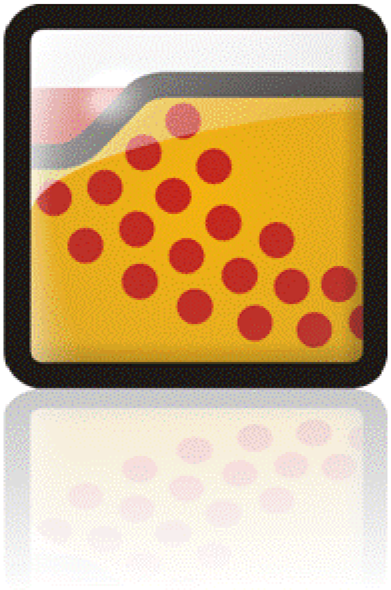

Contaminant Modeling with

CTRAN/W 2007

An Engineering Methodology

Third Edition, March 2008

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1 Introduction

CTRAN/W is a finite element software product that can be used to model the movement of contaminants through porous materials such as soil and rock. The comprehensive formulation of CTRAN/W makes it possible to analyze problems varying from simple particle tracking in response to the movement of water, to complex processes involving diffusion, dispersion, adsorption, radioactive decay and density dependencies.

CTRAN/W is integrated with SEEP/W, VADOSE/W and SIGMA/W, other GEO-SLOPE software products that compute the water flow velocity for a problem. CTRAN/W utilizes the seepage flow velocities to compute the movement of dissolved constituents in the pore-water. CTRAN/W can only be used in conjunction with external seepage data. For a density-dependent analysis, CTRAN/W can only be coupled with SEEP/W. Currently, CTRAN/W does not deal with air phase transport.

1.1 Typical applications

CTRAN/W can be used to model many groundwater contaminant transport problems. This section presents examples of the types of problems that can be analyzed using CTRAN/W. It should be noted that CTRAN/W is designed to use the seepage flow velocities computed due to flow in both the saturated and unsaturated zones. Therefore CTRAN/W is formulated to model saturated/unsaturated contaminant transport.

The next section provides a review of contaminant transport processes to facilitate the later discussion of the applications for which CTRAN/W can be used.

1.2 Contaminant transport processes

The factors which govern the migration of a contaminant can be considered in terms of *transport* processes and *attenuation* processes. The transport processes can be mathematically represented by equations based on flow laws. These equations can be combined into a mass balance equation with those processes causing the attenuation of the contaminant; this yields the general governing differential equation for contaminant migration.

Transport processes

The two basic transport processes are *advection* and *dispersion*. Advection is the movement of the contaminant with the flowing water. Dispersion is the apparent mixing and spreading of the contaminant within the flow system. The advection and dispersion transport processes can be illustrated by considering a steady flow of water in a long pipe filled with sand.

Consider the injection of a slug of contaminant mass into the pipe (Figure 1-1). The mass flows along the pipe with a constant velocity *v*. This transport process is called advection. As the mass moves along with the moving water, it also spreads out (i.e., disperses). The contaminant mass occupies an increasingly longer length of the pipe, thereby decreasing in concentration with time. The spreading out of the contaminant is called dispersion.

Figure 1-2 illustrates the transport process when a continuous source of contaminant mass is injected into the pipe. At some point in the pipe beyond the injection location, the contaminant initially appears at a low concentration and then gradually increases until the full concentration is reached. If only the advection process is considered, the contaminant would arrive at some point in the pipe as a plug with full concentration. Because of dispersion, however, the full concentration arrives at a time later than the first appearance of the dispersed contaminant, as shown in the figure.

Theoretically, the plug flow arrival time corresponds to the time when the fifty-percent concentration arrives. The time difference between the first arrival of the dispersed contaminant and the arrival of the plug flow increases as the distance from the injection point increases.

While the advection process is simply migration in response to the flowing water, the dispersion process consists of two components. One is an apparent "mixing" and the other is molecular diffusion.

The mixing component, often called *mechanical dispersion*, arises from velocity variations in the porous media. Velocity variations may occur at the microscopic level due to the friction between the soil particles and the fluid and also due to the curvatures in the flow path, as illustrated in Figure 1-3. These velocity variations result in concentration variations. When the concentration variations are averaged over a given volume, the contaminant appears to have dispersed.

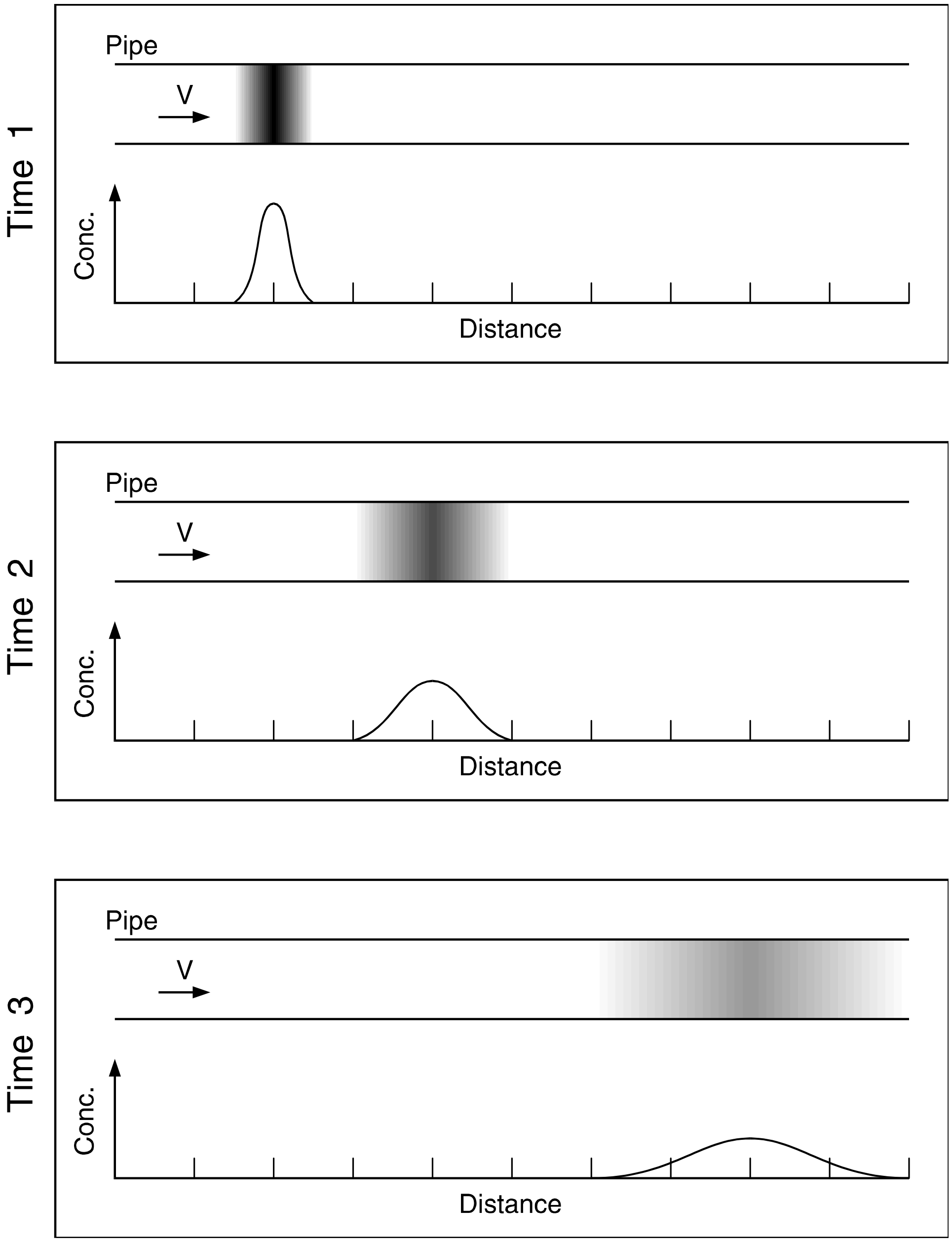


Figure 1-1 The Migration and spreading of a contaminant slug in a fluid flowing with velocity V

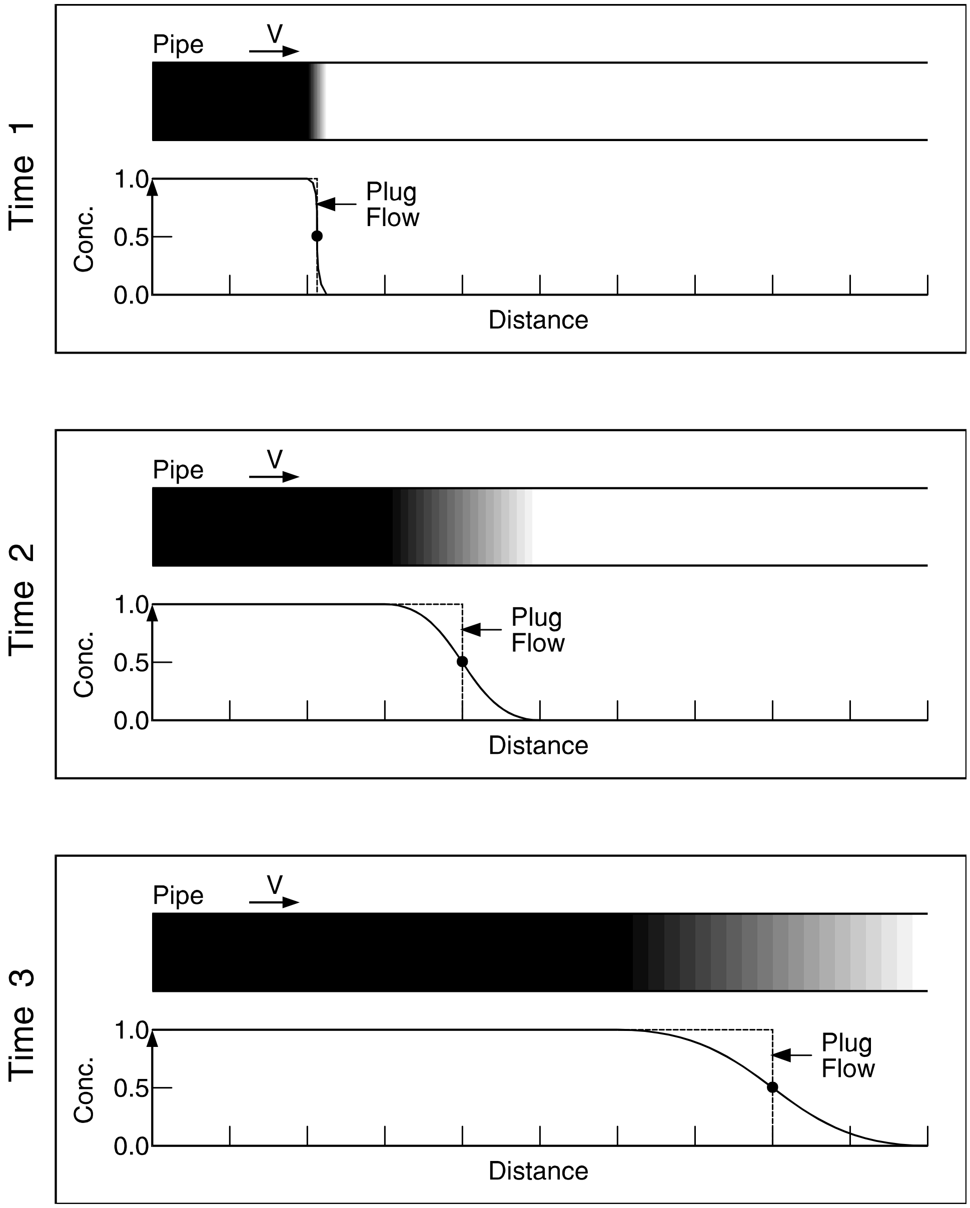


Figure 1-2 Contaminant migration and spreading from a continuous source in a fluid flowing with velocity V

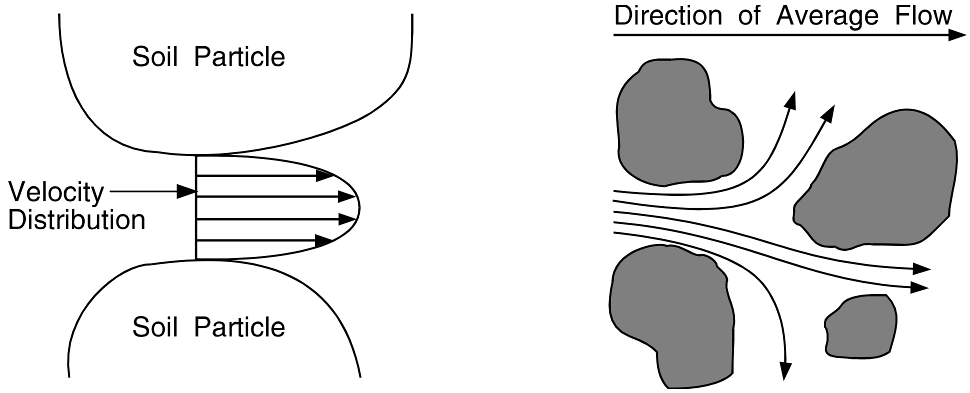


Figure 1-3 Factors causing mechanical dispersion

Molecular diffusion results in the spreading of contaminant due to concentration gradients. This process occurs even when the seepage velocity is zero. Molecular diffusion is dependent on the degree of saturation or volumetric water content of the porous medium, an example of which is shown in Figure 1-4.

In equation form, the dispersion process is characterized as:

$$D = \alpha v + D^*$$

where:

D = coefficient of hydrodynamic dispersion,

v = average linear velocity of the flow system,

α = dispersivity of the porous medium, and

D^* = coefficient of molecular diffusion.

Attenuation processes

Contaminant migration in a porous medium is attenuated by chemical reactions taking place during transport. These reactions can occur between the contaminant mass and the soil particles or between the contaminant mass and the pore fluid. Among these reactions, the process of adsorption is believed to be the most important factor in attenuating the migration of contaminant.

Adsorption causes contaminant mass to be withdrawn from the moving water, reducing the dissolved concentration and overall rate of contaminant movement.

The amount of adsorption that occurs is a function of the contaminant concentration within the porous medium. This relationship is described by an adsorption function which relates the adsorption to the concentration. An example of this relationship is shown in Figure 1-5.

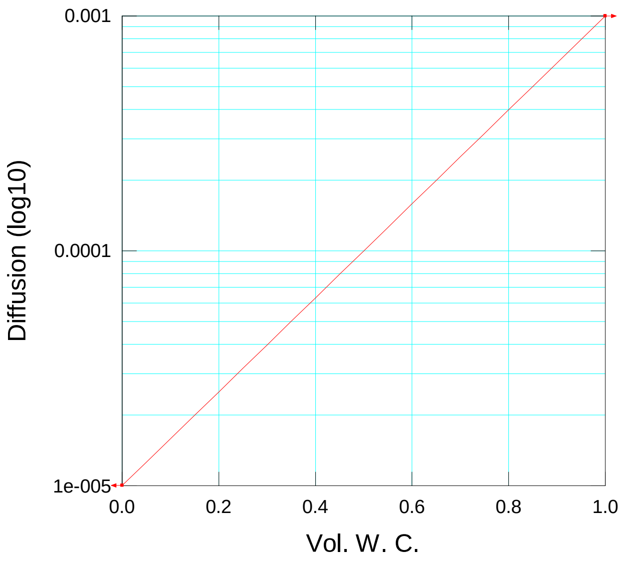


Figure 1-4 Example of molecular diffusion as a function of water content

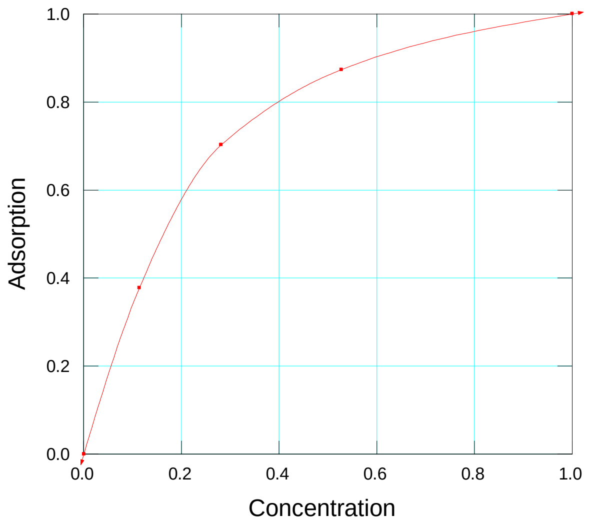


Figure 1-5 Example of adsorption as a function of concentration

In general, the adsorption characteristic of a contaminant in a soil is represented by a function of S vs. C, where S is the mass of contaminant adsorbed per unit mass of soil particles, and C is the concentration of the contaminant in the porous medium. In the case of a linear function, the slope is called the distribution coefficient, K_d The slope represents the partitioning of the contaminant mass between the solid (soil particles) and fluid phases of the porous medium. The chemical reactions that cause the partitioning are assumed to be instantaneous and reversible.

Another important attenuation process in the case of a radioactive contaminant mass is *radioactive decay*. Radioactive decay causes a loss of contaminant mass from the flow system. However, unlike adsorption, the decayed mass is proportional to the travel time and is irreversible.

1.3 Advective contaminant transport

As described above, contaminant transport in soils involves the processes of both advection and dispersion. Early in a contaminant transport analysis, it is often useful to isolate the magnitude of purely advective transport without the extra data input and computational requirements of including dispersion. It is impossible to numerically solve the advection-dispersion equation when the dispersive component is small relative to the advective component, because the numerical solution is unstable in these cases. To overcome this difficulty, CTRAN/W has an option to simulate the purely advective contaminant transport process using particle tracking.

In particle tracking, the dissolved solutes are represented by particles. Figure 1-6 presents an example of a particle tracking analysis. For each time step, the particles are moved in space proportionally to the water flow velocity and the time step size. The particle flow paths provide a graphical representation of the contaminant plume movement caused by purely advective transport. The effects of dispersion, adsorption, decay and density are not considered in a particle tracking analysis.

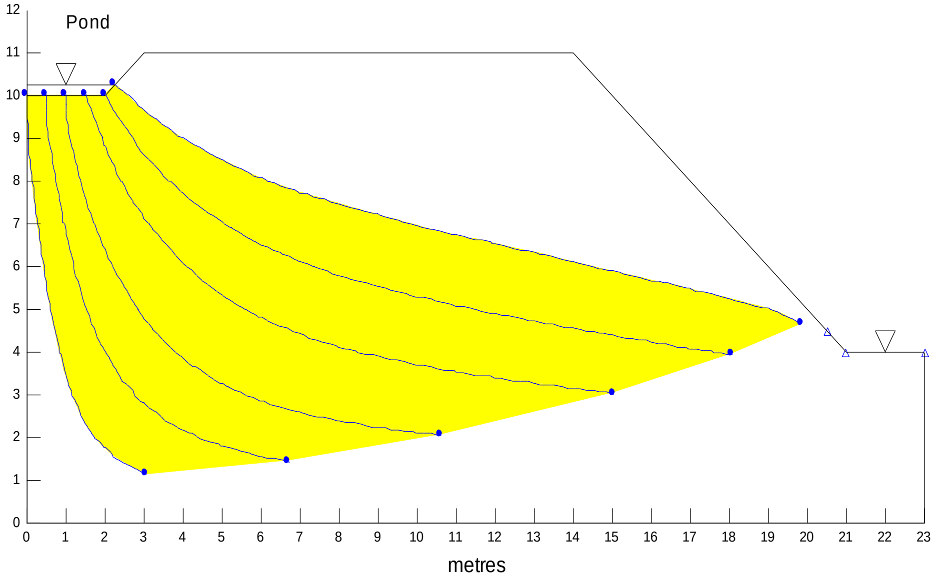


Figure 1-6 Example of a particle tracking analysis

1.4 Advective-dispersive contaminant transport

Quantification of the magnitude of advective flow is useful as a preliminary analysis of contaminant transport. A more realistic analysis also includes the effect of hydrodynamic dispersion. Hydrodynamic dispersion causes dilution of contaminants both longitudinally, (in the direction of groundwater flow), and transversely, (perpendicular to the direction of flow). Contaminant dilution caused by dispersion is a very significant component of contaminant transport and therefore cannot usually be ignored. CTRAN/W provides the capability for modeling contaminant transport with hydrodynamic dispersion.

The transport of certain contaminants, such as dissolved hydrocarbons, is attenuated by reversible reactions with soil particles, such as adsorption. Other contaminants, such as radioactive contaminants, undergo non-reversible decay reactions that remove them from the groundwater during transport. CTRAN/W is formulated to include the effects of absorption and decay type reactions during contaminant transport.

Figure 1-7 shows the results of an advection-dispersion analysis of contaminant migration from a surface pond.

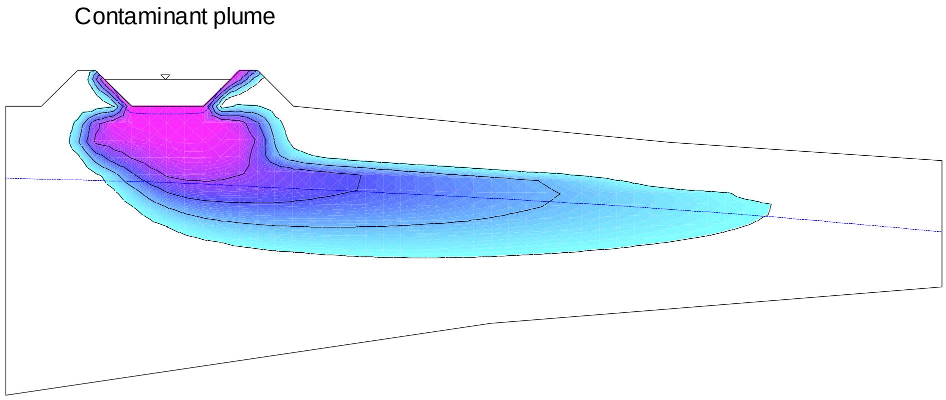
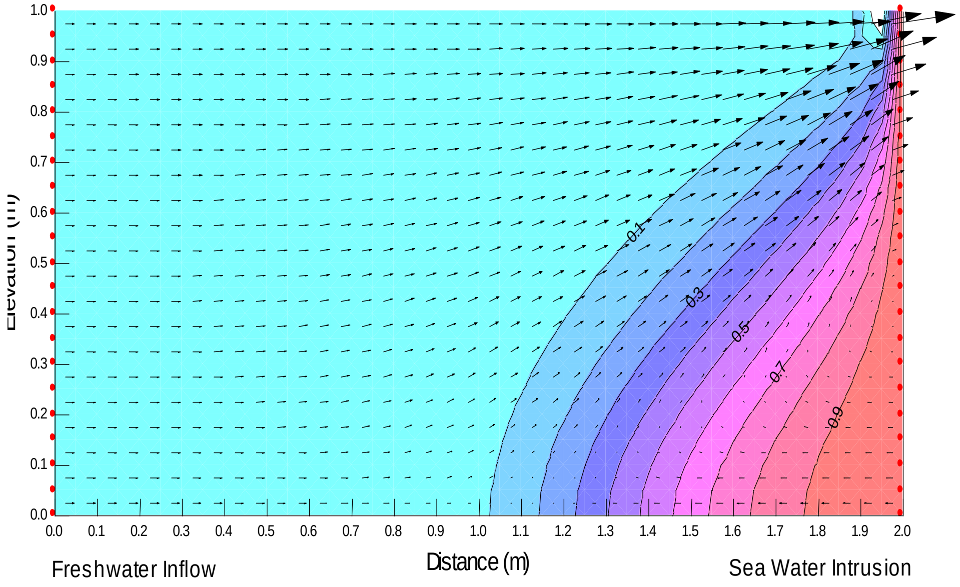


Figure 1-7 Contaminant transport from a surface pond

1.5 Density-dependent contaminant transport

For problems where the dissolved solute density is significant, CTRAN/W has the capability of performing density-dependent flow analyses. Density-dependent problems include sea water intrusion into coastal aquifers, brine transport and landfill leachate migration, to name just a few.

Figure 1-8 illustrates the CTRAN/W solution to the classic Henry's problem for sea water intrusion. At the left boundary, freshwater enters at a constant rate while the right boundary of the aquifer is exposed to sea water constant head conditions. The top and bottom boundaries have no flow. The contours show the relative concentration of sea water, and the vectors show the relative magnitude and direction of the water flow.



Contours indicate relative concentration of sea water.

Figure 1-8 Sea water intrusion into a coastal aquifer

1.6 About this book

Modeling the movement of contaminants through soil with a numerical solution can be very complex. Natural soil deposits are generally highly heterogeneous and non-isotropic. In addition, boundary conditions often change with time and cannot always be defined with certainty at the beginning of an analysis. In fact, the correct boundary condition can sometimes be part of the solution as is the case for an exit review boundary, where the direction of groundwater flow may change between source and sink.

The movement of contaminants can not be modeled without a valid model for groundwater flow in the system. That is why the MOST important aspect of this type of model is to first be confident in the seepage solution. This book is NOT about seepage modeling and it is assumed from this point onward, that the reader is familiar with and has read either the SEEP/W or VADOSE/W Engineering Methodology books. This book is not a stand-alone reference.

While part of this document is about using CTRAN/W to do transport analyses, it is also about general numerical modeling techniques. Numerical modeling, like most things in life, is a skill that needs to be acquired. It is nearly impossible to pick up a tool like CTRAN/W and immediately become an effective modeler. Effective numerical modeling requires some careful thought and planning and it requires a good understanding of the underlying physical fundamentals. Aspects such as discretization of a finite element mesh and applying boundary conditions to the problem are not entirely intuitive at first. Time and practice is required to become comfortable with these aspects of numerical modeling.

Chapter 2 of the SEEP/W and VADOSE/W books is devoted exclusively to discussions on the topic of How to Model. The general principles discussed in that book apply to all numerical modeling situations, even though the discussion there focuses on seepage analysis.

Broadly speaking, there are three main parts to a finite element analysis. The first is discretization – dividing the domain into small areas called elements. The second part is specifying and assigning material properties. The third is specifying and applying boundary conditions. Details of discretization are provided in the SEEP/W or VADOSE/W book, while material properties and boundary conditions as pertaining to transport analysis are discussed in detail in their respective chapters here.

Transport modeling is numerically challenging because of the presence of a first order transport term in the main differential equation. For this reason, it is important to have an understanding of how that term affects the solution of the equation and, in particular, how mesh size and time steps are critical to that solution. The importance of the Peclet and Courant numbers will be introduced and discussed, along with other numerical considerations in a chapter titled Numerical Issues.

Two chapters have been dedicated to presenting and discussing illustrative examples. One chapter deals with examples where geotechnical solutions are obtained by integrating more than one type of analysis, and the other chapter presents and describes how a series of different geotechnical problems can be solved.

A full chapter is dedicated to theoretical issues associated with transport and the solution the finite element equations. Additional finite element numerical details regarding interpolating functions and infinite elements are given in Appendix A of the SEEP/W and VADOSE/W books.

The chapter entitled “Modeling Tips and Tricks” should be consulted to see if there are simple techniques that can be used to improve your general modeling method or to help gain confidence and develop a deeper understanding of finite element methods, CTRAN/W conventions or data results.

In general, this book is not a HOW TO USE CTRAN/W manual. This is a book about how to model. It is a book about how to solve transport problems using a powerful calculator; CTRAN/W. Details of how to use various program commands and features are given in the on line help inside the software.