional method of characteristics- could be derived for nearly any form of the dispersive transport equations that theory might suggest. Such models might require considerable computation to derive and use, but on the whole should be a straightforward programming exercise. Random-walk models, on the other hand, would prove more rigid in this respect since they are always Fickian in the limit of many time steps. Inflexibility in this regard does not by any means disqualify random-walk models from consideration since, as with the other modeling methods, spatially and temporally varying dispersion coefficients may be employed, and by this means, a number of different dispersive behaviors simulated. Other than their inherently Fickian nature, random-walk models are even more flexible than other method of characteristics models since fewer averaging algorithms must be specified.

Criterion 6: Cost Considerations

Computers are rapidly becoming less expensive (in real terms) and capable of faster and larger computations. Larger scale and more intricate modeling efforts are now possible or soon will be. Despite this progress, cost will

always be an important factor. As noted early in this section, an arbitrary degree of accuracy could be obtained if economics allowed enormous computational burdens to be handled easily; however, there is nearly always a trade-off between economics and accuracy to be made.

Of the model structures discussed so far, finite difference and random-walk models are by far the simplest and quickest models to implement. Both are based on relatively transparent computations and logic. Most of the difficulty in a finite difference model lies in the actual solution of the linear model equations. The equations themselves are generally easy to derive. Random-walk models are characterized by extremely simple equations and "solution schemes" and require their most complicated machinations in preparation of the solution for presentation in an intelligible fashion or usable form. Somehow the locations of many tracer particles must be converted to a concentration profile or some other meaningful representation. On the other hand, finite element models are generally more complicated and time consuming to derive than the other model structures. The traditional method of characteristics lies somewhere between these extremes.

In terms of computational burden in applications, finite element models are often very efficient, both because of their extreme flexibility with respect to element size, orientation and shape and because the linear model equations can quite often be configured so that very efficient solution methods are applicable. Flexibility with respect to element geometry is an important advantage since the many nodes that are necessary in a detailed finite difference model can be avoided by the proper choice of a finite element geometry. Finite difference models tend to rank second in efficiency largely because of the very efficient solution schemes that are available for linear systems.

The accuracy of the method of characteristics depends on the number of particle/packets advected. Traditional method of characteristics models may require as few as 2 packets per grid interval (Gardner et al. 1964), but at this level, the danger of instabilities in concentration estimates becomes important (Reddell, 1970). Generally, the larger the number of packets per grid interval, the more stable the model results will be. This relationship may mean that for the whole model, a large number of packets may have to be advected with current positions and concentrations maintained in memory for each. The large memory requirements, in addition to the computational burden imposed by the dispersive component of the model, make the traditional method of characteristics a potentially expensive model structure to employ. Random-walk models are even more dependent on the number of particles advected. Thousands of particles are required to achieve accurate results in complicated and rapidly varying systems. Again, memory requirements can be prohibitive. On the other hand, computationally these models are simple, although thousands of repetitive calculations need to be carried out, since advection and dispersion are handled in a few lines of programming.

CONCLUSIONS

The models discussed vary considerably in their degrees of accuracy under conditions in which advection and/or concentration gradients are large. Finite difference and finite element models are particularly susceptible to numerical errors such as numerical dissipation and overshoot. Models based on the method of characteristics are largely free of these errors; however, these models encounter statistical stability difficulties unless a large number of particle packets are simulated by the advective component of the models. The situations in which numerical difficulties arise are largely the same for all the models discussed, with the exception of the random-walk model. Three coefficients which are indicative of the modeling situation are suggested which serve as a warning that numerical difficulties should be anticipated: dimensionless velocity (the Courant number),

$$U = \frac{u \Delta t}{\Delta x}$$

a dimensionless dispersion coefficient

$$D = \frac{D \Delta t}{\Delta x^2}$$

and the ratio of the two,

$$D/U = \frac{\alpha}{\Delta x}$$

When U is of order unity or when D is a small fraction of U , numerical difficulties can be expected unless special precautions are taken. Random-walk models begin to lose the physical reasonableness of the analogy on which they are based as U and D get large; eg. as the time step length gets large.

Generally, finite difference transport models seem to be more susceptible to numerical errors such as overshoot. Finite elements and the method of characteristics follow. A serious aspect of the numerical problems discussed above is that the inaccuracies may not be apparent to the modeler. Numerical dissipation is particularly insidious in this respect since it looks like natural dispersion effects and is only detected by comparison to analytical or laboratory results. Because numerical dissipation and overshoot are not present in well constructed random-walk models and because of the simplicity of their design, this modeling approach is recommended in terms of accuracy.

Random-walk models, however, can be quite expensive to employ. Ahlstrom et al. (1977) stated that in their experience random-walk models require more computational time than finite difference and finite element models, particularly if the ever present statistical error is to be held at a reasonable level. Despite this potential for additional computational costs, we

recommend the random-walk model for use in the largely untested field of regional transport modeling. If the cost burden grows too large, we next recommend finite element models because of their efficiency and accurate prediction in most modeling situations.

MODELING STRATEGIES

In addition to the above considerations regarding theoretical accuracy and cost of different transport models, two major decisions concerning the strategy by which models are applied should be faced. The first of these is the question of how much physical detail should be modeled. Given the modeling capabilities, physical understanding of the processes at work, ability to estimate and verify model parameters, and the level of accuracy desired, the best answer to this question is not, "As much physical detail as possible should always be included in the model". The second strategy decision is the question of whether or not to include in the modeling effort certain experiments or procedures that will allow the accuracy of the model simulations and predictions to be assessed. If such analyses are to be carried out, what options are available? In the next few paragraphs these strategy issues will be discussed in the context of regional transport modeling efforts.

Perhaps the most important consideration in a decision about the level of detail required in a transport model is the problem of obtaining parameters for intricate numerical models. Other considerations, such as modeling capability and the level of accuracy, are generally secondary because, for instance, numerical methods have long since outstripped the ability to observe the properties of aquifers being modeled. Similarly, even apparently modest accuracy requirements are stymied by the prevalent lack of data with which to calibrate models. In light of the long times and distances that are being modeled in the course of waste repository assessment and the importance of the results to future generations, the accuracy required in this particular application of transport modeling should be anything but modest. Thus a critical factor in transport modeling is the level of detail that can be parameterized.

It appears that two critical and difficult parameters required in a model application are hydraulic conductivity or transmissivity and dispersion coefficients. It was noted in an earlier section on the macro-dispersion phenomena that whatever detail is not included in the advection model finds its way into the calibrated value of the dispersion coefficient and that the largest unmodeled details play a large part in determining that value. In view of that discussion, it seems clear that the detail with which conductivity can be modeled should be consciously traded off against the size of the dispersion coefficient in many field applications. Unless mandated by complex boundary conditions or an interest in localized concentration variations, nothing is gained by using models with numerous conductivity links if there is little information available about conductivity values or variability. This statement is particularly true if good estimates of the dispersion coefficient applicable at that level of model detail are not available. On the other hand, if there is no information about appropriate macro-dispersion coefficients available, then hydraulic conductivity should be modeled

1. with as much conductivity detail as can be meaningfully obtained in a liberal parameter estimation process (ie., give it everything you have got),
2. at a different level of detail at which the macro-dispersion coefficients are understood (even if this means less detailed models), or else
3. probabilistic models might be considered.

The major difficulty in carrying out this trade-off is that accurate estimators of the dispersion coefficient are not yet available; theoretical results are weak and incomplete while field studies have shown wildly erratic results. In view of its importance, a more complete review of approaches to estimating macro-dispersion coefficients is presented in Chapter V. Probabilistic modeling is discussed below.

The trade-off between the conductivity detail modeled and the size of the dispersion coefficient should not be viewed as an even trade. The larger the dispersion coefficient in a numerical model, the more likely are unphysical results to be obtained. As discussed in Appendix B, the extensive "mixing zones" resulting from macro-dispersion processes are not exactly described by any large constant coefficient. For example, some models tend to predict dispersion upstream of point sources; these effects can be avoided to a certain extent by using time variable coefficients that increase as the mixing zone increases; however, parameterization soon becomes unwieldy in this approach. Thus, as larger and larger dispersion coefficients are applied, a situation is eventually reached at which point further increases in the value invalidate the model. In this case, the important conductivity variability must be included in the advection model rather than the dispersion model. A method for including a great deal of variability in the advection model is proposed in the following discussion of probabilistic modeling.

Given the delicacy with which the matter of nuclear waste disposal and repository siting must be presented to a concerned public, there is little doubt that model structure, simulations, and predictions must be critically assessed, whenever possible, during the modeling process from conceptualization to application. A simple prediction will most likely be unsatisfactory. Some indication, preferably quantitative, of the truth value or likelihood of the prediction will allow criticism to be met rationally and will put the results into a more meaningful perspective.

The alternatives available for assessing numerical model prediction veracity include, as important examples,

- a. simple sensitivity analyses
- b. Monte Carlo or conditional simulations, and
- c. analyses of the statistical descriptions of predictions which can be derived from statistical descriptions of the aquifer and constituent properties.

Sensitivity analyses are common modeling practice and involve running the model with a variety of different parameter values. Large changes in the model results indicate high sensitivity to certain parameters which in turn suggests that the model will predict poorly if these parameters are even slightly in error. Small changes indicate that errors in these parameters will be less important to model accuracy. Monte Carlo and conditional simulations are essentially extensive sensitivity studies which try parameter values chosen at random from the probability distribution which describes the variability of and/or the uncertainty of the parameter values. The resulting array of predictions represent the probability distribution of the prediction, and thus the likelihood may be estimated that a particular event will occur as modeled. Statistical analyses involved estimating, through analytical or semi-analytical approaches, statistics such as mean value and variance that describe a particular prediction when the parameters employed are uncertain. The result is something like the R^2 value calculated for a linear regression. This R^2 value represents that part of the dependent variable's variability or uncertainty that is explained by a particular set of independent parameters. Similarly, the results of statistical analyses of numerical models are estimates of the uncertainty that is added to model predictions by uncertainty in model parameters.

Of these alternatives, we suggest sensitivity studies be conducted during the modeling process since it is a well established modeling procedure. Because of the large sources of uncertainty among model parameters, we further suggest that a Monte Carlo simulation be carried out to detail reliability of the model simulations. Because of the presence of great uncertainty with respect to dispersion coefficient values and because of the complexity and size of the numerical models employed in regional radionuclide transport simulation studies, we cannot, at this point, recommend other statistical approaches. We do, however, suggest that the applicability and advantages of the various probabilistic approaches be reviewed in a separate study.

The random-walk model, recommended earlier for its accuracy, has been applied with good advantage by Schwartz (1977) in a probabilistic framework. He used the model under Monte Carlo conditions to determine and investigate macro-dispersion in a two-dimensional medium. Recently Schwartz has begun an investigation into extensions of this approach, and it appears that a valuable method of parameterizing (and conceivably bypassing) dispersion coefficients would be to apply the model with more hydraulic conductivity detail than can be estimated or parameterized with deterministic assurance. This "overly-detailed" model could be used to carry out a series of Monte Carlo simulations in which the conductivity parameters employed are chosen at random from a probability distribution which is believed to describe possible states of the actual physical medium. By this approach, apparent dispersion coefficients due to the simulated but unobserved conductivity variability and its effect on advection rates and directions could be determined. Thus, if the hydraulic conductivity in the field is understood statistically, this knowledge could be used to generate more meaningful estimates of the dispersion coefficient.

To be more explicit, the technique would result in a series of simulation results, each of which is computed with a different conductivity field assumed. As noted above, the conductivity fields would each be chosen at random from a probability distribution describing possible states of the true system. Each of the simulation results could be used to calculate an apparent dispersion coefficient. The resulting series of dispersion coefficients in turn could be used to infer the probability distribution of the "true" apparent dispersion coefficient, i.e., the macro-dispersion coefficient. Alternatively, the simulation results could be compiled directly to calculate a probability distribution of likely outcomes. Thus, a most likely concentration profile could be deduced and the need for a very large apparent dispersion coefficient avoided.

Statistical descriptions of aquifer material properties, such as permeability and porosity, have been attempted with varying degrees of success in the past by numerous hydrologists (eg., Bakr, 1976). At a regional scale, such work has not been reported so that it is not yet clear how well we will be able to estimate the statistics of aquifer property and model parameters.

To summarize this discussion of modeling detail and model parameter uncertainty considerations, we conclude that a conscious trade-off should be made between the detail with which the porous medium is modeled and the value of dispersion coefficients applied. It is suggested that special studies be made regarding the importance of uncertainty in important parameters on the reliability of predictions and simulations. Finally, it is concluded that given a statistical description of the aquifer, a random-walk model can be readily used to carry out a statistical assessment of the appropriate range that dispersion coefficients may take on in a particular model and, in effect, provide a means of avoiding the continued use of physically inappropriate parameter values. Further study will be required to develop methods for obtaining aquifer property statistics.

V. DETERMINATION OF DISPERSION COEFFICIENTS FOR REGIONAL TRANSPORT MODELS

INTRODUCTION

It has been shown that macro-dispersion processes are very likely to play a substantial role in regional mass transport models and thus cannot be neglected. To include the processes, however, estimates of appropriate values of the parameters used to describe the processes must be made available to modelers. In the past, many investigators have conducted laboratory experiments in efforts to parameterize dispersion processes. Field measurements have also been used and are described in Chapter III. Also, a number of transport models have been calibrated to field situations, thus providing working estimates of the desired coefficients. Finally some researchers, as noted in earlier sections, have attempted to estimate dispersion coefficients using theoretical methods. In this section, appropriate methods of acquiring dispersion coefficients for use in regional models will be discussed in light of the explanations and expected behavior of macro-dispersion processes that were reviewed earlier.

MEASURING MACRO-DISPERSION

First of all, measurements of macro-dispersion processes must be made in the field. It has been noted repeatedly, in earlier sections of this report, that the coefficients obtained using laboratory measurements of dispersion processes bear little resemblance to values estimated from field measurements. The accepted explanation for this behavior is that laboratory measurements are made using nearly homogeneous porous media. Even in those cases where specifically heterogeneous media are employed, the scale of the imposed heterogeneities is still small compared to those found in the field. For example, in Greenkorn's (1970) laboratory studies of dispersion in heterogeneous packings of glass beads, heterogeneities of the order 1 inch were used. In the field, hydraulic conductivities might be expected to vary over distances of meters or less within individual strata, over tens of meters between stratigraphic units, and over even larger distances as the scale

of interest increases. Because column or other laboratory tests cannot be used to represent naturally heterogeneous aquifers and because these laboratory results cannot be meaningfully extrapolated to the aquifer scale, laboratory results have little immediate use in present studies of transport processes.

Nearly all of the measurements reported in Table 1 are based on field observation of tracers that have been artificially injected into the aquifers of interest. These measurement techniques are discussed and described in the review of these results presented in Chapter III. These "artificial" measurements have the advantage that they can be conducted anywhere if the injection and observation wells are available or can be drilled. They can be conducted over short time periods and yield results that have a relatively clear-cut interpretation.

Matheron and deMarsily (1979) and Gelhar et al (1979) have, however, cast some doubts on the validity of tracer tests. Both research groups have achieved theoretical results which suggest that the distance scale of measurements have an important influence on the estimated dispersion coefficients. Although their work is limited to one-dimensional conditions, this particular objection makes good sense. Two well tracer tests, for example, certainly cannot measure the effects of variations in aquifer properties that have a length scale considerably longer than the distance between wells. That sort of "slow" variation has little or no effect on flow or transport between wells; variation of properties would, however, effect flow and transport through the aquifer for distances greater than the variation length scale. The variation length scales, as noted above, tend to range from meters to kilometers. Since the largest scale variations that are included in the measurement distance may dominate the macrodispersion coefficients measured, it is expected that multiple well tracer tests will yield results that are primarily indicative of dispersion along distances equivalent to the measurement scale. For this reason, values of dispersivities tend to grow along with the measurement scale, and it

must be concluded that tracer tests should be carried out at the same distance scale as the transport process/situation to be modeled.

Matheron and deMarsily (1979) also show that, based on their theory, dispersion coefficients could not be economically or meaningfully measured by multiple-well tracer tests at the scale required by even small scale regional models. They estimate natural travel times of over 100 days under reasonable conditions for advection covering 600m. By their theory, an asymptotic value of the dispersion coefficients might be approximately applicable by that time. Even so, such an experiment is not feasible for economic reasons. If the tracer is injected under pressure in order to reduce travel times, the flow field will be substantially altered, and it is not certain that the dispersion coefficients will apply once the natural flows are resumed. In fact, the analytical theories of both Matheron and deMarsily (1979) and Gelhar et al (1979) suggest that the values obtained will depend critically on the flow configuration during the measurement period. This dependence on flow configuration is currently of an unknown functional form.

It appears then that if macro-dispersion is to be measured in a meaningful experiment, it will have to be measured through observations of environmental tracers. Use of environmental tracers is not a well established science and so our definite suggestions are few. Variations of isotopic concentrations, salinities, temperatures, and ionic concentrations are potential tracers. Winograd and Pearson (1976) considered a wide range of such tracers in their study of flow in a regional aquifer in South Central Nevada and concluded that a large variation in carbon-14 content in springwater in the area suggests large scale variations in permeabilities. Schwartz (1979) is currently carrying on megascale macro-dispersion studies involving observations of isotopic variations between old and new groundwater under the Canadian Great Plains. As noted when the notion of environmental tracers was first raised in Chapter III, environmental tracers, in order to be useful, must be observable and be configured on a spatial scale so that the concentration profiles are applicable for model calibration or direct calculation of coefficients.

In addition, we suggest that experiments involving environmental tracers be planned and interpreted with the possible asymptotic behavior of dispersion coefficients (as discussed above) in mind. It appears that one of two interpretations of results may be assumed:

1. observations lead to values that are applicable to a narrow range of transport situations exhibiting the same distance scale as the scale of observation or transport of the tracer, or
2. observation length scales may be such that asymptotic behavior predominates; in which case, all transport situations with larger length scales can be described by the measured coefficients.

In the second case, upper limits on asymptotic behavior may also occur, at which point aquifer variations of a new larger scale become important and the dispersion coefficients start to vary again. The choice between these two interpretations of results should be made on the basis of testing at several different length scales, whether through a more gross view of the tracer configuration or through attention to finer details.

Finally, we suggest that transfers of values of dispersion coefficients developed through field observations be carried out rather conservatively. Even within an aquifer, macro-dispersion can be expected to progress at different rates from site to site. Certainly in practice, the extent of this coefficient variation will not be known in any detail and, in fact, many aquifers will be modeled without benefit of observations of dispersion processes. It is important, however, because of the wide range of values that dispersion coefficients can assume, that coefficients only be used in aquifers which are similar in terms of the various "parameters" of macro-dispersion time and distance scales, variability of aquifer properties, etc.

THEORETICAL PARAMETERIZATION

In this report several attempts to theoretically parameterize the macro-dispersion process have been discussed. All of these parameterizations depend on statistical descriptions of aquifer properties, the flow field boundary conditions, and local dispersion coefficients. Although these theoretical parameterizations are currently incomplete, they do provide an excellent idea of the kinds of information that will be required to

1. predict coefficients, as theory develops, and
2. specify conditions under which aquifers are "similar" with respect to macro-dispersion processes.

The theoretical parameterizations require a statistical description of the variability of aquifer properties and, in particular, hydraulic conductivity. This statistical description must include not only the extent of variation (generally in terms of a variance) but spatial statistics of the property. The most commonly employed spatial statistics are the two-point correlation structure and the related statistic, the covariogram. Unfortunately, such statistical descriptions are not common and have only been obtained for a few aquifers. These descriptions have been compiled using either well log data (Bakr, 1976) or well field data (Delhomme, 1979). Very intricate and detailed well logs are carried out in petroleum reservoir studies but, due to the high cost of these studies, few have been carried out for groundwater purposes.

A similar lack of appropriate data and accepted procedures must be dealt with in providing information about flow fields at reasonable aquifer scales. In particular, local seepage velocities are difficult to estimate given uncertainties concerning aquifer properties and the difficulties inherent in estimating piezometric gradients in the absence of numerous observation wells (Anderson, 1979).

On a more optimistic note, local dispersion coefficients have been measured in good detail in a variety of different laboratory porous media. The number of values that have been obtained for consolidated, natural materials is quite small (see Fried and Combarnous, 1971), but it appears that these properties could be measured relatively easily. Notice, for instance, the single well measurements made by Pickens et.al.(1977). It is also likely that local dispersion coefficients are transferable from laboratory results to field situations.

A note that should be made at this point regarding theoretical parameterization of the macro-dispersion process: Matheron and deMarsily (1979) have suggested that a set of constants $D(t_0)$ may be a more appropriate descriptor of the macro-dispersion process than the more familiar Fickian coefficient. These constants would be specified so that when substituted into the dispersion equation or model, the resulting predicted concentrations at Time t_0 are accurate. Simulations leading to a prediction of concentrations at some other time t' would require another coefficient $D(t')$ if accurate results were to be insured. This approach would be very complicated and is very foreign from usual approaches to transport modeling; however, this approach is somewhat implicit in our decision that measurements of dispersion coefficients should be made at the same scale as the transport situation to be modeled. This measurement policy would lead to a value of the coefficients that is valid within a restricted time or advected distance regime and seems to assure neither efficient nor flexible modeling efforts. Until the current doubts concerning the Fickian nature of macro-dispersion processes are dispelled or a new, valid set of governing equations for these processes is available, it seems reasonable to recognize in measurement and modeling schemes that macro-dispersions coefficients are functions of the length scale of interest.

A final "theoretical" approach is to estimate coefficients through Monte Carlo simulations. At the conclusion of Chapter IV, a numerical statistical approach to parameterizing macrodispersion and testing a range of values for macro-dispersion coefficients in particular modeling applications was outlined. The

Monte Carlo procedure discussed would add confidence with regards to the prediction accuracy by yielding a range of possible outcomes of the simulation given the existing uncertainty with respect to the "real" value of the dispersion parameters. The approach, however, will be expensive.

A less expensive means of providing confidence about simulation results is through application of conservative or "worst-case" values of the uncertain parameters. In this approach, a single group of physically believable parameter values are input to the model (numerical or analytical) which produce the "worst" outcome. If this outcome is acceptable, then it is assumed that for any of the possible parameter values the outcome will be acceptable. *The worst-case approach, however, cannot be encouraged in light of the difficulties in obtaining coefficient values discussed in this chapter.* Coefficients show enough variability from report to report that obtaining demonstrably conservative parameters would be difficult. This is especially true in light of analytical predictions of infinite coefficients and observations of channeling in regional scale studies. Either of these phenomena lead to a complete breakdown of "worst-case" analyses.

Because of these difficulties, we must suggest, at this point, that either a defensible coefficient value must be obtained or else a probabilistic study should be made. Simply proposing "conservative" parameters may lead to misleading simulations and the potential for eventual release of large doses of radionuclides to the biosphere as a result of repository siting and licensing decisions based on inadequate understanding of the system developed through these simulations.

MODEL CALIBRATIONS

Many of the values of dispersivities that have been cited for field use were obtained during the iterative calibration of numerical transport models. These estimates were chosen to be the coefficient values which result in the

"best" simulations and/or reproduction of observed concentration profiles. Because calibrated values of dispersion coefficients tend to be used in tuning the model to achieve accurate results, their final values include the influence of the model structure and approximations active in the advective components of the model. For this reason, the coefficients obtained during model calibration are the "best" values, given the errors in observations, the particular discretization scales employed, and numerical errors and approximations in the model being employed.

If employed in another model or in the same model with different discretization lengths or grid geometry, dispersion parameters would lead to different and potentially meaningless model results. Calibration should ideally be carried out separately for each model structure and geometry that is employed. Where this is not practical, values should be transferred between models that have similar numerical error behavior for the transport problem being solved and are employing similar solution grid geometries. Thus, if a model is being used at the limits of its numerical accuracy, it should be assumed that many errors are being compensated for by the value of dispersivities, etc., being employed. Use of the same value of dispersivity in an inherently more accurate model will be likely to produce noticeably different results. For models that are producing accurate results, transfer of coefficients will be less hazardous. In any such transfer, the safest course of action will be to attempt to duplicate some of the results of the model application from which the coefficient is obtained. This will serve as a test of whether or not the models are similar enough to allow the transfer of calibrated parameters.

A number of different calibration procedures are available. In large part, how the term "best parameter value" is defined controls the methods by which iterative calibration procedures progress and are terminated. The final criterion by which "best" is judged is generally the analyst's or modeler's judgement. Before application, absurd values are culled by the conscientious modeler. In trial and error calibration, the modeler's judgement is the entire criterion for choosing parameter values. More complex automatic procedures are also available which employ nonlinear optimization techniques

in arriving at values (Murty and Scott, 1977). It should be noted that deterministic optimization procedures tend to rely heavily on constraint sets if physically plausible constraints are imposed. This can lead to unstable iterations. Alternatives to automatic deterministic calibration schemes are probabilistic estimators such as maximum likelihood estimators, optimization under uncertainty (Yeh, 1971), and extensions of linear filtering algorithms (Wilson et al, 1978). To date, these estimators have been developed primarily for the calibration of transmissibilities in groundwater flow values, but it is likely that they could be extended to dispersivity values in transport models. In any case, it should be reiterated that the "best" value, whatever the calibration procedure, depends on the model structure, calibration data, and persistence of the calibrator.

At this point, it should be noted that since model parameters include the effects of model approximations and errors, they should not be expected to correspond exactly to field values (Robson, 1974). The relationship between the two will generally be quite complex and if, for convenience or some other reason, field measured values of the macro-dispersion coefficients are employed in a numerical model, it should be expected that numerical approximation and error effects will appear in other model parameters whose "true" values are even less well known.

Finally, in Chapter III, the insensitivity of the dispersion coefficients in large scale models was commented upon. As noted in that section, this insensitivity implies that

1. these coefficients will be difficult to calibrate accurately, but that
2. accuracy will be less important to the proper performance of the model than parameters to which the model is more sensitive.

On this more or less encouraging note, we will conclude the discussion of model calibration.

GENERAL NOTES ON OBTAINING MACRO-DISPERSION COEFFICIENTS

The primary conclusion to be derived from the discussion thus far in this section is that, no matter how they are arrived at, the value of dispersion coefficients obtained is crucially dependent on:

1. the model being applied (whether analytical, analog, or numerical), and
2. the scale of the transport that is being modeled.

This variation of coefficient values presents modelers with a technically challenging problem. If a variety of coefficient values are required to complete a simulation of the history of a contaminant plume, then the transfer of the model parameters to other conditions is limited and the task of describing the parameterization process becomes much more difficult.

Eventually, the conclusion may well be reached that the Fickian model is not valid as applied to aquifer scale transport. A method based on Monte Carlo simulations was proposed at the end of Chapter IV to extend the usefulness of the Fickian analogy and include more of the variability of flow rates in the advection model. This approach could in some sense yield an expected or most likely value of concentration profiles while at the same time providing a statistical description of all possible outcomes. Model results would be based on model assumptions that face less criticism--the structure of the advection model, dispersion processes at smaller scales and statistical descriptions of aquifer properties. In a sense, this proposed approach would dispense with the aquifer or multi-aquifer macro-dispersion coefficients and replace them with a statistical model of what we really believe is happening in the aquifer. This process would be expensive, but we believe that it would result in truly meaningful results and parameterization of the transport model in terms of parameters that have some physical basis.

VI SUMMARY

This technical memorandum was developed as a result the evaluation by CDM of problems associated with dispersion processes in regional ground-water models.

We have concluded that modelers of radionuclide transport at the regional scale will find it necessary to include dispersion processes in their computations. The term, dispersion, refers to a group of processes which lead to irreversible mixing during transport through porous media. Three problem areas with respect to modeling dispersion processes in groundwater aquifer systems are identified and discussed in this memorandum: modeling local scale dispersion and diffusion processes, modeling regional scale dispersion processes, and numerical errors inherent in mathematical solution techniques.

Local scale dispersion processes which dominate in transport over distances ranging from centimeters to a few meters are diffusion processes and mechanical or hydrodynamic dispersion. These processes are accessible to laboratory studies and, therefore, their physics and effects are relatively well understood compared to regional scale processes. Problems associated with modeling these processes include model parameterization and numerical model problems that arise when advection dominates transport. The problems are easily handled relative to the problems arising at the regional scale.

A review of the sorts of numerical errors that plague many transport models is presented; in particular, we review conservation of mass in numerical models, stability problems, numerical dissipation, overshoot and undershoot, flexibility and cost considerations. Comparison of these numerical problems as associated with the four main transport modeling techniques: finite difference, finite elements, method of characteristics and random walk models, lead to the conclusion that random walk models are probably best suited for Lawrence Livermore Laboratory's needs and capabilities. Finite element models rank second, but are also very attractive in terms of the criteria employed.

One of the most complex problems that will be encountered in modeling regional transport is the parameterization and simulation of regional scale dispersion. Dispersion at this scale is dominated by mixing due to heterogeneities in aquifer properties. Also important at this scale are sampling errors, model assumptions concerning aquifer homogeneity and even numerical approximations and errors. In large part, what we call regional dispersion processes are the cumulative effects of the details that are not included in models of advective processes, whether because they are not known, unpredictable or because the modeling technique is inadequate to incorporate them.

Because of the complex origins and nature of these macro-dispersion processes and because of the long distances over which they are active, it was found that the process is difficult to parameterize for use in groundwater models. The descriptive coefficients used in such models should theoretically be functions of aquifer property heterogeneity magnitude and length scale, the flow field predominant in the aquifer, the length scale of the transport being modeled, and local scale dispersion processes. After a review of the possible approaches to parameterization, the conclusion is reached that parameterization should be based on field measurements made at the distance scale of the transport phenomena to be modeled or else the coefficients should be bypassed as much as possible through development of a probabilistic advection model. The proposed probabilistic transport model is based on a series of Monte Carlo simulations of transport through media that are believed to be possible realizations of the actual medium. The model results would consist of a statistical description of the possible concentration configurations at each simulation; the macro-dispersion coefficients required would be substantially reduced and represent processes that have somewhat more substantial physical bases.

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APPENDIX A.
DETAILS OF A 1-D RANDOM-WALK MASS TRANSPORT MODEL

INTRODUCTION

In Chapter III, a simple conceptual model of a one-dimensional macro-dispersive medium is presented. A numerical model of mass transport through the medium was developed for use on the Tektronix 4051 computer graphics system and ten simulations performed. The general conclusions which were inferred from the results of these simulations were summarized in Chapter III. In this appendix the numerical modeling method applied in those simulations is described, and the model input parameters and graphic outputs are outlined. In the next appendix, the simulation results will be discussed in detail.

DESCRIPTION OF THE RANDOM-WALK MODEL ALGORITHM

The numerical model developed to simulate transport through layered media for the purposes of investigating macro-dispersive processes is based on the simplest simulation approach available: the random-walk method of solution of the advective-dispersion equation. In Chapter IV, it is noted that this simulation technique is also among the most dependable of the methods considered.

Transport is modeled in the random-walk model by following the progress of a number of tracer particles as they are advected and dispersed along the length of the flow, i.e., along the x-axis, from initial positions at $x = 0$. The position of each of the particles is calculated at time intervals Δt and is

$$X_i(t + \Delta t) = X_i(t) + V(y_i(t)) \Delta t + \epsilon_{xi} \quad (A-1a)$$

$$Y_i(t + \Delta t) = Y_i(t) + v \Delta t + \epsilon_{yi} \quad (A-1b)$$

with $X_i(t)$, $Y_i(t)$ equal to the x and y coordinates of the ith particle at time t, $V(Y_i(t))$ equal to the x-component of seepage velocity in the layer which contains the plane $Y = Y_i(t)$, and v equals the y-component of velocity (due to J_y) which is constant throughout the aquifer.

The terms ϵ_{xi} and ϵ_{yi} are random distances that are added to the x- and y-position of the ith particle after each advection time step. ϵ_{xi} and ϵ_{yi} are normally distributed with zero mean and variances,

$$\sigma_x^2 = 2\alpha_L V(Y_i(t))\Delta t \quad (A-2a)$$

$$\sigma_y^2 = 2\alpha_T V(Y_i(t))\Delta t \quad (A-2b)$$

The local dispersion processes are simulated in the model by these random components.

The random-walk method of modeling advective-dispersive transport is based on the fact that if many tracer points are randomly displaced according to a Gaussian probability distribution from a single starting location, the resulting distribution of points will resemble a cloud whose density (or concentration) is described by the same Gaussian distribution. As noted in Chapter II, solutions to Fick's Law in the absence of advection (2-2) are generally related to the Gaussian distribution. In fact, they are quite often convolutions of that function. Advection is superimposed on this solution in the random-walk model with the result that the tracer points form a cloud with a density profile that approximates a concentration plume subject to the advection-dispersion equation (2-10). This method of transport modeling is easily implemented and provides simulations whose accuracy are limited only by the number of particles that can be traced. The advantages of this method are discussed further in Chapter IV.

The top and bottom boundaries of the medium in our conceptualization are the only place where the x- and y-position equations 3-1a and 3-1b do not necessarily apply. In the hypothetical situation illustrated in Figure 1a and 1b, these boundaries are assumed to be impermeable to the tracer and flow, and special checks must be included in the model code to assure that the model is, in fact, simulating that condition. The impermeable boundaries are handled in our code by a simple constraint on the positions to which a particle can be advected or dispersed. In other situations, infinite media could be simulated by choosing a very large number of layers. Ideally, even in a finite medium if boundaries are not of interest in a simulation, the system chosen should be large enough so that tracer points do not reach the boundaries.

The simulation results in our model are compiled and presented as if the tracer is being observed continuously along the entire length of the layered medium. The observations do not differentiate between concentrations in the individual layers. As we noted in the discussion of Table 1, this type of observation leads to results that are depth averaged and dispersion coefficients that are representative of local dispersion processes and the effects of stratification. On the basis of the mean and variance statistics of the cloud of tracer points, the apparent longitudinal dispersivity, α , is calculated according to the equation:

$$\alpha = \frac{\sigma^2}{2d} \quad (A-3)$$

where d is the mean position of the particles and σ^2 is the variance in their positions.

MODEL INPUT PARAMETERS

The simple random-walk model coded for this study simulates mass transport through a porous medium composed of horizontal layers with different hydraulic conductivities. All of the layers are assumed to be of uniform thickness. Along the length of this medium a regional hydraulic gradient J is imposed which induces flow through the system. In addition, a vertical gradient, J_v , can be included if a small component of flow across the layers is desired. All layers are assumed to share the same porosity N , local transverse dispersivity α_T and local longitudinal dispersivity α_L . The model simulates transport of the tracer from an instantaneous point or line source at time 0 along the x-axis ($x = 0$) perpendicular to the layering. Transport is modeled at discrete time steps Δt as indicated in Equations 3-1 and 3-2.

Each simulation is initiated by inputting the following parameters:

- Number of tracer points.
- Number of layers.
- Thickness of layers.
- Hydraulic conductivity of each layer.
- J , the regional hydraulic gradient along the x-axis.
- J_v , the vertical component of the regional hydraulic gradient.
- N , the medium porosity.
- α_L , local longitudinal dispersivity.
- α_T , local transverse dispersivity.
- The initial distribution of points along the x-axis ($x = 0$).
- Time step length.

These parameters together with assumptions based on the conceptual model underlying the simulations are sufficient to describe the transport situation.

DESCRIPTION OF 1-D RANDOM-WALK MODEL OUTPUT

The results for each simulation with our simple random-walk model, e.g., Figure 2, are presented as a series of histograms which represent the number of tracer points to be found within evenly spaced intervals (50m long) along the direction of flow (or horizontal axis) at 50-year intervals. These histograms are plotted with the number of points located within a given interval along the flow on the vertical axis. The axes all have their origins at 0 points and 0.0m. Cross hatched elements of the histograms found to the left of the origin represent points located at positions $x < 0.0m$. A box labeled "INPUT PARAMETERS" reports the model parameters applied in the simulation, including a plot of hydraulic conductivity K versus distance perpendicular to the layers y . Also shown in this plot is the distribution of tracer points along the line perpendicular to the layers initially and after 200 years. The initial positions are indicated by the line of points parallel to the y -axis next to the "IC" label in the "INPUT PARAMETERS" portion of the output graphics and the positions after 200 years are indicated by the array of points parallel to the y -axis next to the "FC". For the purposes of comparing the behavior of macro-dispersion under varying conditions, a simple linear regression is carried out for the σ^2 versus d curve of each simulation from time 0 to 200 years. The resulting slope s is used in the equation

$$\alpha = \frac{1}{2} s = \frac{1}{2} \left(\frac{\sigma^2}{d} \right) \quad (A-3a)$$

to calculate a coefficient value that is comparable from simulation to simulation. The calculated coefficient represents a time-averaged value taken on by the apparent dispersivity of the medium and is reported as "APPARENT DISPERSIVITY" at the bottom of each simulation output.

Also reported in each simulation output is the value

$$\alpha = \frac{1}{2} \left[\frac{\sigma^2(t)}{d(t)} \right] \quad (A-3b)$$

as calculated using the individual values of variance and mean reported at 50, 100, 150 and 200 years. These values represent the longitudinal dispersivity value that would have to be assumed in a model of the medium with uniform hydraulic conductivity to duplicate the statistics of the tracer cloud at each of the times shown. These values are reported in the simulation outputs as "α=" printed in the histograms for the corresponding time periods.

APPENDIX B.
SIMULATIONS OF TRANSPORT THROUGH A LAYERED POROUS MEDIUM

INTRODUCTION

In this appendix the results of ten simulations of mass transport through a simple layered medium are described and discussed. First, the conditions that were simulated are presented and then the simulation results are discussed.

DESCRIPTION OF SIMULATED CONDITIONS

Table 4 presents the values for the eight key input parameters in the ten simulations that were conducted. The number of tracer points in every simulation was one hundred and the porosity was assumed to be 0.01. The medium was assumed to be a total of 10 meters thick in all simulations.

Simulation F.2 is the baseline simulation. All of the other simulations involve a change in one or more of the baseline input parameters. The model parameters are described in Appendix A. Comparisons of the simulation results to the baseline results indicate how the varied parameters effect macro-dispersive mixing in the layered medium.

In the baseline simulation, flow through the medium is assumed to be strictly parallel to the layers, that is, parallel to the x-axis. The hydraulic gradient in that direction is 0.005 and there is no hydraulic gradient perpendicular to the layers. The local longitudinal and transverse dispersivity values are equal to 1cm and 3mm, respectively. These local values are representative of the dispersion within the individual layers, each of which is a homogeneous material. Thirty of these layers, each with its own hydraulic conductivity and each 0.33m thick, make up the porous medium. The hydraulic conductivities of these layers vary arbitrarily with a mean value $\bar{K}$ of 6.1 m/yr and a standard deviation of 2.22 m/yr. The initial condition (IC) for the baseline simulation has all 100 points located at $x = 0$ and distributed uniformly over layers 4 through 9.

TABLE 4. Key parameters applied in 1-D random-walk model simulations.

Simulation ID	<u>Hydraulic Gradients</u>		<u>Local Dispersivities</u>		Thickness of Layers	<u>Conductivity</u>		Initial Condition Perpendicular to Layering
	J	Jy	Longitudinal	Transverse		Standard Deviation	Mean	
F.2 (Baseline)	0.005	0	0.01m	0.003m	0.33m	2.22m/yr	6.1m/yr	Spread evenly over layers 4 through 9
F.3	b	b	b	0.0m	b	b	b	b
F.4	b	b	0.1m	0.3m	b	b	b	b
F.5	b	0.00004	b	b	b	b	b	b
F.6	0.0025	b	b	b	b	b	b	b
F.7	b	b	b	b	b	b	4.6m/yr	b
F.8	b	b	b	b	b	2.96m/yr	b	b
F.9	b	b	b	b	b	b	b	Point source in layer 5
F.10	b	b	b	b	b	b	b	Layers 4 through 25
F.11	b	b	23.8m	b	10m	b	b	Same positions as baseline

b = same value as in baseline simulation

All other simulations represent changes in the input parameters for comparison with the baseline simulation. In Simulations F.3 and F.4, the effects of using high and low local dispersivities are tested; in Simulation F.5 and F.6 the effects of varying the hydraulic gradients, both parallel and perpendicular to the layers, are observed. In Simulations F.7 and F.8, the standard deviations and mean values of the hydraulic conductivities in the layered medium are varied from their baseline values. Simulations F.9 and F.10 represent experiments to determine the effects of initial conditions on macro-dispersive behavior. Finally, Simulation F.11 illustrates an experiment that includes much less detail in the model.

DISCUSSION OF SIMULATION RESULTS

Before proceeding to discuss the simulation results, a word of caution concerning the generalizations that will be drawn is necessary. The model employed in these analyses is a very simple representation of the tremendously complex causes and effects of macro-dispersion. The model, to a certain extent, has been limited to this simple form by the resource constraints of this study, but also has been kept simple in order that it remain an instructive conceptual model. The simulations were not intended to prove any of the trends in macro-dispersive behavior; rather, their purposes is to evoke thought concerning the processes involved. Within the framework of the simple one-dimensional conceptual model on which the computer code is based, we hope that the following discussion will expedite understanding of why certain aquifer and transport model parameters are important in determining the extent and nature of dispersive mixing in heterogeneous porous media.

Simulation F.2

The results of the baseline simulation, F.2, are discussed in Chapter III where it is noted that the tracer is being spread over much longer distances than can be explained by the local dispersion processes. This extensive spreading is caused by the heterogeneity of the hydraulic conductivity.

Simulation F.3

In order to illustrate how conductivity heterogeneities lead to dispersive behavior, Simulation F.3 was performed. In this simulation the local transverse dispersivity is assumed equal to zero and as a result no mixing between the layers occurs. Figure 5 presents the results of this simulation. Notice that the position of the tracer points perpendicular to the layering after 200 years, indicated by the set of points next to the "FC" in the input parameters box in Figure 5, is the same as their initial positions (IC), indicating that no lateral movement of the tracer points has occurred.

Notice that Figure 5 reports an apparent dispersivity for Simulation F.5 of 40.6m, which is substantially greater than the baseline result of 23.8m. Notice also that the "cloud" of tracer points in Simulation F.3 does not resemble the "cloud" in the baseline simulation F.2, illustrated in Figure 2. Rather, in Simulation F.3 the tracer is transported through the medium in the form of a small number of pulses. Both of these results are to be expected since in the absence of mixing between layers, as time progresses the tracer points in layer i tend to be a distance along the medium

$$d_{ij} = (u_i - u_j)t \quad (B-1)$$

from points in layer j (with u_i the seepage velocity in layer i). Tracer in each layer is advected over longer or shorter distances than the tracer in surrounding layers depending on the hydraulic conductivity of those layers. The average distance that the entire mass of tracer is advected is

SIMULATION ID : F. 3
X TIC INTERVAL = 50
Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
IN EACH PLOT.

APPARENT DISPERSIVITY : 40.6 M

FIGURE 5 Distribution of tracer at 50 year intervals as it is transported along a layered porous medium with no mixing between layers.

NOTE: This simulation shows a complete breakdown of the concept of macro-dispersion when local dispersivity is assumed negligible and channeling becomes the mode of transport.

$$d = \bar{u}t = \frac{KJ}{n}t \quad (B-2)$$

where $\bar{u}$ is the average seepage velocity in the layers along which the tracer is being advected and $\bar{K}$ is the average hydraulic conductivity in the same layers. The spreading of the tracer points may be measured by the variance of their locations around the average location,

$$\sigma^2 = E[(ut - \bar{u}t)^2] \quad (B-3a)$$

where $E[\cdot]$ denotes "the expected or average value of". This may be reduced to

$$\begin{aligned} \sigma^2 &= E[(u - \bar{u})^2 t^2] \\ &= E[(u - \bar{u})^2] t^2 \\ &= E \left[\left(\frac{KJ}{n} - \frac{\bar{K}J}{n} \right)^2 \right] t \\ &= E[(K - \bar{K})^2] \frac{J^2 t^2}{n^2} = \sigma_K^2 \frac{J^2 t^2}{n^2} \end{aligned} \quad (B-3b)$$

where σ_K^2 is the variance of the hydraulic conductivity of the layers in which the tracer is advected. Thus, when no mixing between layers occurs we expect spreading over a distance of roughly 4 standard deviations which is equal to

$$4\sigma = \frac{4\sigma_K Jt}{n} = \frac{4\sigma_K}{\bar{K}} d \quad (B-4)$$

The corresponding apparent dispersivity would be

$$\begin{aligned} \alpha &= \sigma^2 / 2d = \frac{\sigma_K^2 J^2 t^2}{n^2} \bigg/ 2 \left(\frac{K Jt}{n} \right) \\ &= \frac{\sigma_K^2}{2\bar{K}} \frac{Jt}{n} = \frac{\sigma_K^2}{\bar{K}^2} \frac{ut}{2} = \frac{\sigma_K^2}{\bar{K}^2} \frac{d}{2} \end{aligned} \quad (B-5)$$

Thus, in our layered medium, in the absence of mixing between layers the apparent dispersivity and distance over which the tracer spreads are increasing (linear) functions of time or its surrogate distance advected. The result also suggests that the more heterogeneous the medium, i.e., the larger $\frac{\sigma_K^2}{K}$ becomes, the larger will be the apparent dispersivity and spreading. In Simulation F.3, the variance of the hydraulic conductivities in the contaminated layers is $3.35 \text{ m}^2/\text{yr}^2$ and the average is $4.15 \text{ m}/\text{yr}$; therefore, the apparent dispersivity should be

$$\alpha = \frac{\sigma_K^2}{K} \frac{ut}{2} = \left(\frac{3.35 \text{ m}^2/\text{yr}^2}{4.15 \text{ m}/\text{yr}} \right) \frac{(2.075 \text{ m}/\text{yr})t}{2}$$

$$= (0.202 \text{ m}/\text{yr})t \quad (\text{B-6})$$

or approximately 40.4m by the year 200. The value reported for the simulation is 40.6m, the difference between the two being attributable primarily to the effects of local longitudinal dispersion.

The results of Simulation F.3 might be compared in a certain sense to the channeling phenomena discussed above in connection with Winograd and Pearson's work. Channeling as discussed above is the result of the presence in a region of relatively well defined channels or conduits of material with advection rates much higher than surrounding materials. Channeling occurs when a contaminant is advected through the region by means of these well defined conduits quickly enough so that little mixing with the rest of the region occurs. In Simulation F.3 we have, by neglecting mixing between layers, insured that all layers act as independent channels. Under channeling conditions, Fickian models of regional mixing are generally not applicable. A major reason is demonstrated by the pulse-like distributions in Figure 5. With no mixing between layers and relatively little longitudinal mixing within each layer, the tracer travels along each layer suffering little or no dilution from its initial concentration. The tracer moves through the medium in undiluted pulses with a pulse from each contaminated layer arriving in

turn at the monitoring wells. This behavior is considerably different from the smooth concentration profiles showing considerable dilution from input concentrations that are encountered in the laboratory, in the field when channeling is not important and, in short, where mixing may be approximated by Fick's Law. The considerable difference between transport with channeling and without renders the phenomenon a threat to the accuracy and applicability of conventioned mass transport modeling approaches.

While it is relatively simple to derive analytical estimates of the extent of tracer spreading and to estimate the apparent dispersivity when mixing between layers is neglected, inclusion of mixing greatly complicates the process of deriving such estimates. In Chapter III results obtained by two research groups applying state-of-the-art methods to this problem were outlined. Through the simulations to be discussed below we will attempt to identify and justify parameters and trends of the dispersion process when lateral mixing is included without attempting to formally derive the results.

Simulation F.4

Comparison of the baseline simulation results with the results of Simulation F.3 in which, as discussed above, no lateral mixing occurs suggests that inclusion of lateral mixing in a simulation decreases the apparent dispersivity. Simulation F.4 was conducted to further explore the role of mixing between layers on the macro-dispersion process. Figure 6 illustrates the result of Simulation F.4 in which local dispersivities are increased by an order of magnitude. The resulting apparent dispersivity is 3.2m for this simulation which is much less than the values of 23.8m in the baseline Simulation F.2 and 40.6m in Simulation F.3. Figure 7 illustrates the effect that lateral dispersivity has on the curve of variance versus the mean distance that the tracer has been transported in the simulated medium. It is clear from

SIMULATION ID : F.4
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

APPARENT DISPERSIVITY : 3.2 M

FIGURE 6. Distribution of tracer at 50 year intervals as it is transported through a layered porous medium with relatively large local dispersivity values, ($\alpha_T = 3$ cm).

NOTE: This simulation shows a reduction in longitudinal dispersal of the tracer as a result of increased lateral mixing.

these curves that decreasing the transverse dispersivity and therefore lateral mixing increases the spreading (or variance) of tracer along the medium. Recalling that the dispersivity is defined to be the slope of the σ^2 versus d curve; Figure 7 shows that apparent dispersivity may be increased by decreasing local transverse dispersivity.

FIG. 7. Effect of local transverse dispersivity values on longitudinal dispersion along a layered medium.

The decrease in the longitudinal dispersal of the tracer with increasing local mixing between layers seen in Figure 7 is the intuitively correct trend. When lateral mixing is increased, the distance that each component of the tracer cloud (or each tracer point) tends to approach the average distance for the entire cloud. Consider, for example, the extreme case in which lateral mixing has become so extensive that each component of the tracer cloud is equally likely to be found in any of the layers at any given time. As a result of this mixing, each component or tracer point may be expected to spend very nearly the same amount of time in

every layer during the period of transport. In our model, this might imply that each tracer point spends approximately 1/30 of its time in each layer during the 200 year simulation period. The average distance that each point would be advected is

$$d = \frac{200}{30} u_1 + \frac{200}{30} u_2 + \dots + \frac{200}{30} u_{30}$$

$$= 200 \bar{u} \quad (B-7)$$

where

u_i = seepage velocity in layer i , and

$\bar{u}$ = average seepage velocity.

Since all points would be subjected to this mixing, all points would be advected this average distance plus or minus a relatively small distance attributable to the randomness of the mixing process, that is, attributable to the scatter of times spent by each point in each layer around the value 200/30 years. Increasing the rate of lateral mixing causes the rate of transport of each point in the tracer cloud to converge to the average advection rate, and the result is a relatively small apparent dispersivity. At the other extreme is the case discussed above in which no mixing between layers occurs. In that case, the "cloud" is composed of many components each of which is advected at a well defined rate. The entire cloud has an average rate of advection (although not necessarily equal to $\bar{u}$ above) but most components are not advected at that rate. The "cloud" as we have seen above is composed of neatly spaced, undiluted pulses of tracer and the apparent dispersion of the tracer is the result of the different advection rates of these well defined pulses. The apparent dispersivity in this case can become infinitely large. Between these two extremes, it is reasonable to expect that as mixing between layers increases, the travel times of the tracer points will be increasingly equalized and thus longitudinal spreading will be decreased.

Simulation F.5

Figure 8 illustrates the results of Simulation F.5 and shows the effect on longitudinal dispersion of imposing a small component of advecting flow perpendicular to the layers. A small regional vertical gradient of 0.00004 is assumed to be superimposed on the longitudinal gradient of 0.005. Although this vertical gradient is over two orders of magnitude smaller than the longitudinal gradient, it leads to an immediate and significant decrease in the apparent dispersivity in comparison to the baseline case. The two dimensional nature of the flow field in Simulation F.5 is the dominant force in causing lateral mixing. Because it is an effective force in causing tracer points to spend time in many different layers, the apparent dispersion due to velocity differences is averaged out and reduced considerably. Generally, two-dimensional velocity fields tend to act as very efficient mixing agents. This effect, as will be discussed later in connection with Matheron and de Marsily's (1979) theoretical results, suggests that the one dimensionality of the flow field and conductivity variations in our model places severe limitations on the physical validity of the results obtained. Figure 9 illustrates the effect that the small vertical gradient has on longitudinal dispersion of the tracer. The slope of the σ^2 versus d curve is significantly decreased when the small vertical gradient is included. As in Simulation F.4, increased lateral mixing results in less extensive longitudinal dispersal and smaller values of the apparent dispersivity of the medium.

SIMULATION ID : F.5
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

APPARENT DISPERSIVITY : 4.7 M

FIGURE 8. Distribution of tracer at 50 year intervals as it is transported through a layered porous medium in a flowfield that is not exactly parallel to the layering.

NOTE: This simulation shows a large reduction in longitudinal dispersal of the tracer due to the small component of flow across the bedding.

FIG. 9. Effect of a small vertical hydraulic gradient on longitudinal dispersion of the tracer.

Simulation F.6

Figure 10 illustrates the results of a simulation (F.6) in which the regional gradient along the layer is reduced to half the baseline value of 0.005. This reduction reduces the seepage velocities and therefore the advection rates through all layers to half their baseline values. Although the apparent dispersivity for the simulation is 19.4m which is not very different from the baseline value (F.2) of 23.8m, comparison with the baseline results suggests that in Simulation F.6 the longitudinal dispersal of tracer after 100 years is very nearly the same as in the baseline simulation after 50 years. Similarly after 200 years in Simulation F.6 the dispersal approximates that found after 100 years in the baseline case. It appears that reducing the regional gradient by half results in a

SIMULATION ID : F.6
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

B-15

APPARENT DISPERSIVITY : 19.4 M

FIGURE 10. Distribution of tracer at 50 year intervals as it is transported along a layered porous medium driven by a hydraulic gradient that is half the baseline value ($J = 0.0025$).

NOTE: Mixing in this simulation proceeds at half the rate reported in the baseline simulation.

general reduction of the rate of tracer dispersal. Figure 11 illustrates that the longitudinal dispersal (or variance) of the tracer is almost identical in the two simulations when the two advection distances are equal. Thus, although it is often convenient to consider the dispersivity of a heterogeneous medium to be a function of time, it is perhaps more meaningful to recognize the average distance that the tracer is advected as a parameter of the process. It is likely that if the output interval for the baseline simulation were 25 years rather than 50 years the σ^2 versus d curves in Figure 11 would match even more closely.

FIG. 11. Effect of a reduction in the regional hydraulic gradient on longitudinal dispersion of the tracer.

Reducing the regional hydraulic gradient J reduces the rate of advection in each layer

$$u_i = \frac{K_i J}{n} \quad (B-8a)$$

and also reduces the rate of the local dispersion processes which depend on

$$D_i = \alpha u_i = \frac{\alpha K_i J}{n}$$

where u_i is the seepage velocity in the i -th layers and D_i represents a local dispersion coefficient in this instance. With the rates of both underlying processes reduced by half, the macro-dispersion processes proceeds at half the baseline rate. In light of this it is apparent that the rate of tracer dispersal could also be decreased by half, by doubling the porosity.

Simulations F.7 and F.8

Figure 12 presents the results of a simulation (F7) in which the hydraulic conductivities throughout the medium are uniformly reduced so that the mean conductivity $\bar{K}$ is 4.6 m/yr or 3/4 of the average value in the baseline simulation. The apparent dispersivity reported for Simulation F.7 is 60.0m, a value which is considerably larger than the baseline value.

Reducing the mean conductivity results in a reduction in the average advection rate but apparently does not simply slow down the transport processes. As discussed in Chapter III and throughout this Appendix, it is the variability of conductivity which drives the macro-dispersion process. As a result, the way that the mean conductivity affects the macro-dispersion process is very different from the influence of the porosity, regional hydraulic gradient or other uniform parameters of the advection process. -Reducing the mean conductivity without altering the

SIMULATION ID : F.7
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

FIGURE 12 Distribution of tracer at 50 year intervals as it is transported along a layered porous medium with an average hydraulic conductivity that is 75% that of the base-line average.

NOTE: Decreasing the average hydraulic conductivity without reducing the variability results in a larger apparent dispersivity.

variability of hydraulic conductivity from layer to layer, as in Simulation F.7, serves to increase the effect of the variability. The range over which hydraulic conductivity varies becomes a larger proportion of the average as does the range of advection rates. The importance of this proportion commonly measured by the coefficient of variation ($\sigma_K/\bar{K}$) is, for example, indicated by Equation B-5 which states that mixing due solely to advective differences is described by a dispersivity

$$\alpha = \frac{\sigma_K^2}{\bar{K}^2} \frac{d}{2} \quad (B-5)$$

Another way of affecting the coefficient of variation is to increase the standard deviation of the conductivity variations σ_K . This too will increase macro-dispersion. Simulation F.8, whose results are presented in Figure 13 is a simulation in which the standard deviation of the hydraulic conductivities is increased from the baseline value 2.22m/yr to 2.96m/yr. This increase is accomplished without altering the mean value or the spatial correlation structure of the conductivities. The apparent dispersivity reported in this case of 76.1m which is even larger than the dispersivity reported for Simulation F.7.

The results of the two simulations may be compared to the baseline case and each other in Figure 14 which presents the σ^2 versus d curves for the three simulations. The baseline curve is very different from the other curves because under baseline conditions the coefficient of variation of the conductivities is only 3/4 that of the other two. The dispersion processes in Simulations F.7 and F.8 are, as illustrated in Figure 14, very similar functions of distance advected d . Thus, we surmise that the coefficients of variation of hydraulic conductivities or advection rates in the layered medium are appropriate parameters of the macro-dispersion process.

SIMULATION ID : F.8
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

FIGURE 13. Distribution of tracer at fifty year intervals as it is transported along a layered porous medium with hydraulic conductivity values that are 4/3 as variable as the baseline values.

NOTE: Increased hydraulic conductivity variability leads to increased variation of advection rates from layer to layer and, as a result, a larger apparent dispersivity.

FIG. 14. Effect of increasing the coefficient of variation of the hydraulic conductivities in the medium on longitudinal dispersion.

Simulations F.9 and F.10

The effect of the initial location of the tracer on the macro-dispersion process may be investigated through a comparison of the results of Simulations F.9 and F.10, in conjunction with the baseline Simulation F.2. In Simulation F.9, whose results are presented in Figure 15', the entire mass of tracer is located at time 0 at a single point two meters from the bottom of the medium ($y = 2\text{m}$) and at $x = 0.0\text{m}$. The baseline initial condition has the tracer scattered evenly over approximately 2 meters along the line $x = 0$ While in Simulation F.10, whose results are presented in Figure 16, the tracer is initially evenly spread over approximately 7 meters along the line $x = 0$. Simulation F.9 results in an apparent dispersivity of 19.6m while Simulation F.10 yield a value of 20.2m. Neither of these values is substantially different from the baseline result (23.8m). Notice that there appears to be

a trend from the tracer profiles reported in Figure 15 for Simulation F.9, which are skewed toward the positive x- (longitudinal) direction, to the negatively skewed profiles found in Figure 16 for Simulation F.10. Between these extremes lies the baseline simulation which exhibits more or less symmetric profiles by the year 200. Figure 15 presents the σ^2 versus d curves for the three simulations and shows that, after a time, differences between the slopes of the curves becomes quite small (relative to the differences seen in Figures 7, 9, and 14). This result suggests that the effect of initial conditions on apparent dispersivity may be transient. Intuitively it might be suggested that the initial conditions will be of importance only for a period of time whose extent depends on such factors as the rate of advection, the extent of lateral mixing and the heterogeneity of the medium.

Fig. 15. Effect of initial distribution of tracer perpendicular to layers on longitudinal dispersion along a layered medium.

SIMULATION ID : F.9
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

APPARENT DISPERSIVITY : 19.6 M

FIGURE 16 Distribution of tracer at fifty year intervals as it is transported along a layered porous medium from an initial point source.

NOTE: The effects of initial conditions on the macro-dispersion process appear to be transitory.

SIMULATION ID : F. 10
 X TIC INTERVAL = 50 M
 Y TIC INTERVAL = 1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

FIGURE 17 Distribution of tracer at fifty year intervals as it is transported along a layered porous medium from a widely spread line source.

NOTE: The effects of initial conditions on the macro-dispersion process appear to be transitory.

Simulation F.11

A final experiment with the model was performed to demonstrate the problems involved in attempting to apply the apparent dispersivity as a parameter in a transport model. In Simulation F.11, the layering of the medium was not included in the model and, in order to compensate, the local longitudinal dispersion coefficient was assumed equal to the apparent dispersivity in the baseline case. The hydraulic conductivity of the medium was assumed equal to the average value in the baseline case, 6.1m/yr. The resulting tracer profiles are illustrated in Figure 18. The apparent dispersivity reported in 24.7m for Simulation F.11 while the assumed local dispersivity was 23.8m. The difference between these two values is statistically insignificant; for example, the difference between the assumed and calculated values is well within the confidence bounds of the linear regression on which the calculated value is based.

Notice that during the first 100 years components of the tracer cloud are found upstream of the initial pulse of concentration, a result that is not found in the more detailed baseline simulation (Figure 2). This problem was also reported by E. S. Simpson (1978) and apparently is a common difficulty when large constant apparent dispersivity values are applied in transport models. This suggests that at least during the early time steps apparent dispersivity coefficients must be small if physically meaningful results are to be obtained from transport models. After a time, however, Figure 19 shows that the simple model of the medium employed in Simulation F.11 reproduces the rate of dispersion in the baseline case fairly well. This suggests that after the dispersivity in the layered medium has stabilized, the simple unlayered model of the medium with a large assumed dispersivity can be used to predict certain aspects of tracer transport. It appears that, after the early time steps, the unlayered model of the medium with a large assumed dispersivity can be used to predict certain aspects of tracer transport. These results suggest that accurate models of macro-dispersive media will require time varying coefficients at least during the early time steps. Since "early times" may be quite extensive given the slow nature of groundwater systems, this problem needs to be addressed very carefully. As we have seen above,

SIMULATION ID : F.11
 X TIC INTERVAL ~50 M
 Y TIC INTERVAL ~1 POINT

NOTE: THE VERTICAL SCALE IS DIFFERENT
 IN EACH PLOT.

FIGURE 18 Distribution of tracer at 50 year intervals as modeled replacing the layered porous medium with a uniform medium with large local dispersivity ($\alpha_L = 23.8$ m).

NOTE: During the first 100 years fictitious upstream transport is predicted by this simplified model.

many parameters of the medium may be expected to play a role in determining just how long the "early times" last and how the coefficient will vary during this time.

FIG. 19. Comparison of results of a layered model of the medium to a homogeneous model of the medium.

Finally, notice that the tracer profiles in Figure 18 tend to approximate a Gaussian distribution. This shape is to be expected given the very simple Fickian model applied. None of the other simulation results are as symmetric or as "bell-shaped". The tracer profiles in all other simulations are distorted and show the effects of the medium layering; that is, to some extent, all show the tendency to separate into pulses as in Figure 5. This behavior is the result of the finite thickness of the layers, the limited number of layers, the limited time span modeled and the statistical nature of the numerical model.

After a long time, the layered model could lead to Gaussian profiles if the distance that each component of tracer is advected in each layer (or alternatively the times spent in each layer) during the simulation period are considered to be randomly distributed. By the Central Limit Theorem the total distance transported might tend to be distributed according to a Gaussian or normal probability distribution. The Central Limit Theorem states that,

"Under very general conditions, as the number of variables in the sum becomes large, the distribution of the sum of random variables will approach the normal probability distribution,"

which applies

- "1. If the variables involved are independent and identically distributed;
2. if the variables are independent, but not identically distributed (provided that each individual variable has a small effect on the sum); or
3. if the variables are not independent at all, but jointly distributed such that correlation is effectively zero between any variable and all but a limited number of others."

(Benjamin and Cornell, 1970).

If sufficient mixing occurs and the conductivities and advection rates are sufficiently random, the entire mass of tracer (or in our case all tracer points) may be expected to approach a concentration profile that approximates a normal curve. The tracer profiles in Figures 2 (Simulation F.2), 6 (Simulation F.4) and 7 (Simulation F.5) show a slight tendency toward this "bell" shape. The tracer profiles in the other simulations show the effects of other factors such as the discrete layering of the model and thus do not closely approximate this shape.

These considerations suggest that, in the presence of conductivity heterogeneities, the simple Fickian model will very likely fail to model the details of the concentration profiles, even if it is calibrated to duplicate the extent and simple statistics of the macro-dispersion process. After a very long time, however, within certain restrictions the layered model may approach the Gaussian profiles exhibited by the simple Fickian model.