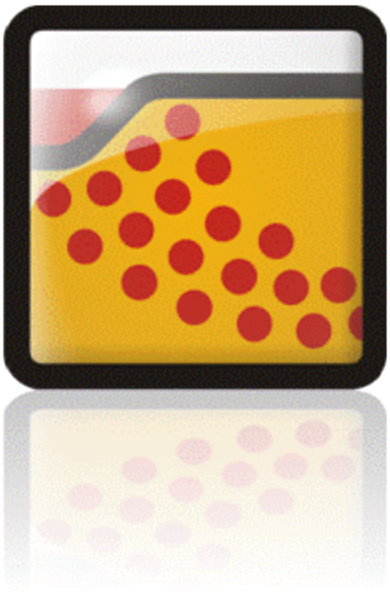

Contaminant Modeling with CTRAN/W

An Engineering Methodology

February 2012 Edition

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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.

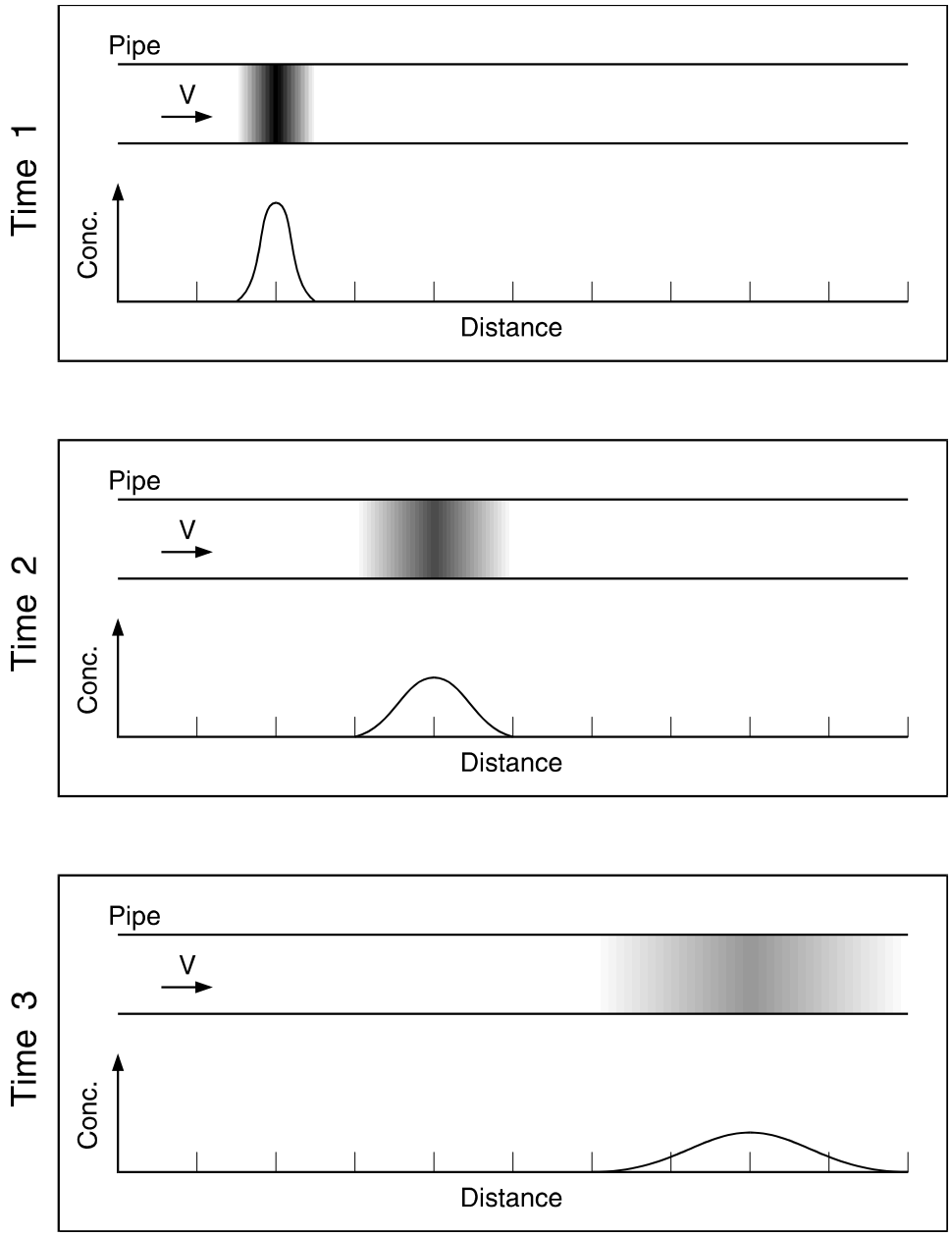


Figure 1-1 The Migration and spreading of a contaminant slug in a fluid flowing with velocity V

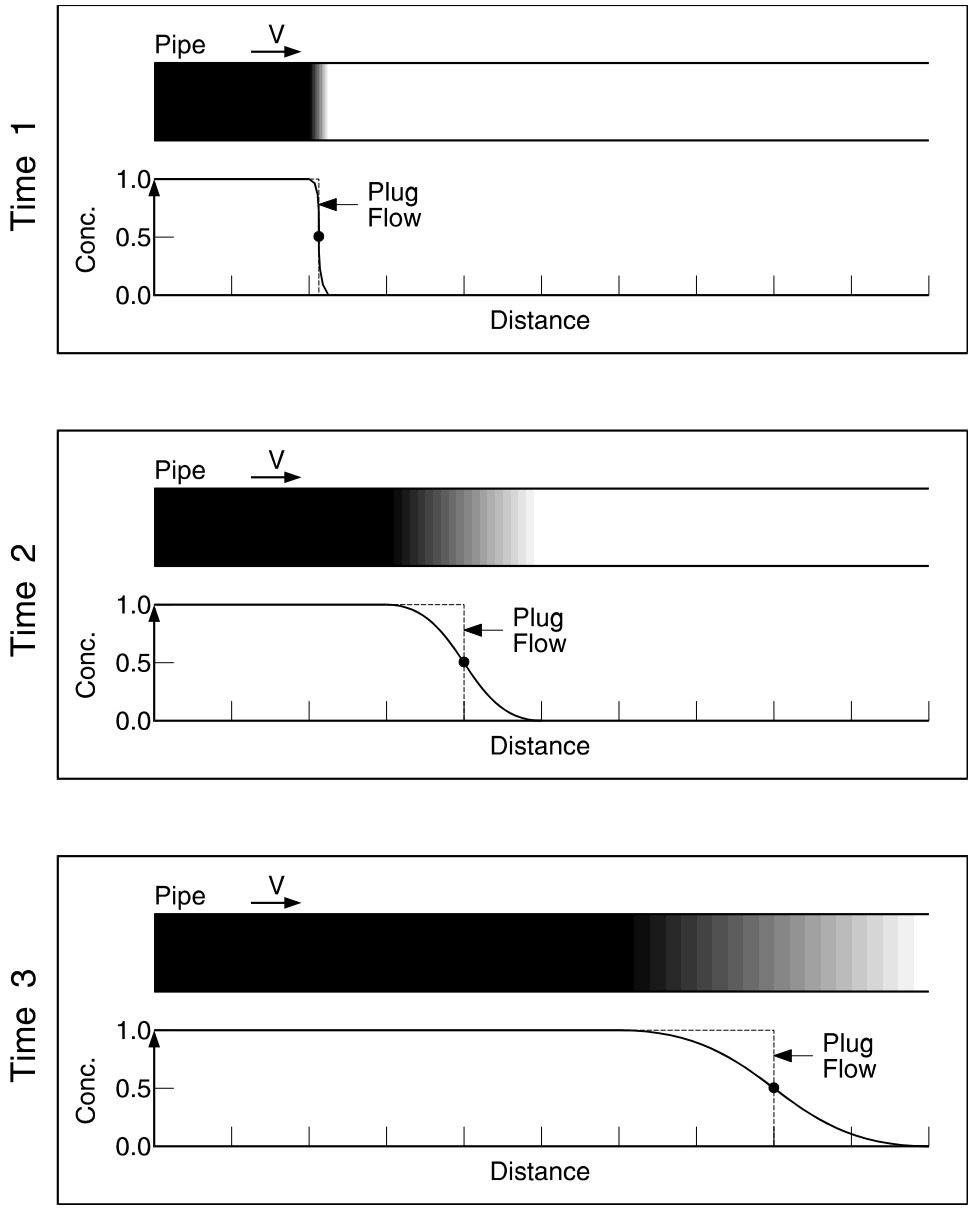


Figure 1-2 Contaminant migration and spreading from a continuous source in a fluid flowing with velocity V

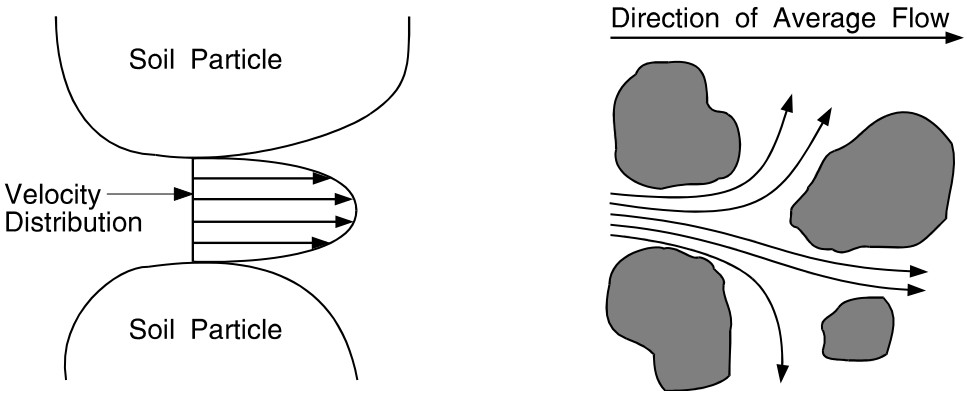


Figure 1-3 Factors causing mechanical dispersion

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.

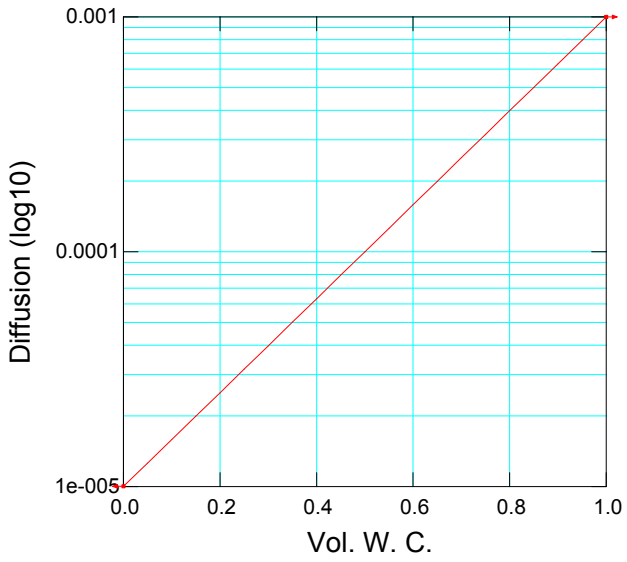


Figure 1-4 Example of molecular diffusion as a function of water content

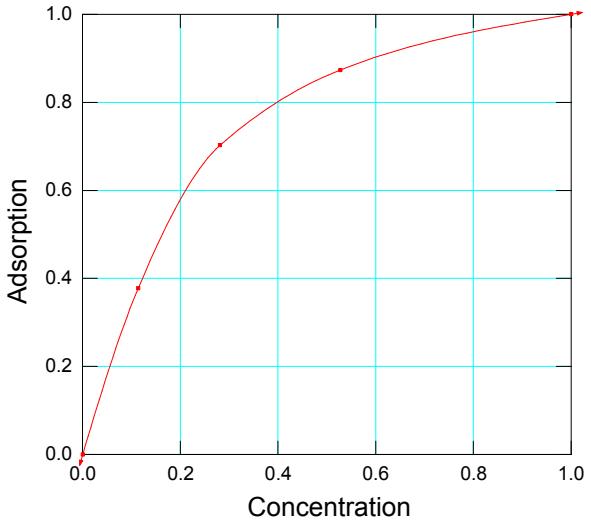


Figure 1-5 Example of adsorption as a function of concentration

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.

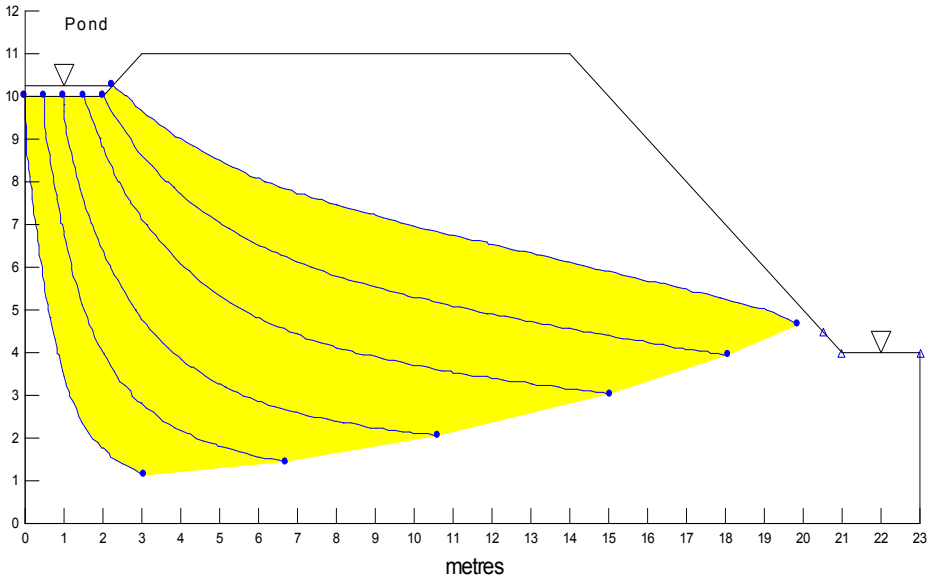


Figure 1-6 Example of a particle tracking analysis

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.

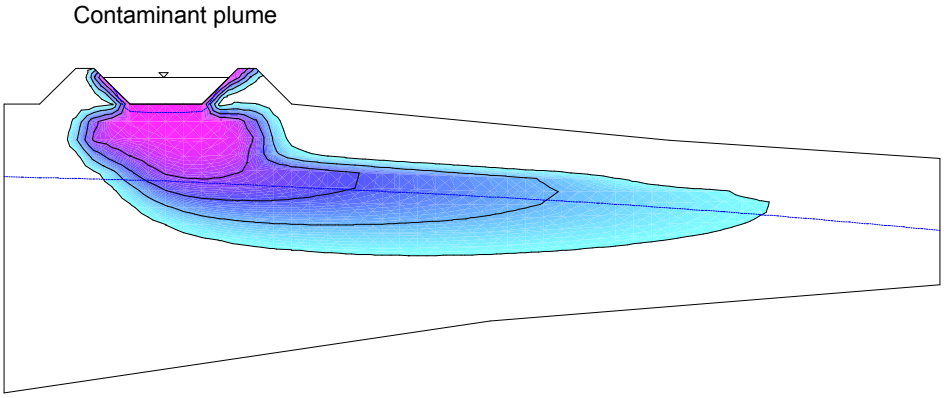


Figure 1-7 Contaminant transport from a surface pond

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.

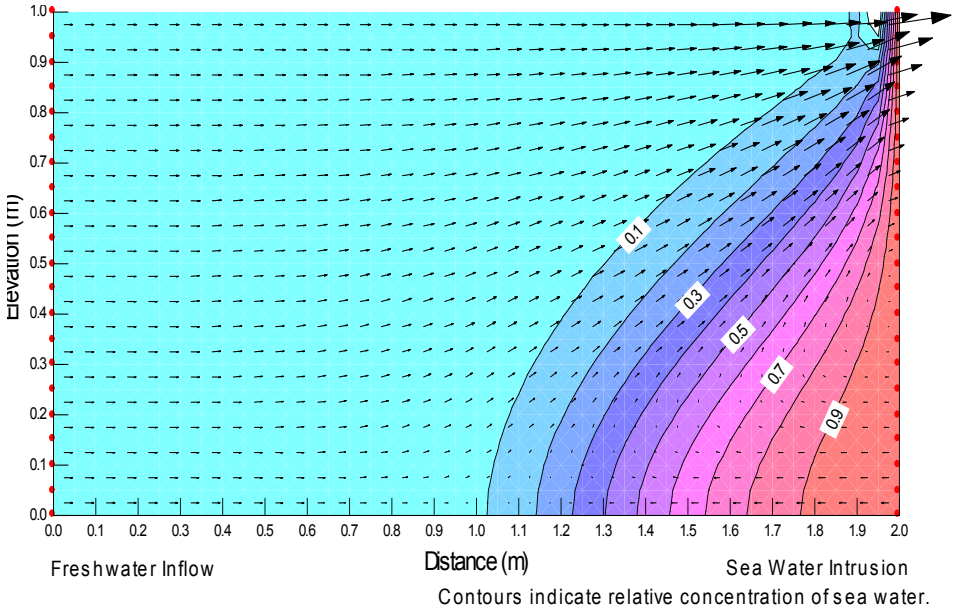


Figure 1-8 Sea water intrusion into a coastal aquifer

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.

2 Material Properties

This chapter describes the various soil transport properties that are required in the solution of the CTRAN/W partial differential equation. It is important to have a clear understanding of what the soil properties mean and what influence they have on the type of results generated. This chapter is not meant to be an all inclusive discussion of these issues. It is meant to highlight the importance of various parameters and the implications associated with not defining them adequately.

Well defined soil properties can be critical to obtaining an efficient solution of the finite element equations. When is it acceptable to guess at a function and when must you very carefully define one? This chapter will address these issues.

2.1 Dispersivity and diffusion

For one-dimensional flow, the hydrodynamic dispersion coefficient *D* is defined above as:

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

where:

α = dispersivity (material property),

v = D'Arcy velocity divided by volumetric water content (U/Θ), and

D^* = coefficient of molecular diffusion.

Dispersivity is the ratio of the hydrodynamic dispersion coefficient (d) divided by the pore water velocity (v); thus a = d/v and has units of length. Typically, the dispersivity varies from 0.1 to 100 m however field and laboratory tests have indicated that dispersivity varies with the scale of the test. Large scale tests have higher dispersivity than small lab column tests. An approximate value for dispersivity is 0.1 times the scale of the system (Fetter, 1993). If you are simulating contaminant transport in a 1 m long laboratory column, then dispersivity ~ 0.1 m. However, if you are simulating transport in a large aquifer greater than 1 km in extent, then use dispersivity ~ 100 m.

Dispersion in the direction of the water flow is usually higher than dispersion perpendicular to the flow direction. Two dispersivity values are therefore required to define the spreading process. Dispersivities in the flow directions are designated as the longitudinal dispersivity α_L and the transverse dispersivity α_T.

In CTRAN/W if no coefficient of molecular diffusion (D*) is defined, then the dispersion is equal to the diffusivity in the longitudinal and transverse directions respectively.

Diffusion function

In general, the coefficient of diffusion D^* is a function of the volumetric water content, as shown in Figure 2-1. An empirical relationship between D^* and Θ has been proposed by Kemper and Van Schaik (1966), however CTRAN/W allows you to define any desired values of the coefficient of diffusion function as a function of volumetric water content (i.e., the diffusion function).

The D^* parameter and its dependence on water content is of significance only in unsaturated flow and when the water flow rate is very low. The value of the hydrodynamic dispersion coefficient is often governed by the water flow rate. Therefore, it is often adequate to assume that D^* is independent of Θ, and to define the relationship by a constant horizontal function.

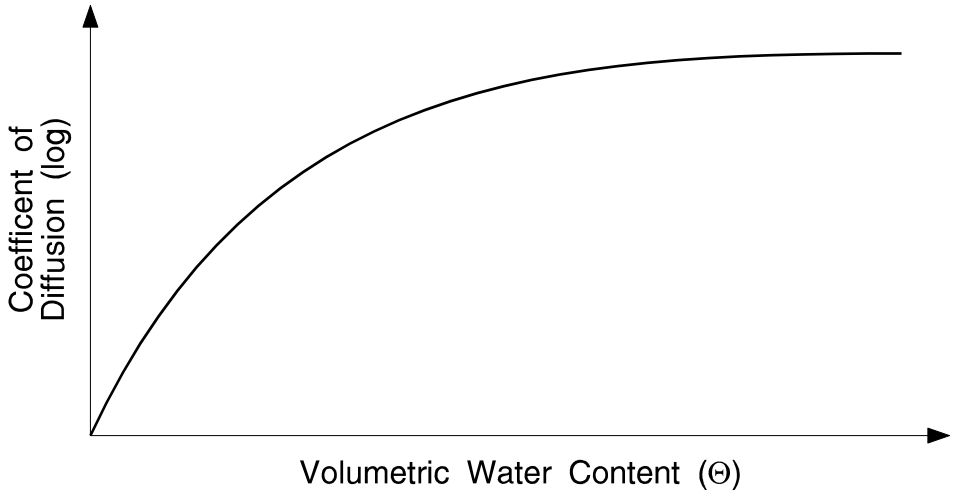


Figure 2-1 Illustration of a diffusion versus water content function

2.2 Adsorption function

For the transport of a reactive substance, the movement of the mass is also affected by the adsorption of the solute by the soil particles. As discussed above, the amount of mass adsorbed can be defined in terms of the mass density of the soil particles. From relationships developed in the Theory chapter, the adsorbed mass *M*s is:

$$M_s = S\rho_d$$

The rate of change of the adsorbed mass is:

$$\frac{\partial M_s}{\partial t} = \rho_d \frac{\partial S}{\partial t}$$

The adsorption *S* is a function of concentration *C* with experimental results usually plotted as *S* vs. *C*, as shown in Figure 2-2. The slope of the *S* vs. *C* relationship is $\partial S / \partial C$ and in the case of a linear relationship is usually referred to as the distribution coefficient K_d.

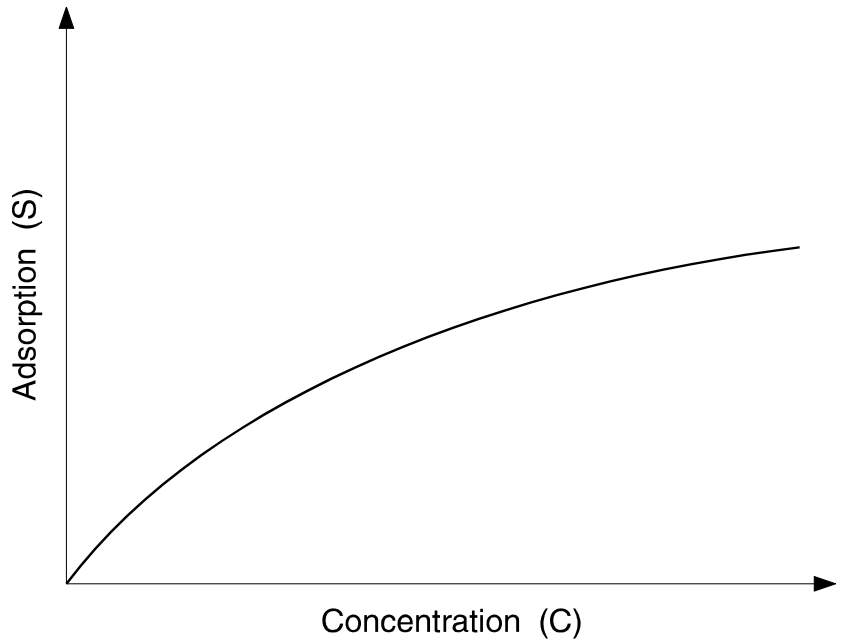


Figure 2-2 Relationship between adsorption and concentration

For many dissolved contaminant and soil combinations, adsorption of contaminant on the soil particles is linearly related to concentration (e.g. the K_d term). CTRAN/W, however, allows a more general relation to be used to specify the chemical partitioning by allowing the adsorption to be specified as a function of concentration. The actual slope used in the solution of the equations will be obtained from the function for any given concentration.

Dry density

The dry density term is the dry mass density of the porous medium. It is multiplied by the adsorption quantity in the governing equation. The units of dry density are (M/L^3) must be consistent with the units of mass and length.

2.3 Decay half life

For the transport of a radioactive substance, mass may be lost during the transport process due to radioactive decay of ions in the pore fluid and decay of ions attached to the soil particles. The reduced concentration resulting from radioactive decay, in terms of the initial concentration, is:

Equation 2-1 $C = C_0 e^{-\lambda t}$

where t is the elapsed time and λ is the decay coefficient. The decay coefficient λ can be related to the half-life T of a decaying material. By definition, the half-life T is the elapsed time when the concentration of $C/C0 = 1/2$. Therefore:

$$\frac{C}{C_0} = \frac{1}{2} = e^{-\lambda T}$$

which can also be written as:

$$\lambda = \frac{\ln 2}{T} = \frac{0.693}{T}$$

Differentiating Equation 2-1 with respect to time leads to:

$$\frac{\partial C}{\partial t} = -\lambda C$$

The amount of radioactive mass in the pore-water *M*w in an elemental unit volume is ΘC, (see above), or:

$$M_w = \Theta C = \Theta C_0 e^{-\lambda t}$$

The decay half-life must be specified in units of time that are consistent with the units of diffusion. For example, if the diffusion coefficient is in meters per second (m/sec), then the half-life must be specified in seconds.

3 Boundary Conditions

3.1 Introduction

Specifying conditions on the boundaries of a problem is one of the key components of a numerical analysis. This is why these types of problems are often referred to as "boundary-valued" problems. Being able to control the conditions on the boundaries is also what makes numerical analyses so powerful.

Solutions to numerical problems are a direct response to the boundary conditions. Without boundary conditions it is not possible to obtain a solution. The boundary conditions are the driving force. What causes contaminant to transport? It is the concentration difference between two points or some specified rate of contaminant flux into or out of the system. The solution is the response inside the problem domain to the specified conditions on the boundary.

Sometimes specifying conditions is fairly straightforward, such as defining the concentration or contaminant flux conditions that exist on a year-round basis at the leakage point beneath a waste collection pond. Many times, however, specifying boundary conditions is complex and requires some careful thought and planning. Sometimes the correct boundary conditions may even have to be determined through an iterative process, since the boundary conditions themselves are part of the solution, as for instance, the contaminant flux from a seepage face where the seepage face is not active continually.

Due to the extreme importance of boundary conditions it is essential to have a thorough understanding of this aspect of numerical modeling in order to obtain meaningful results. Most importantly, it is essential to have a clear understanding of the physical significance of the various boundary condition types. Without a good understanding, it can sometimes be difficult to interpret the analysis results. To assist you with this aspect of an analysis, CTRAN/W has tools which make it possible verify that the results match the specified conditions. In other words, do the results reflect the specified or anticipated conditions on the boundary? Verifying that this is the case is fundamental to confidence in the solution.

This chapter is completely devoted to discussions on boundary conditions. Included are explanations on some fundamentals, comments on techniques for applying boundary conditions and illustrations of boundary condition types applicable for various conditions.

3.2 Fundamentals

All finite element equations just prior to solving for the unknowns untimely boil down to:

$$[K]\{X\} = \{A\}$$

where:

[K] = a matrix of coefficients related to geometry and materials properties,

{X} = a vector of unknowns which are often called the field variables, and

{A} = a vector of actions at the nodes.

For a transport analysis the equation is,

Equation 3-1 $$[K]\{C\} = \{Q\}$$

where:

$\{C\}$ = a vector of the concentration at the nodes, and

$\{Q\}$ = a vector of the contaminant flux quantities at the node.

The prime objective is to solve for the primary unknowns, which in a transport analysis are the concentrations at each node. The unknowns will be computed relative to the C values specified at some nodes and/or the specified Q values at some other nodes. Without specifying either C or Q at some nodes, a solution cannot be obtained for the finite element equation. In a steady-state analysis, at least one node in the entire mesh must have a specified C condition. The specified C or Q values are the boundary conditions.

A very important point to note here is that boundary conditions can only be one of two options. We can only specify either the C or the Q at a node. It is very useful to keep this in mind when specifying boundary condition. You should always ask yourself the question: "What do I know? Is it the C or the contaminant flux, Q?" Realizing that it can be only one or the other and how these two variables fit into the basic finite element equation is a useful concept to keep in mind when you specify boundary conditions.

As we will see later in this chapter, flux across a boundary can also be specified as a gradient or a rate per unit area. Such specified transport boundary conditions are actually converted into nodal Q values. So, even when we specify a gradient, the ultimate boundary condition options still are either C or Q.

Remember! When specifying transport boundary conditions, you only have one of two fundamental options – you can specify C or Q. These are the only options available but they can be applied in various ways.

Another very important concept you need to fully understand is that when you specify C, the solution to the finite element Equation 3-1 will provide Q. Alternatively, when you specify Q, the solution will provide C. The equation always needs to be in balance. So when a C is specified at a node, the computed Q is the Q that is required to maintain the specified C. When Q is specified, the computed C is the C that is required to maintain the specified flux Q.

Recognizing the relationship between a specified nodal value and the corresponding computed value is useful when interpreting results. Assume you know the specified flux across a surface boundary. Later when you check the corresponding computed concentration at that node you may find that it is unreasonably high or low. You would use your knowledge of the problem to assess if the contaminant flux applied was reasonable. The C values are computed based on Q and the soil properties, so it must be one of three things. Knowing what to look for helps you to judge whether that is reasonable or not.

CTRAN/W always provides the corresponding alternative when conditions are specified at a node. When C is specified, Q is provided, and when Q is specified, C is provided. The computed Q values at nodes where a concentration is specified are referred to as Boundary Flux values with units of mass of contaminant per time (e.g. M/t). These Boundary Flux values are listed with all the other information provided at nodes.

A third important fundamental behavior that you need to fully understand is that when neither C nor Q is specified at a node, the computed Q is zero. Physically, what it means is that the contaminant flux coming towards a node is the same as the flux leaving the node. Another way to look at this is that no contaminant is entering or leaving the system at these nodes. Contaminant leaves or enters the system only at nodes where C or a non-zero Q has been specified. At all nodes for no specified condition, Q is always zero.

This, as we will see later in this chapter, has important implications when simulating features such as point sources of contaminants at a single node.

The concentrations in a transport analysis are the primary unknowns or field variables. A boundary condition that specifies the field variable (C) at a node is sometimes referred to as a Type One or a Dirichlet boundary condition. Transport gradient (flux) boundary conditions are often referred to as Type Two or Neumann boundary conditions. You will encounter these alternate names in the literature but they are not used here. This document on transport modeling simply refers to boundary conditions as concentration (C) or contaminant flux (Q) boundary conditions. Later we will differentiate between nodal flux Q and specified gradients (rates of flux per unit area) across an element edge.

3.3 Boundary condition locations

In GeoStudio, all boundary conditions must be applied directly on geometry items such as region faces, region lines, free lines or free points. There is no way to apply a BC directly on an element edge or node. The advantage of connecting the BC with the geometry is that it becomes independent of the mesh and the mesh can be changed if necessary without losing the boundary condition specification. If you keep the concept of BC's on geometry in mind, you will find that you can specify any location for a BC quite easily. Consider the following examples which show the desired location of boundary conditions, the boundary condition applied to the geometry, and finally the underlying mesh with boundary conditions visible.

If you look carefully at Figure 3-2 and Figure 3-3 you will see that the BC symbols along the slope edge are spaced differently. In the view with no mesh visible, the BC's are displayed at a spacing that depends on the scale and zoom factor of the page. In the image with the mesh visible, the BC's are drawn exactly where they will appear. They are always at a node for this type of BC. Notice also that the free point location forces a mesh node to be at the exact location. This way, you can always define a BC anywhere you want and when the mesh changes, the BC location will remain fixed.

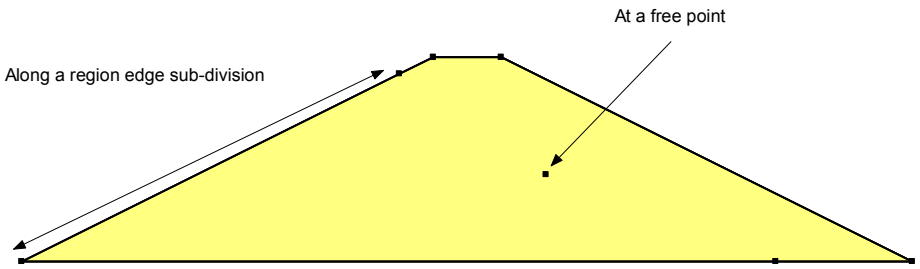


Figure 3-1 Desired BC locations

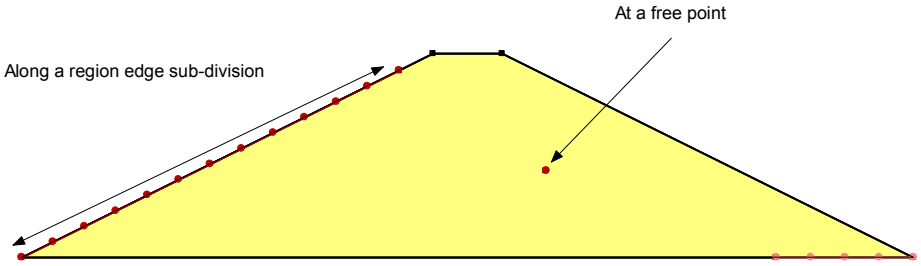


Figure 3-2 BC's attached to geometry

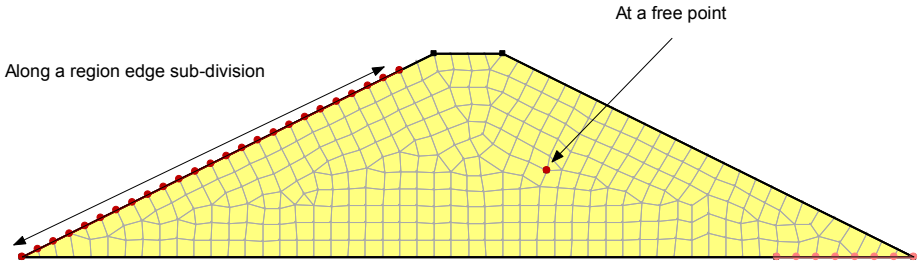


Figure 3-3 BC's with underlying mesh visible

Region face boundary conditions

A flux or stress boundary condition, which is given in units per area, can be applied to the "face" of a region. GeoStudio uses the contributing area that surrounds each node to calculate the corresponding flow rate or force. For example, a stress boundary condition applied to a region face is multiplied by the area that surrounds a node and converted into a force at the nodes. Similarly, a heat flux rate of 1 kJ/m2/day would be converted into a flow rate (kJ/day) after integration.

3.4 Sources and sinks

There is another type of boundary condition called a source or a sink. These boundary conditions are sometimes referred to as a Type 3 boundary condition. A typical sink might represent a drain at some point inside a mesh where contaminant is added or removed. The important concept about sinks and sources is that they represent mass flux into or out of the system.

In CTRAN/W flux boundary conditions can be applied along outside edges or nodes of the mesh, or along inside edges or nodes. There is no difference in how the equations are solved in either case. The only thing to watch for is that you have an understanding of the area that the contaminant transports across.

There are a couple special types of boundary conditions that have been formulated directly in CTRAN/W: the surface mass accumulation condition and the exit review condition. These are discussed in more detail below.

3.5 Advection and dispersion considerations

When you specify the boundary conditions in a contaminant transport analysis, it is important to recognize that there are two processes by which mass is carried across a boundary: one is by advection and the other is by dispersion. The advective component is due to the water movement across a boundary while the dispersive process is due to the chemical (concentration) gradients between the boundary nodes and the nodes immediately inside the boundary.

The advective component of the boundary mass flux is related to the water flux (*Q*w) across the boundary. This information is obtained from a SEEP/W analysis. CTRAN/W uses the nodal *Q*w values from the SEEP/W file to compute the advective boundary flux.

When specifying boundary conditions for a transport analysis, you will often find it useful to first get a clear picture of the water flux across the boundaries. A clear understanding of the boundary water flux is essential in the specification of boundary conditions and the interpretation of computed results.

3.6 Source concentration

Consider the case illustrated in Figure 3-4 where the leakage from the lagoon is the source of the contamination. If the concentration of the contaminated fluid in the lagoon is known, you can specify the boundary condition type as *C*s (the concentration of the source).

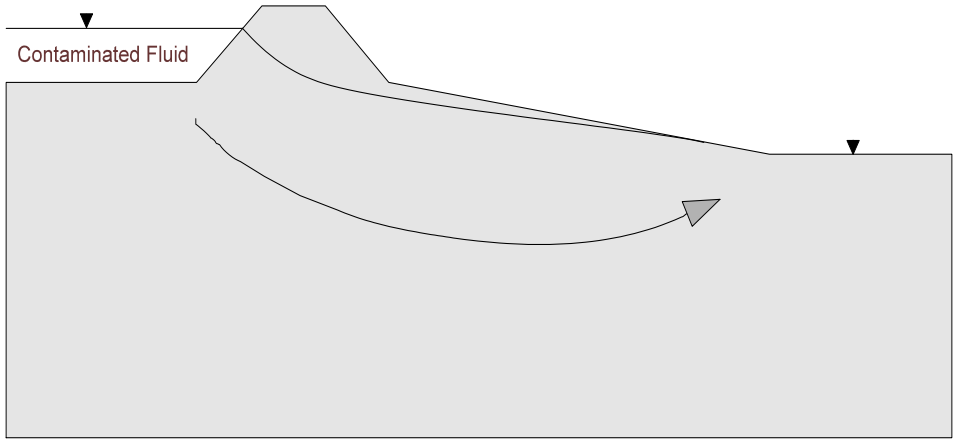


Figure 3-4 Illustration of a lagoon with contaminated fluid

When you specify *C*s as the boundary condition type, CTRAN/W uses the concentration of the source to compute a nodal mass flux at the boundary. The mass flux is computed as:

$$Q_{mass} = Q_w * C_s$$

where:

Qmass = nodal total mass flux,

Qw = nodal water flux from SEEP/W, and

Cs = user-specified concentration of the source.

Specifying a *C*s boundary at the nodes is different than specifying a *C* boundary with a value equal to *C*s. By specifying *C*s at a boundary, you are actually defining a mass flux type boundary. When specifying *C*, you are defining a specified concentration type boundary.

When you specify *C*s at a node, the computed nodal concentration will be less than *C*s during the early stage of the transport process. After some time, the computed concentration will become equal to *C*s. However, if you specify a *C* boundary with a value equal to *C*s, the computed nodal concentration will be equal to *C*s immediately.

In general, using *C*s as a boundary condition is a more realistic option than simply specifying concentration at the nodes. In addition, it has the advantage of not creating excessive initial concentration gradients, as is the case with specified concentration boundaries. The gradual build-up of concentration at *C*s nodes tends to reduce numerical difficulties that may arise from excessively high concentration gradients.

NOTE: Specifying a *Cs* boundary in a node with zero nodal flux is the same as specifying the node as a zero mass flux boundary (i.e., *Q*m = 0.0 or *q*m = 0.0).

3.7 Surface mass accumulation

Slow, contaminated moisture flow to the ground surface (or evaporative water flux) can result in an accumulation of the solute on the surface boundary. In such cases, the water evaporates, but the solute remains and accumulates with time, as illustrated in Figure 3-5.

The solute accumulation at the ground surface can be simulated with CTRAN/W by specifying a zero mass flux at the surface (i.e., *Q*m = 0.0 or *q*m = 0.0). A zero mass flux means that no mass gain or loss is allowed across the boundary. In other words, contaminant mass carried by the water flow to the boundary is not allowed to leave; consequently, the mass accumulates at the boundary.

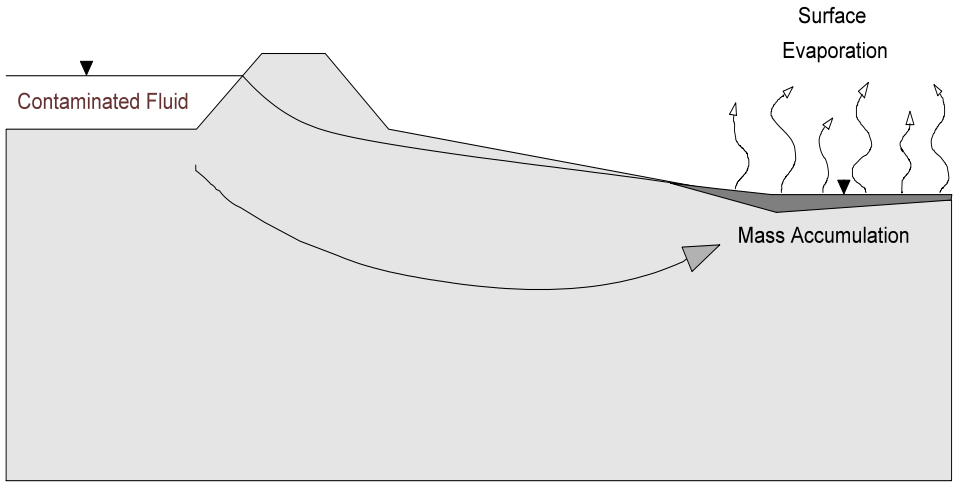


Figure 3-5 Illustration of mass accumulation on evaporative ground surface

In technical terms, the advective flux carries the contaminant solute to the boundary. Physically, the water flux will cause advective mass loss across the boundary; however, because of the specified zero mass flux boundary condition, the boundary develops a reverse dispersive mass flux equal in magnitude but opposite in direction to the advective mass loss. The reverse dispersive mass flux causes the increase in concentration.

For the mass to accumulate at the boundary there must be water flux loss across the boundary. There will be no solute accumulation if there is no water flow across the boundary (i.e., *q*w = 0.0).

The default boundary condition in CTRAN/W is a no-mass flux condition, (i.e., *Q*m = 0.0 or *q*m = 0.0). Specifying a boundary type as *none* is the same as specifying *Q*m or *q*m equal to zero.

3.8 Exit review

At a boundary where neither the mass flux nor the concentration are known, or where the nodal water flux may reverse in direction during the transport process, you may specify the boundary as an Exit Review boundary. When a boundary node is specified with Exit Review, the node is checked to see if an exit boundary should be applied at each time step. If the water flux of the node is negative (i.e., water flux is exiting at the boundary), the boundary condition of the node will be changed to an exit boundary. If the water flux of the node is zero or positive, the boundary condition of the node is not changed.

CTRAN/W offers two types of exit boundaries. The first and simplest option is one that ignores the dispersive flux across the exit boundary (Qd = 0), and is often referred to as a zero dispersive mass flux exit boundary. With this type of exit boundary, contaminant mass is assumed to leave the exit boundary by advection only. As a result, the concentration gradients at the boundary are forced to be zero, which causes the concentration contours to be perpendicular to the exit boundary. The second type of exit boundary condition accounts for both advective and dispersive mass flux at the boundary (Qd > 0), and is referred to as a free exit boundary. A free exit boundary accounts for both advective and dispersive mass flux across the boundary, which generally gives more realistic results. It is best to use the free exit boundary unless there is a specific reason for using the zero dispersive mass flux exit boundary.

The “Example” problem in the Illustrative Examples chapter illustrates a typical situation where an exit boundary is required. Contaminant mass is existing at the downstream toe of dam. Since neither the mass flux nor the concentration are known at the boundary, the boundary is specified as Qm =0 conditions with review for free exit boundary (Qd > 0).

The Exit Review feature is particularly useful in a density-dependent flow problem. Using Henry’s sea water intrusion problem presented in the Illustrative Examples chapter, sea water may enter the flow system along the bottom portion of the sea water boundary and freshwater may exit along the upper portion. Since the interface between the sea water and the freshwater is not known, it is best to specify the entire vertical boundary as *Cs* = 1 and review for free exit boundary.

Figure 3-6 is the solution to Henry’s sea water intrusion problem when the right boundary is simulated as a *C* boundary condition with no exit review. Figure 3-7 is the solution to the same problem except that the right boundary is specified as a *Cs* boundary type condition with exit review Qd > 0. In the latter case, the nodes along the upper portion of right boundary were converted to an exit boundary by the exit review feature.

Allowing the sea water boundary to be reviewed for free exit boundary conditions provides a more physically realistic solution than when the concentration is specified along the sea water boundary. The difference between the two solutions is primarily in the concentration distribution along the upper portion of the sea water boundary. Without exit review, the concentration of the nodes along the upper portion of the right boundary are equal to your specified value at all times; whereas with exit review, the nodes may be converted to free exit boundary, and the concentration is solved for at each time step.

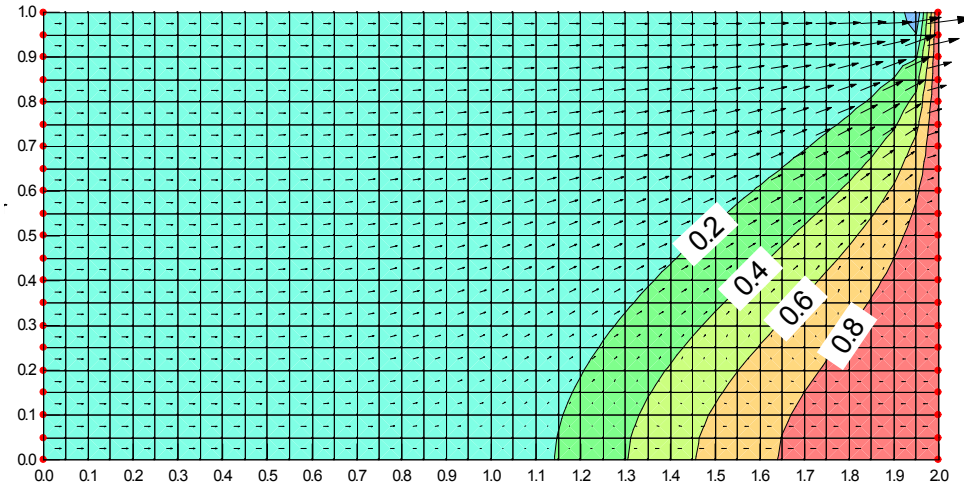


Figure 3-6 contour of Henry's problem, no exit review

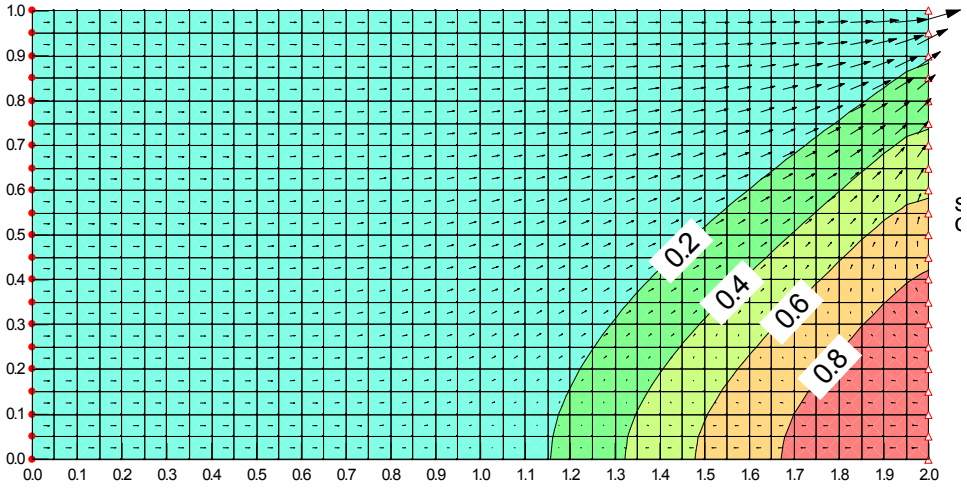


Figure 3-7 Concentration contour of Henry's problem with exit review

Note that Exit Review specification is only allowed for mass flux type boundary conditions, (i.e. *Q*m, *q*m and *Cs*), where the nodal concentration are computed.

Exit boundaries should only be applied to regions with four-noded quadrilateral elements and must be specified along only the edge defined by elements with two nodes. When each element matrix equation is calculated in SOLVE, a surface integral term is formed for element edges that are exit boundaries. This surface integral *cannot* be formed for higher order elements; and therefore, application of exit boundaries to higher ordered elements is invalid.

The exit surface integral can be formed for three-noded triangular elements if two of the three nodes are on an exit boundary. However, using an exit boundary on a triangular element often is of limited value, since any adjacent triangular elements usually have only one node on the exit boundary. In this case, the surface integral is formed only for every second triangular element.

In summary, the best exit boundary results are obtained with four-noded quadrilateral elements. Three-noded triangular elements can be used but do not give the best results and higher-order elements cannot be used along an exit boundary.

3.9 Concentration vs. mass function

A special type of boundary function can be used to simulate, for example, the case where a contaminant flows into a body of fresh water. Figure 3-8 illustrates this example. Initially, the boundary condition of the fresh water pond can be specified as a zero concentration boundary, (i.e. C=0). As the contaminant flows into the pond, the concentration of the water increases with time.

The concentration boundary condition of the pond therefore has to be modified with time. The concentration of the pond can be computed at any time if you know the accumulated mass discharged into the pond and the volume of the pond. In equation form, the pond concentration is:

$$C_{pond} = \frac{accumulated\ mass}{pond\ volume}$$

This relationship can be used to develop a *C vs. mass* function, (Figure 3-9), which can be specified as a boundary condition.

When using this boundary type, CTRAN/W computes the accumulated mass that flows into the pond at the end of each time step. This value, together with the boundary function, is then used to compute the boundary concentration at the start of a new time step.

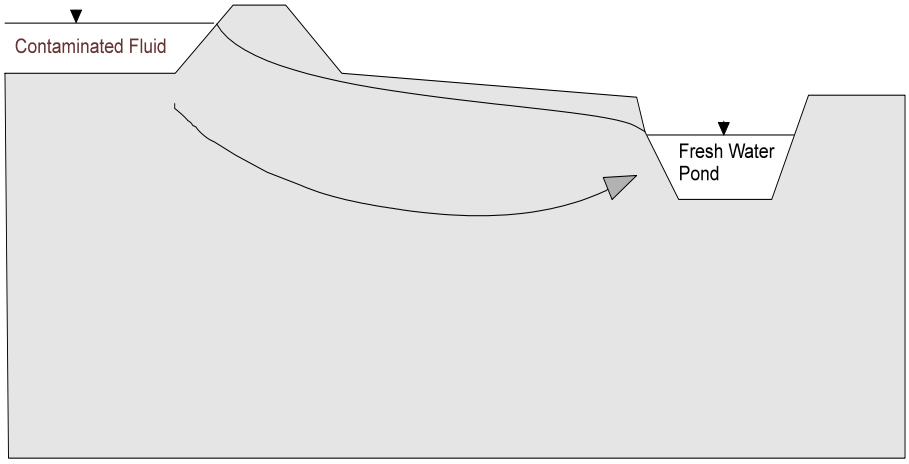


Figure 3-8 Illustration of contaminant discharge into a fresh water pond

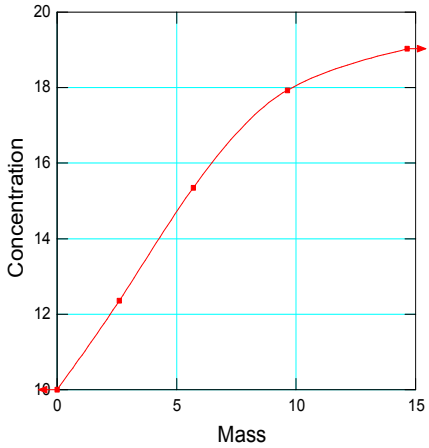


Figure 3-9 Illustration of a concentration versus mass boundary function

3.10 Boundary functions

CTRAN/W is formulated to accommodate a very wide range of boundary conditions. In a steady state analysis, all of the boundary conditions are either fixed concentrations or fixed flux values. In a transient analysis however, the boundary conditions can also be functions of time or in response to transport amounts exiting or entering the transport regime. CTRAN/W accommodates a series of different boundary functions. Each one is discussed in this section.

3.11 Time activated boundary conditions

There are situations where the actual position of a boundary condition may change with time. A typical case may be the placement of mining tailings. The thickness of the tailings grows with time and yet there is always some water on the surface. The position of the head equal elevation (zero pressure) changes with time. Another case may be in the simulation of constructing an embankment in lifts. The hydraulic boundary condition changes with time. This type of boundary condition is only useful when elements are activated or deactivated with time for the purpose of simulating fill placement or constructing an excavation.

Time activated boundary conditions are currently under development for a future version of GeoStudio.

3.12 Null elements

There are many situations where only a portion of the mesh is required. Parts of the mesh that are not required in a CTRAN/W analysis can be flagged as null elements. Consider a case where you want to use a similar mesh in different GeoStudio analyses. In the case of a cutoff wall to prevent water flow, you could set those elements as NULL in the seepage analysis. This would treat the elements as if they were not a part of the mesh and water would not flow around them. However, if you now wanted to model the contaminant transport in this scenario, you would turn the elements back on in CTRAN/W and assign them valid properties.

Elements present but not required in a particular analysis can be assigned a material type (number) that does not have an assigned conductivity function. Elements with this uncharacterized material are treated as null elements. As far as the main solver is concerned, these elements do not exist.

4 Analysis Types

There are two fundamental types of finite element contaminant transport analysis: advection / dispersion, or density-dependent. A further option for simple particle tracking is also available. In terms of the seepage solution used with CTRAN/W, it can be steady state or transient. Full details of steady state and transient seepage analysis are provided in the SEEP/W or VADOSE/W engineering books. A description of each type of contaminant analysis and the implications associated with each type are discussed in this chapter.

4.1 Seepage solution interpolation

The accuracy of the contaminant transport solution is directly dependent on the accuracy of the seepage solution. In other words, you must be able to obtain a reasonable seepage solution of a flow system first before conducting the transport analysis.

CTRAN/W relies on a seepage solution generated by either SEEP/W or VADOSE/W to perform the contaminant transport analysis. For a steady-state seepage analysis, the seepage solution is assumed to be constant during the transport process. For a density-dependent analysis, the time steps specified in the CTRAN/W data file are used to compute the seepage solution in SEEP/W (VADOSE/W does not support density-dependent analysis). For transient seepage analysis, CTRAN/W interprets the seepage solution as a step function. For example, if seepage solutions are only available for three elapsed time steps at 100, 200 and 400 minutes, in a transport analysis, the seepage solution is assumed to be constant between 0 to 100 minutes, 100 to 200 minutes and 400 minutes or more.

In situations where the boundary condition is not constant and a more precise seepage solution is required, you may be required to do one of the following:

- Use smaller time step increments, especially in a period in which changes in boundary condition are anticipated. The approximation error resulting from the step function decreases as the time step increments become smaller.
- Use the same time step increments in both the seepage model and CTRAN/W, so that the exact seepage solution at a certain time is computed rather than interpolated.

4.2 Initial conditions

The initial concentration of all nodes must be defined in a transport analysis regardless of whether it is an advection-dispersion or density-dependent problem. CTRAN/W allows you to specify the initial conditions by either reading the data from an initial conditions file, or by specifying the initial concentration as a material property. By default, when initial conditions are not specified, CTRAN/W assumes the initial concentration of all nodes to be zero. A zero initial concentration condition represents a clean flow system at the beginning of a transport process.

NOTE: The initial concentration of a node is independent of the boundary condition of the node. In other words, a particular node may have an initial concentration of 100 units specified, with a C boundary condition of 0 units also specified.

Using an initial conditions file

With this option, you specify an initial conditions file by choosing the file name in the analysis settings command dialogue. You can choose a parent file within the same project or an external file.

Activation concentrations

If you have new soil region becoming active and you know it has a certain initial concentration, you can use the material property activation concentration value to initialize the concentrations in that region. This value is only applied the first time a new region is active in the analysis. This approach can be used to set initial concentrations at the start of any analysis, not just a construction sequence analysis.

Spatial function for the initial conditions

A third option is to specify directly what you think the starting concentrations conditions will be by applying a spatial function. You can define a spatial function for concentrations and have the solver point to this function result. An example of a spatial function is shown below. Most of the functions data points indicate a concentration of zero with a small contaminated zone at the base of the slope.

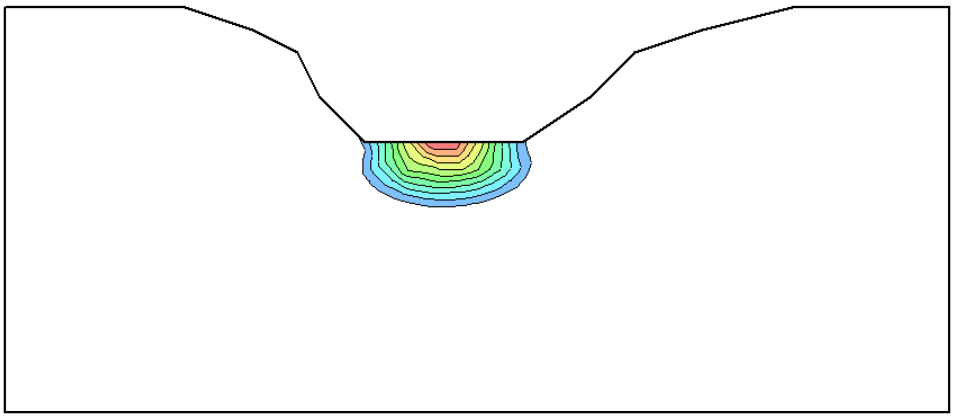


Figure 4-1 Spatial function for initial concentrations

4.3 Particle tracking analysis

In the initial stages of performing a contaminant transport analysis, it is sometimes useful to isolate the advective component of contaminant transport to get an idea of the contaminant travel distances and travel times. CTRAN/W includes a particle tracking analysis capability for just this purpose.

The particle tracking feature analyzes purely advective transport problems. A number of particles can be arbitrarily introduced to the flow system at any position. Particles are assumed to be attached to the water and move in the direction of the water flow with the same speed as the water flow.

You may track the movement of the particles forward in the direction of water flow, or backward in the opposite direction, toward the entrance or source boundaries. You may select the forward or backward tracking option using the KeyIn Analysis Control command when defining the problem.

With the forward tracking option, particles are usually introduced at the source boundaries. CTRAN/W computes the new positions of the particles according to the average linear velocity of the groundwater. Forward tracking is useful for determining where a particle of contaminant may end up and approximately how long a particle may take to arrive at a new position. It is also useful for delineating the possible flow paths or contaminant plume from the source boundaries. Figure 4-2 illustrates the migration of particles from the lagoon to the right exit boundary using forward tracking. A total of seven particles are used in this example.

With the backward tracking option, particles are usually introduced at the sink or exit boundaries and are tracked backward to the source boundaries. For example, Figure 4-3 illustrates particles that arrived at the right exit boundary not only come from the lagoon but can also come from the upstream boundary. Therefore, the backward tracking option is particularly useful in delineating the possible sources of contamination to the sink or exit boundaries in transport problems with multiple source boundaries.

NOTE: Backward tracking function is only valid in a steady-state seepage solution.

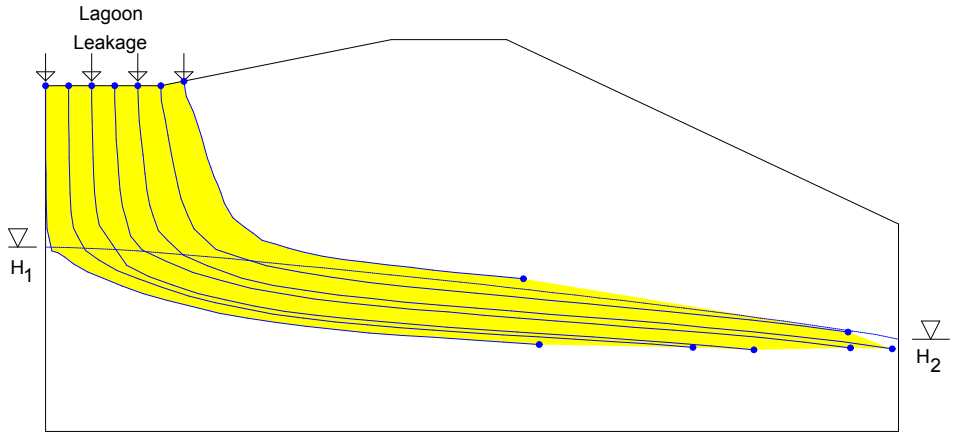


Figure 4-2 Illustration of particle flow path and plume using forward tracking

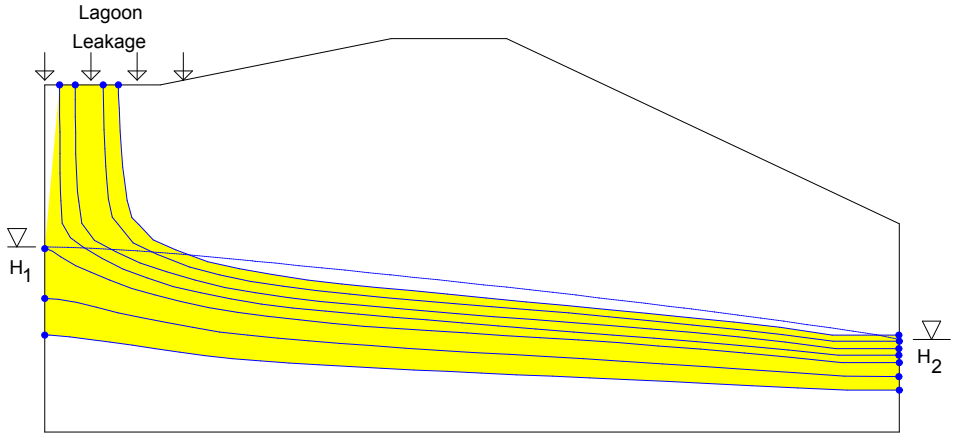


Figure 4-3 Illustration of particle flow path and plume using backward tracking

NOTE: Particle tracking simulates the transport of contaminant by the advection process, (water movement), only. Other transport processes such as dispersion, adsorption and decay are not considered. You may use the View Particle information command in CTRAN/W CONTOUR to look at the computed results of any particle at any location. The elapsed time of a particle at any location can be interpreted as time required to move a dissolved contaminant molecule from the starting position when dispersion, adsorption and decay are neglected.

4.4 Advection-dispersion analysis

Advection refers to the process by which solutes are transported by the bulk motion of flowing groundwater. Dispersion refers to the phenomenon of contaminant spreading from the path that it would be expected to follow according to the advective hydraulics of the flow system. Virtually all contaminant transport analyses require computation of advection and dispersion.

Adsorption refers to contaminant adsorption onto the solids of the porous medium. Decay refers to removal of the contaminant by some form of decay reaction, such as radioactive decay. Reactive, (adsorbing), or decaying contaminants may have a significant effect on the contaminant concentration in groundwater.

4.5 Density-dependent analysis (with SEEP/W only)

For problems where the density of the contaminant is significantly different than water, CTRAN/W has the capability of performing density-dependent transport analyses. This feature is useful for solving problems such as sea water intrusion, brine transport and landfill leachate migration, among others. Contaminant density is modeled as varying linearly with concentration. Contaminant density can be lower, higher or equal to the density of the native groundwater.

In density-dependent transport analyses, the flow velocities are dependent on the contaminant concentration distribution and the concentrations are dependent on the flow velocities. This circular dependence, or non-linearity, requires that the seepage flow velocities and the contaminant concentrations be solved for simultaneously by iterating at each time step. This type of non-linearity does not exist for advection-dispersion transport analyses, where the flow velocities are independent of the contaminant concentration distribution. For advection-dispersion analyses, the seepage velocities may be computed for all time steps before calculating the contaminant transport.

To allow for the seepage velocities to be calculated at each time step during a density-dependent analysis, CTRAN/W SOLVE starts and controls an instance of SEEP/W SOLVE to perform the velocity calculations at each time step. Therefore to perform a density-dependent transport analysis using CTRAN/W, you must select the analysis type as Density-Dependent in both SEEP/W and CTRAN/W.

In SEEP/W DEFINE you must specify the relative density of the contaminant at a specified reference concentration. The relative density refers to the density of contaminated water at the specified reference contaminant concentration. The density of the contaminated water is assumed to vary linearly with increasing contaminant concentration.

A relative density larger than 1.0 means the contaminant has a higher density than water. Similarly, a relative density smaller than 1.0 means the contaminant has a lower density than water. By default, the relative density of the contaminant is 1.0, meaning that there is no density contrast between freshwater and contaminated water as a function of concentration. Doing a density-dependent analysis with relative density equal to 1.0 is essentially the same as doing an advection-dispersion transport analysis, except that the seepage velocities will be re-calculated within each iteration.

The time step increments specified in CTRAN/W DEFINE are used in the analysis for both SEEP/W and CTRAN/W. Time step information defined in SEEP/W DEFINE is ignored in a density-dependent analysis. Similarly, the maximum number of iterations allowed within a time step is specified in CTRAN/W DEFINE. The maximum number of iterations specified in SEEP/W is not used in density-dependent analyses.

It is important to recognize that the interpretation of head potentials in the seepage solution of a density-dependent transport problem is somewhat different than the usual interpretation in an advection-

dispersion (density-independent), transport problem. For density-dependent analyses, the total head at a node is interpreted as the equivalent freshwater head. As the name implies, equivalent freshwater head is an equivalent total head potential of freshwater. The density contrast between contaminated water and freshwater adds a "body force" term on the finite elements in the mesh. Therefore if density of the contaminated water relative to freshwater increases with concentration (relative density greater than 1.0 at some concentration), then the equivalent freshwater head will increase with contaminant concentration. Similarly, if the density of the contaminated water relative to freshwater decreases with concentration, (relative density less than 1.0 at some concentration), then the equivalent freshwater head will decrease with contaminant concentration.

A good example to illustrate the equivalent freshwater head is the static saltwater column example in the chapter on Illustrative Examples. Although there is an upward gradient in the equivalent freshwater head within the column, the upward gradient is balanced exactly by the downward gradient caused by the body force. As a result, there is no flow in the column.

4.6 Problem geometry orientation

The orientation of the defined problem in CTRAN/W will depend on what it was specified as in the SEEP/W or VADOSE/W problem. More detailed discussion of each type of view is provided in those other engineering books. A brief review of the possible types of geometry views follows.

Axisymmetric view

An axisymmetric analysis can be used to simulate three-dimensional problems with symmetry about a vertical axis of rotation. The problem is defined in two dimensions, but for analysis, it is as if the section is rotated about a vertical central axis.

For an axisymmetric analysis, the computed mass flux is per unit radian if the element thickness is specified as 1.0. If you want the computed flux value for the entire circumferential area, you must either specify the element thickness as 6.2832 (i.e., 2 pi radians) before you do the analysis, or simply multiply the above value by 2 pi after the solution is finished. You can change the element thickness for the entire mesh with the Draw Element Properties command.

Plan view

A plan view analysis views the finite element mesh as lying on its side instead of standing upright in a vertical plane. In CTRAN/W the only difference between a plan view and a 2D view analysis is the way the area of a unit "q" contaminant mass flux boundary is computed.

In a plan view, the area by which the "q" contaminant mass flux rate is multiplied comes from the plan view areas of each element that contribute data to the "q" specified nodes. The solver will compute the element areas and apply the flux, Q, to the nodes.

2D view

In a 2D view, the area by which the "q" contaminant mass flux rate is multiplied comes from the length of the element edges that the boundary condition is specified. This length is then multiplied by the specified thickness of the element (typically unit thickness into the screen) to obtain a total flux, Q, to apply at the relevant nodes.

4.7 Staged / multiple analyses

Multiple analyses can be included in a single GeoStudio project. Fundamentally, multiple analyses in a single Project allows different material properties and different boundary conditions to be specified across time and space. This facilitates the modeling of staged construction in which soil is added or removed over time and/or boundary conditions or material properties that change with time. Including multiple analyses in a single Project can be used for a variety of reasons such as:

1) Conducting sensitivity analyses for variations in material properties and boundary conditions;

2) Analyzing staged construction;

3) Establishing initial conditions for a transient analysis;

4) Integrating various GeoStudio products; and,

5) Linking together multiple transient analyses.

GeoStudio uses a parent-child terminology to describe the relative position of each analysis within a Project. Figure 4-4 displays an example of an Analysis Tree for a slope stability project. The SEEP/W steady-state analysis is the Parent and is used to define the initial pore-water pressure conditions for the two transient SEEP/W analyses. The indentation in the tree indicates that both analyses 2 and 3 have the same Parent. SLOPE/W analyses 2a and 3a are children of transient SEEP/W analyses. This naturally suggests that the pore-water pressure conditions for both stability analyses are defined using the transient seepage results.

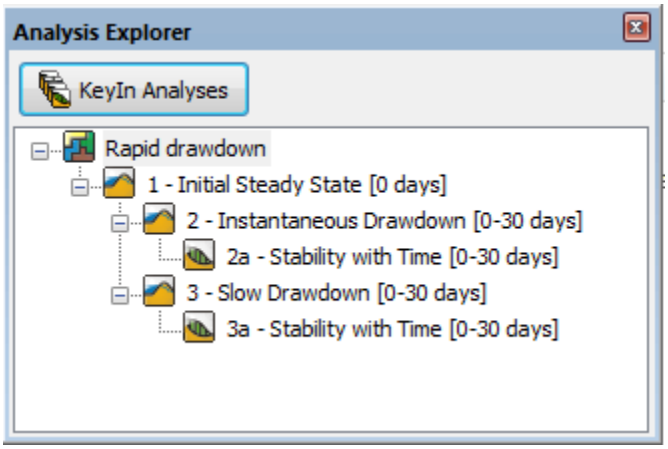


Figure 4-4 Example of an Analysis Tree in GeoStudio

One significant benefit of the Analysis tree is that all analyses related to a specific project are contained within a single file. It is no longer necessary to reference other files to establish initial conditions or integrate the various GeoStudio products.

5 Functions in GeoStudio

User specified functions are used throughout GeoStudio to specify soil material properties, to specify modifier parameters for constants or other functions, or to specify boundary conditions that change over time. It is important to have an understanding of how the functions are specified and used by the solver and also to know what your options are for inputting these functions. A functional relationship between "x" and "y" data can be defined using:

- Natural and weighted splines between data points
- Linear lines between data points
- A step function between data points
- A closed form equation that is based on parameters and does not require data points
- A user written externally complied code (dll library) that connects with GeoStudio data or data from another process (eg, Excel)

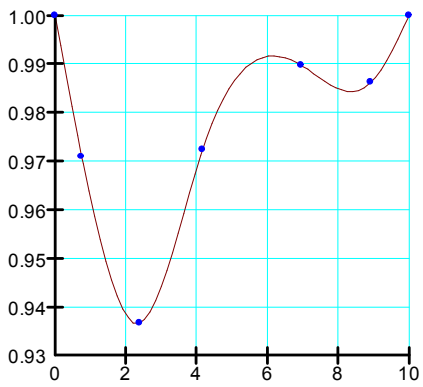
The type of function you choose to use will depend on what your needs are.

In many cases a function you need can be estimated from other data you have input. An example is the hydraulic conductivity function for soils that is based on a user input water content function. Several GeoStudio material models require functions that may be estimated if you do not already have a full set of data.

5.1 Spline functions

A spline function is a mathematical technique to fill in the gaps between adjacent data points with curved line segments. Unfortunately, all our data points do not always fit nicely along a path with a predictable curvature such as a logarithmic or exponential decay. Many of the functions in geo-technical engineering have double curvature with an inflection point between. Consider the water content function that is initially concave downwards, and then at higher suctions is concave upwards. Splining is an advantageous technique to fit lines through these data points because the spline settings can be altered to fit almost any set of data.

In GeoStudio you can control the look of a spline function by adjusting its degree of curvature and its level of fit with the input data points. Consider the two images below.



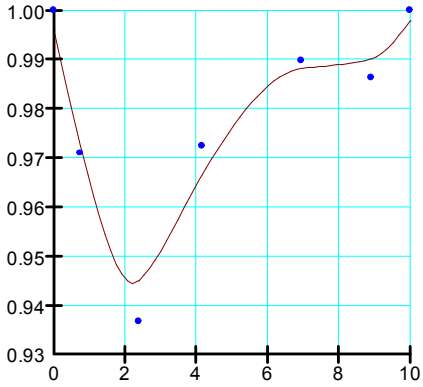


Figure 5-1 Spline functions with different settings

The left image has the spline fit almost exactly through the data points with fairly curved segments. The right image has more linear segments that only fit the data approximately. The range of fit and curvature is controlled by two "slider controls" and can range between values of zero and 100%. The important thing to note is that the solver will use the data represented by the splined fit. What you see in the function set up is EXACTLY what the solver will use when needed.

Slopes of spline functions

Sometimes, the solver does not require the "Y" value of a function at a given "X" value but the slope of the function at a given "X" value. This is the case for the water content function where the slope is used directly in the solution of the transient seepage and air flow equations. You must be careful when setting spline values because while a spline may look smooth, its slope may not be so.

The two images below are the slopes of the two functions shown above. You can see that the more natural curved function (left side images) with 100% curvature and exactness in the spline settings produces a much smoother slope function than the approximated function. While not usually critical, you should know if the function you are using is dependent on its slope being well behaved.

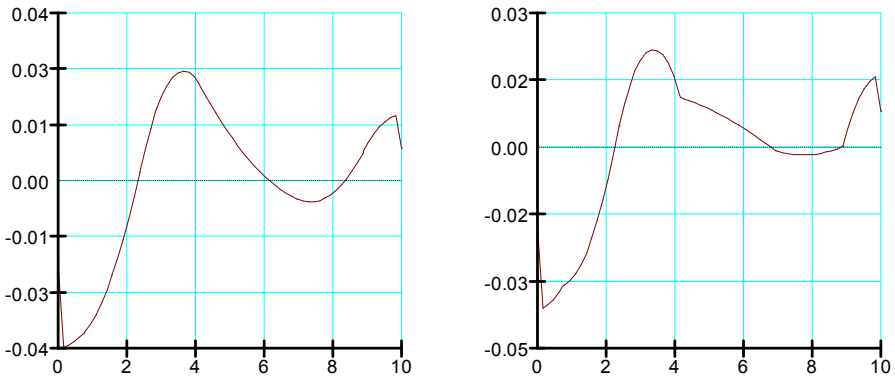


Figure 5-2 Slope of spline functions

5.2 Linear functions

A linear function is a spline function with the curvature setting to 0% and the fit set to 100% exact as shown below.

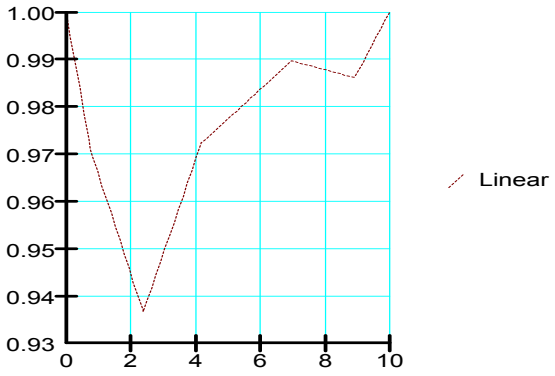


Figure 5-3 Linear fit spline

5.3 Step functions

GeoStudio has an option for functions that result in "steps" between data points. This can be useful if your data changes abruptly over time, for example, rainfall on different days. When you use a step function, you need to be careful of the location of the blue data point. You can see that the functions will assume the starting time of the step is at the data point and that its duration extends just up to but not reaching the next data point.

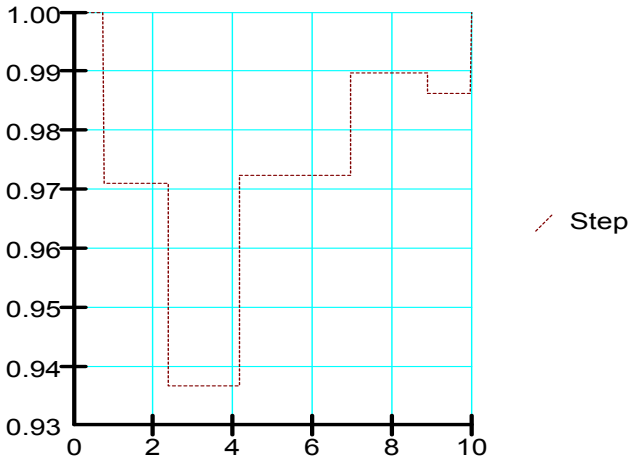


Figure 5-4 Step function

A comparison of all four data point functions is shown below on one image. When multiple functions are viewed simultaneously in GeoStudio, the data points are hidden and just the computed functions are displayed.

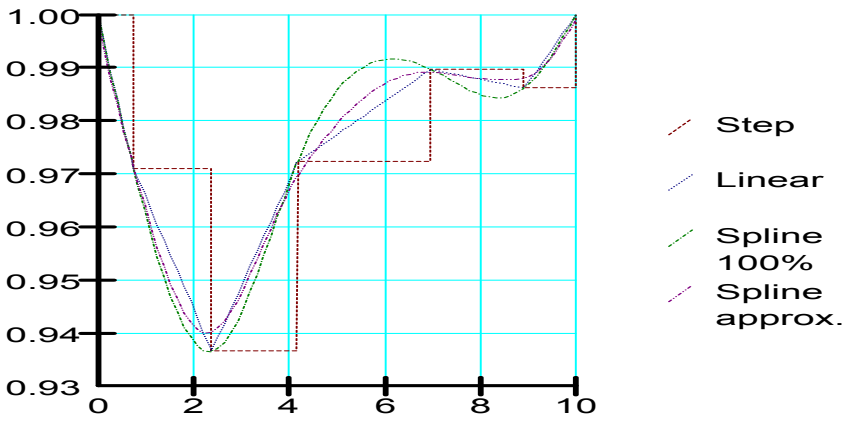


Figure 5-5 Comparison of all data point functions

5.4 Closed form curve fits for water content functions

The storage function is defaulted to be represented by a spline function; however, it is possible to have the function represented by a closed form equation that is fit to the data. Two common methods exist in the literature for water content functions: the Fredlund and Xing method, and the Van Genuchten method. Each of these curve fits require that you enter fitting parameters that are usually published or provided by soil laboratories. The only advantage to using these techniques in GeoStudio is that you do not have to enter a series of data points. If you know the fit parameters, you may enter them directly to obtain the function. More information about these two fit equations are provided in the chapter on Material Models and Soil Properties in this book.

5.5 Add-in functions

GeoStudio Add-Ins are supplemental programs run by the solver as part of a GeoStudio analysis. A Function Add-In is an object that takes the place of a function defined in GeoStudio, and offers the flexibility of computing function results that vary dynamically based on the current analysis state. For example, Add-Ins can be assigned to Slip Surface Slices (via strength functions), Mesh nodes (via boundary condition functions), and Mesh gauss points (via material property functions). Please consult the Add-In Developers Kit (SDK) available on the website (www.geo-slope.com/downloads) for full details.

5.6 Spatial functions

A spatial function in CTRAN/W can be used to establish starting concentration profiles over a two-dimensional domain. When you first create a spatial function you will not see its contoured colors appear on the geometry. However, once you assign the function as the initial condition in Key In Analysis Settings, you can return to the Key In Spatial Function command, make changes and edits to the function data, and see instantly what the new function will look like when applied to your model. An example of this is shown below for initial pore-water pressures which would be applied in the seepage part of the analysis. In CTRAN/W, you can only create a spatial function for initial concentration in this version.

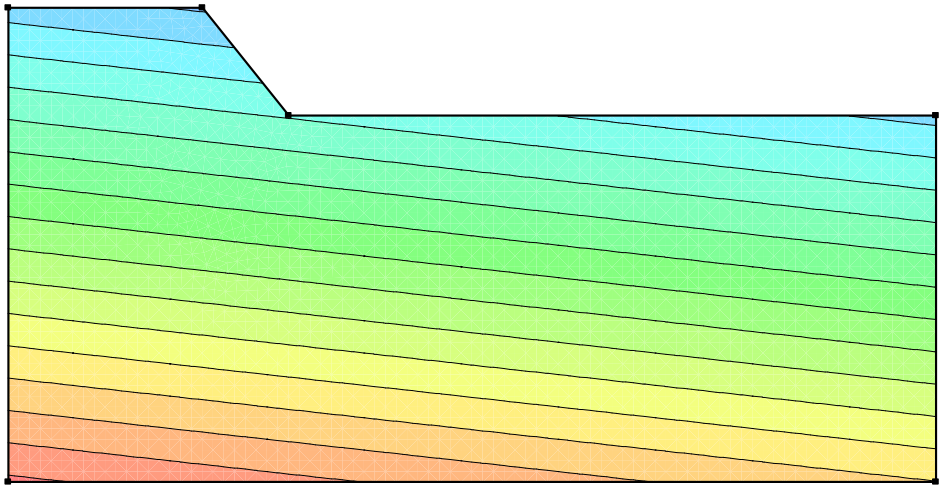


Figure 5-6 Example of spatial function assigned to model

6 Numerical Issues

Entire textbooks can be written on numerical issues related to finite element analysis. While modern computers and powerful graphics can make defining an analysis quite fast and easy, they can not necessarily deal with some of the intricate issues related to the concept of taking a natural process and breaking it down into finite time and special domains (i.e. individual elements within a soil geometry).

There are various ways to deal with many of the numerical issues, but the unfortunate part is that there is no single method, approach, or technique that can deal with all problems. Some numerical issues relate to restrictions in computer hardware such as rounding off of non-integer variables during math operations; some issues relate to non-linearity of soil properties; some issues relate to the fact the physical equations being solved do not apply to all cases (for example, CTRAN/W does not account for contaminants moving in both the air and liquid phases); some issues relate to our inability to discretize a domain to small enough element sizes; and other issues relate to the fact we have made the elements too small!

There are numerical solvers that make use of adaptive meshing or adaptive time stepping or both in attempts to be more suited to a wider range of problems. All of these, however, have their limitations from a sound mathematical perspective – regardless of what the software developer will tell you. If you don't know what the limitations are, it becomes somewhat risky to rely on a solver that claims to "handle it all."

Some finite element solutions attempt to march forward in time by considering soil property values taken from the last, the current or the mid-time step average. Some solvers simply make assumptions that limit their applicability to real life in order to get a solution, such as moving the mesh to find the water table in a seepage program instead of solving for the physics of flow above and below the water table. Finally, some solvers may only work if you put in an initial guess of the solution for the dependent variable being solved that is close to the desired solution, in other words, start off the solution by pointing it in the right direction.

While it may appear all hope is lost, this is far from the case. Sound judgment and common sense can usually overcome most of these challenges and result in meaningful interpretations of how the soil will respond to changes in various parameters.

It is not always possible to get an exact solution in many challenging cases, so you should not necessarily be seeking an exact solution. If the problem is so difficult that it is not solving reasonably, then it is very likely that either mistakes have been made in the input, or, that you are pushing the envelope of the physical theory applied in the model. This chapter looks at some of these issues as they pertain to CTRAN/W.

6.1 Convergence

The objective of solving the finite element equations is to compute the concentration at each node. For linear analyses when the material properties are constant, the nodal concentrations can be computed directly. However, in the cases of nonlinear analyses where there is adsorption as a function of concentration, the correct material properties are not known at the start of the analysis; consequently, an iterative scheme is required to solve the equations.

CTRAN/W uses a repeated substitution technique in the iterative process. For the first iteration, the user-specified initial concentrations are used to define the material properties. The material properties are updated in subsequent iterations using the computed concentration from the previous iteration. The iterative process continues until the iteration number reaches the maximum number specified or until the results satisfy the convergence criteria.

Convergence means repeated solving of the nodal transport equations until the computed solution does not change by more than a specified amount on successive iterations. If the equations want to solve to the same results over and over, then this means that the soil property values used in the solution agree with the computed concentration values at each position in the mesh, and that the influence of the boundary conditions (i.e., adding or removing mass) also are reflected in the correct soil properties and concentrations. Everything must be just right to balance both sides of the transport equation.

Vector norms

CTRAN/W does not use individual nodal concentrations to make the comparison between successive iterations. Instead, it uses the percent change in the vector norm – a process that considers all nodal concentrations simultaneously. The vector norm is computed as the square root of the sum of each nodal concentration value squared, or in equation form:

$$N = \sqrt{\sum_{i=1}^{n} C_i^2}$$

where:

N	=	the vector norm,
i	=	a counter,
n	=	the total number of nodes, and
C_i	=	the individual nodal concentrations.

The percent change in the vector norm is simply the change in the value N between two successive iterations. If the change in N were exactly zero, then there would be no change in solution on successive iterations. In general, there are always very small differences between iterations so it is not reasonable to expect a change in vector norm of zero.

You may wonder why we use the vector norm. It is a powerful way of considering the entire problem in a single comparison, which prevents any individual nodal concentration from potentially failing the convergence test in a solution that really should be considered converged.

When the dependent variable (e.g. concentration in a transport analysis) gets close to zero, very small changes in a single variable between successive iterations can appear to be very big when converted to a percent difference comparison. Consider if a single nodal concentration is changing from 0.01 to 0.02 between successive iterations. This is a change of 100% but likely insignificant from a physical perspective. It's a failure in the logic of checking convergence by individual nodal percent difference, because it lets small physical changes become significant mathematical changes.

During the iterative process, CTRAN/W calculates the percent difference in vector norm; which represents the percent difference in the concentration of all nodes between two consecutive iterations. In an analysis where there is no adsorption or in a particle tracking analysis, the problem is linear and is solved in one iteration. Consequently, convergence parameters are ignored.

6.2 Numerical dispersion and oscillation

Numerical dispersion and oscillation are inherent in the finite element solution of the advection-dispersion equation. The two phenomena are illustrated graphically in Figure 6-1. Numerical

dispersion tends to spread out the contaminant more than what is predicted by analytical solutions. Numerical oscillation produces concentrations higher or lower than the maximum and minimum specified values.

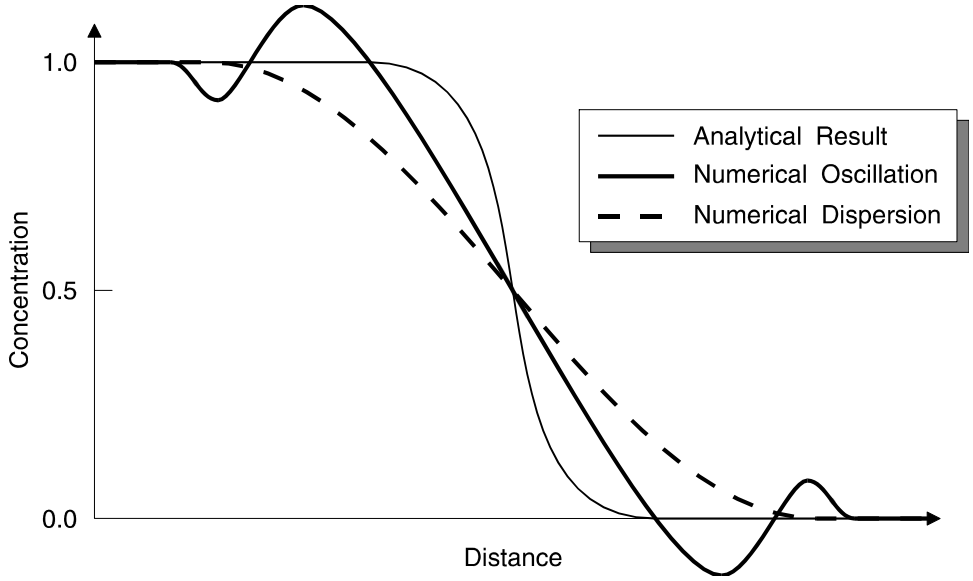


Figure 6-1 The phenomena of numerical dispersion and oscillation

Numerical dispersion and oscillation cannot be eliminated; they can only be controlled or minimized. The two widely used criteria are the Peclet Number and the Courant number constraints. (See Frind and Pinder, 1982, and Daus, Frind and Sudicky, 1983).

6.3 Peclet and Courant number criteria

The Peclet and Courant Number criteria are usually expressed in the one-dimensional form as follows:

$$\text{Peclet Number} = \frac{v\Delta x}{D} \leq 2$$

$$\text{Courant Number} = \frac{v\Delta t}{\Delta x} \leq 1$$

where:

Δx	=	nodal spacing,
D	=	hydrodynamic dispersion coefficient,
v	=	average linear velocity, and
Δt	=	incremental time step.

In two-dimensional analyses, CTRAN/W computes the Peclet and Courant Numbers at each Gauss point of an element using the following equations:

$$P_x = \frac{|v|\Delta x}{D_{11}} \le 2 \quad \text{(Peclet Number in } x\text{-direction)}$$

$$P_y = \frac{|v|\Delta y}{D_{22}} \le 2 \quad \text{(Peclet Number in } y\text{-direction)}$$

$$C_x = \frac{v_x \Delta t}{\Delta x} \le 1 \quad \text{(Courant Number in } x\text{-direction)}$$

$$C_y = \frac{v_y \Delta t}{\Delta y} \le 1 \quad \text{(Courant Number in } y\text{-direction)}$$

where:

Δx = maximum x-distance between the element corner nodes,

Δy = maximum y-distance between the element corner nodes,

D_{11} , D_{22} = hydrodynamic dispersion coefficient,

$|v|$ = magnitude of linear average velocity,

vx = average linear velocity in x direction,

vy = average linear velocity in y direction, and

Δt = incremental time step.

The Peclet and Courant Number constraints provide the necessary conditions for the finite element mesh design and the selection of time steps in transport modeling. The Peclet Number constraint requires that the spatial discretization of the flow regime is not larger than twice the dispersion potential of the porous medium. The Courant Number constraint requires that the distance traveled by advection during one time step is not larger than one spatial increment (i.e., one element).

It is convenient to check for the Peclet and Courant numbers distribution within a flow system by using the Draw Contours command. As a rule of thumb, when the Peclet number is too big, the mesh size should be reduced, or alternatively, the material dispersivity should be increased. When the Courant number is too big, the time step increment should be reduced.

6.4 Backward or central difference time integration

Numerical dispersion and oscillation is also affected by the time integration scheme. The Backward Difference approximation method (BDA) results in less numerical oscillation but more numerical dispersion. On the other hand, the Central Difference approximation method (CDA) results in less numerical dispersion but more numerical oscillation.

A more stable answer can be obtained using the Backward Difference method. However, if numerical stability can be controlled, a more accurate solution can be obtained using the Central Difference method.

In summary, it is best to start with the more stable Backward Difference method and then refine the solution with the Central Difference method once all other factors in the analysis have been modeled correctly. In many cases, the differences between the two methods are relatively small.

6.5 Mesh design

The Meshing chapter of the SEEP/W or VADOSE/W books provides general modeling guidelines for the design of a finite element mesh for seepage analysis. This section provides additional guidelines which should be followed in order to extend the seepage analysis results for contaminant transport modeling.

In order to obtain stable solutions in a transport analysis, both the Peclet Number and Courant number criteria must be considered in the design of the finite element mesh. Rearranging the above Peclet and Courant number equations, the spatial discretization requirements are:

$$\Delta x \leq 2 \frac{D_{11}}{|v|}$$

$$\Delta y \leq 2 \frac{D_{22}}{|v|}$$

$$\Delta x \leq v_x \Delta t$$

$$\Delta y \leq v_y \Delta t$$

The above equations indicate that the spatial discretization of the flow regime should not be larger than twice the dispersion potential of the porous medium and the distance traveled by advection during one time step. In most cases, the time steps can be easily reduced to satisfy the Courant criterion, therefore, the design of the mesh depending primarily on the seepage velocity and the dispersivity of the materials.

Since the equations require knowledge of the average linear velocity, the Peclet and Courant Numbers for each element will not be known at the time you create the finite element mesh. Therefore, these criteria cannot be rigidly applied during creation of the mesh. As a broad rule, the discretization in the major flow direction should be about twice the longitudinal dispersivity α_L of the soil, and the discretization in the minor flow direction should be about twice the transverse dispersivity α_T of the soil.

This will provide a starting point for you to estimate the required spatial discretization. Later, you can confirm the actual Peclet and Courant Numbers computed by CTRAN/W and check that both the Peclet and Courant Number criteria are satisfied in all time steps.

6.6 Time step design

Numerical dispersion and oscillation are directly affected by the time step increments. To minimize numerical dispersion and oscillation, the Courant Number constraint should be satisfied. The Courant Number constraint requires that the distance traveled by the advective component of the transport process during one time step ideally should not be larger than one element; that is, the advective component should not jump across elements in one time step.

In order to satisfy the Courant Number constraint, the time increment should be:

$$\Delta t \leq \frac{\Delta x}{v_x}$$

and,

$$\Delta t \leq \frac{\Delta y}{v_y}$$

As a first approximation, you can estimate the time step increment based on the average size of the elements and the average linear velocity. The Courant numbers computed by CTRAN/W should be checked to confirm that the Courant Number constraint is satisfied in all time steps.

6.7 Use of the Peclet and Courant numbers criteria

The Peclet and Courant Numbers must be viewed as a guide to minimizing numerical dispersion and oscillation. Ideally, the Peclet Number should be less than 2 and the Courant Number should be less than 1. Satisfying these criteria, in general, would ensure a stable solution to the transport problem with minimal numerical dispersion and oscillation. However, satisfying these criteria in all elements for all time steps may be difficult to achieve in some practical problems. It may require thousands of small elements and hundreds of small time step increments depending on the material dispersivity and seepage velocity.

Generally, adherence to these criteria is most important where the concentration gradients are steep, as is often the case during the initial time steps. Away from regions with steep gradients, the criteria can be relaxed without creating major difficulties. (Marsily, 1986) How rigidly you apply these criteria needs to be judged in light of the objectives of a particular project.

Let us use Henry's Problem in the verification chapter as an example. Figure 6-2 shows the computed concentration contours at time step 35, and Figure 6-3 and Figure 6-4 illustrate the contour plots of the Peclet and Courant numbers, respectively.

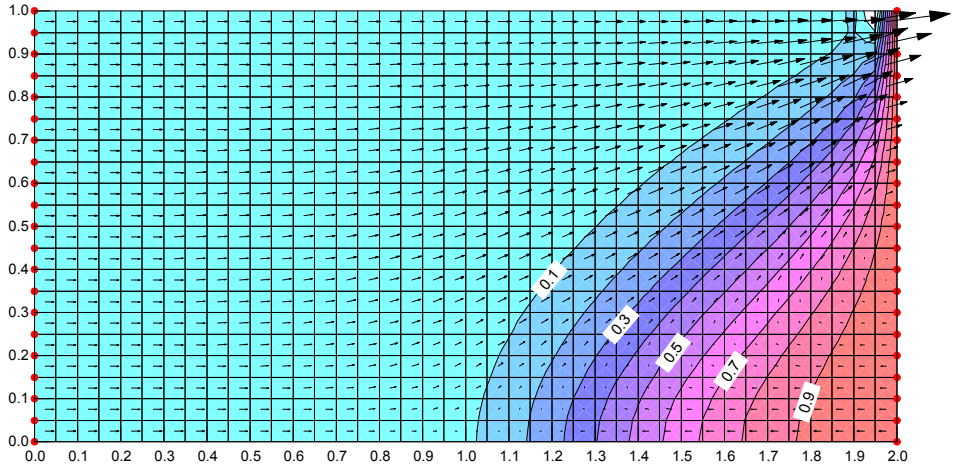


Figure 6-2 Concentration contours in Henry's problem

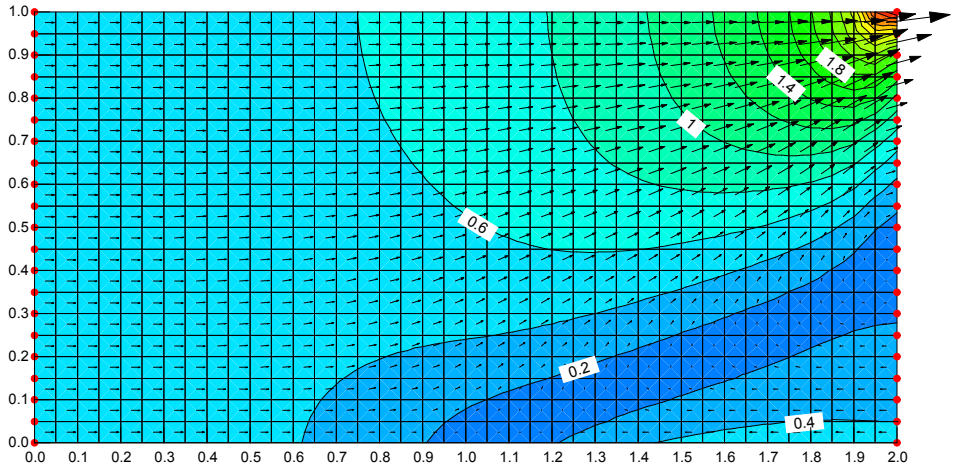


Figure 6-3 Peclet number contours of Henry's problem

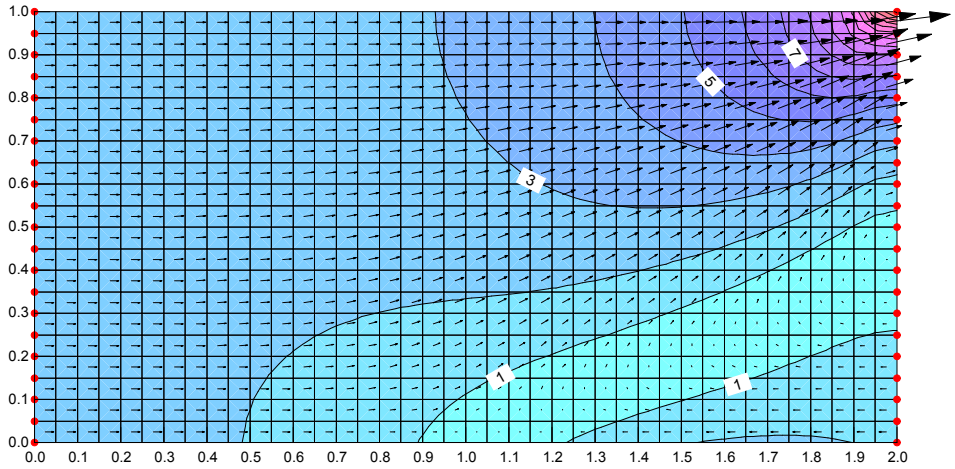


Figure 6-4 Courant number contours of Henry's problem

Near the upper right corner of the flow system, where the seepage velocity is the highest, both the Peclet and Courant numbers criteria are not satisfied. However, within most of the flow system, the Peclet number criterion is satisfied and the Courant number is slightly higher than the suggested criterion. As a result, the concentration contours indicate that a stable solution was obtained within most of the flow system, and a small area with numerical instability is observed near the upper right corner. The numerical instability causes small negative concentration values to be computed at the upper nodes between the 0.1 and 0.2 concentration contour lines. The concentration contours greater than 0.3 are not significantly affected by the instability.

It is possible to improve the simulation such that both the Peclet and Courant number criteria are satisfied and numerical instability is minimized. To do so will require substantial refinement to the mesh especially in the upper right corner, and a much finer time step increment. Since the area of interest of the Henry's

problem is in the lower right portion of the flow system, and only the 0.5 concentration contour line is used in the comparison with other models, we feel that it is not necessary to further refine the analysis.

6.8 Gauss integration order

The details of numerical integration are provided in the appendices, along with a discussion of how different integration orders can affect results for various types of elements. Part of this discussion is repeated here as it pertains to improving solution convergence.

The appropriate integration order is a function of the presence of secondary nodes. When secondary nodes are present, the interpolating functions are nonlinear and consequently a higher integration order is required. Table 6-1 gives the acceptable integration orders.

Table 6-1 Acceptable element integration orders

Element Type	Secondary Nodes	Integration Order
Quadrilateral	no	4
Quadrilateral	yes	9
Triangular	no	1
Triangular	yes	3

It is also acceptable to use four-point integration for quadrilateral elements which have secondary nodes. This is called a reduced integration order (see Bathe, 1982). Acceptable results can be obtained with reduced integration.

It is also possible to use three-point and nine-point integration with elements that have no secondary nodes. However, the benefits of this are marginal, particularly for quadrilateral elements. Nine-point integration for a quadrilateral element involves substantially more computing than four-point integration, and there is little to be gained from the additional computations. As a general rule, quadrilateral elements should have secondary nodes to achieve significant benefits from the nine-point integration.

The situation is slightly different for triangular elements. One-point integration means the material properties and flow gradients are constant within the element. This can lead to poor performance of the element, particularly if the element is a zone of steep concentration gradient and there is active adsorption. Using three-point integration, even without using secondary nodes, can improve the performance, since material properties and gradients within the elements are distributed in a more realistic manner. The use of three-point integration in triangular elements with no secondary nodes is considered acceptable for triangular elements in a mesh that has predominantly quadrilateral elements. This approach is not recommended if the mesh consists primarily of triangular elements with no secondary nodes.

In general, it is sufficient to use three-point integration for triangular elements and four-point integration for quadrilateral elements. In situations where there is adsorption and steep gradients within an element, it is best to use quadrilateral elements with secondary nodes together with nine-point integration.

6.9 Equation solvers (direct or parallel direct)

CTRAN/W has two types of equation solvers built into it; a direct equation solver and a parallel direct equation solver. Both offer certain advantages.

Select the direct equation solver option if you want the system equations to be solved using a Gauss elimination skyline direct solver. The processing speed of the direct solver is bandwidth (the maximum

node number difference of all the elements in a domain) dependent. In other words, the direct solver is very fast when solving simple problems with small bandwidth, but it can be quite slow when solving more complex problems with a large bandwidth. CTRAN/W automatically sorts the nodes so that the bandwidth is the smallest possible value, which helps the solution solve faster using the direct solver. By default, the direct equation solver is selected.

Select the parallel direct equation solver option if you have a larger mesh. The parallel solver will save the matrices in a compressed format to eliminate zero's and it has many advanced schemes to solve large systems of equations more efficiently. It also offers the ability to make use of multiple processors on a computer if they are available. The disadvantage of this solver is that it is a bit slower when the models are smaller in size.

If in doubt, try each solver and choose the one that offers the best performance.

7 Visualization of Results

When you get to the visualization of results stage of a finite element analysis you can congratulate yourself for having completed the hardest parts – setting up the geometry, defining meaningful soil property functions, and applying appropriate boundary conditions to the mesh. If, at this point, you do not have the tools or the understanding of how to interpret the massive amount of data that may have been generated by the solver, then you have wasted your time.

This chapter describes the various types of output data that are computed by the solver and it attempts to get you thinking about what the data is trying to tell you. For example, did the solution solve properly? Did the boundary conditions you applied get reflected in the actual solution? Did the soil respond how you thought it would respond? If not, how to you methodically determine what to check next?

The chapter is structured to explain what type of data is available for visualization. In the various sections, comments are provided that relate they type of result data in question to how is should be used in the overall thought process. It's a good idea to read this entire chapter.

7.1 Node and element information

In order to understand what type of information can be viewed as results output, it helps a bit to know how the data is obtained. To recap, you set up the problem geometry, define material properties, and apply boundary conditions of either known concentration or mass flux. The solver assembles the soil property and geometry information for every Gauss point in every element and applies it to the transport equation that is written for every node. Therefore, at each node we have some applied boundary data, some interpolated soil property data and geometry data. The solver then computes the unknown value in the equation for each node – the unknown value being either concentration or flux. It is the Gauss point data that is used to set up the nodal equations so the Gauss point data written to the output file is the actual data used in the solver.

Figure 7-1 is an illustration of the type of information that can be viewed for each node in the finite element mesh. You can view information about geometry, material properties, seepage results, concentrations and boundary fluxes as well as gradients, water velocities etc. Of significance is the ability to view Courant and Peclet information. This is discussed more in the contouring data section below.

One key point to note in the figure below is that the nodal Boundary Mass Flux quantity is exactly zero. This is an important point to understand because it can help with your overall interpretation of results. This boundary flux is computed by summing the contributing fluxes from each of the four Gauss points that surround this node. So, if mass is flowing out of one Gauss region, it HAS TO be flowing into an adjacent Gauss region. For all internal nodes with no user boundary applied to them, the sum of all the mass fluxes at a node should equal zero in a properly converged solution. In other words, there is mass balance at the node.

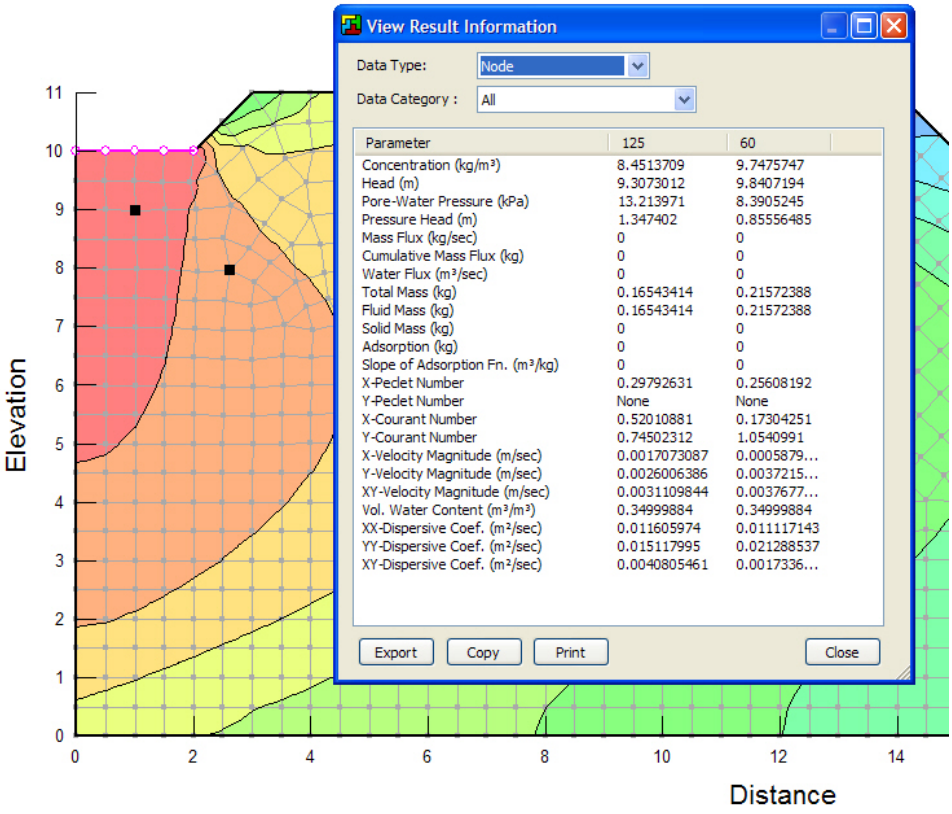


Figure 7-1 Visualization of node information

If the node being viewed is a boundary condition node (not necessarily at the edge of the geometry but with an allowed influx or out flux) then the summation of all the mass fluxes at that node will not be zero because contaminant mass is either gained or lost at that point.

Figure 7-2 is the corresponding Gauss point information for the Gauss point located just above and to the right of the node illustrated in the previous figure. The shaded region in the figure shows the contributing area of that Gauss point and in this case, because the element is rectangular and has no secondary nodes, this Gauss area is equal to one fourth of the total area of the element. The inset in the figure below shows the type of data that can be viewed at each Gauss point. If you consider the water content value of 34.9%, for example, you should realize that this water content is assumed to exist throughout the Gauss point area displayed; and you should next realize that if the element size is increased, the estimate of the water content becomes less accurate as we are averaging it over a larger area. The real trick to getting good finite element analysis results, is to create a finite element mesh with just the right sized elements that are not too big or too small, that can represent the highly non-linear soil properties within them, and that can handle the potentially extreme boundary conditions you apply. It's not always easy and there is no sure quick or automatic method to make that happen.

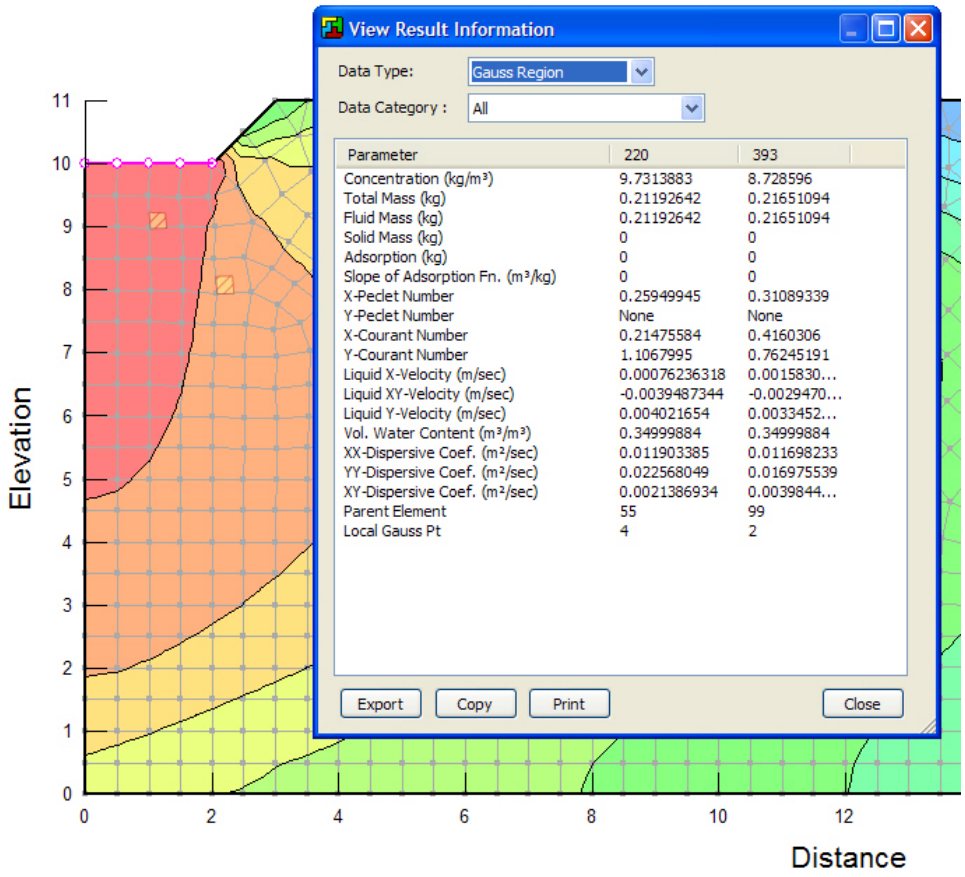


Figure 7-2 Visualization of element Gauss point information

7.2 Particle information

This features displays information about a particle at a specified point in time. When a particle time increment is selected to view, CTRAN/W reads all particle files up to the selected time increment and displays the path over which the particle traveled during these time increments. Using the View Particle Information command, you can select any point along the particle path and view the particle *x*-*y* coordinates, the time at which the particle arrived at the point, the distance the particle traveled up to the point, and the average particle speed up to the point. Figure 7-3 shows the type of data that can be accessed.

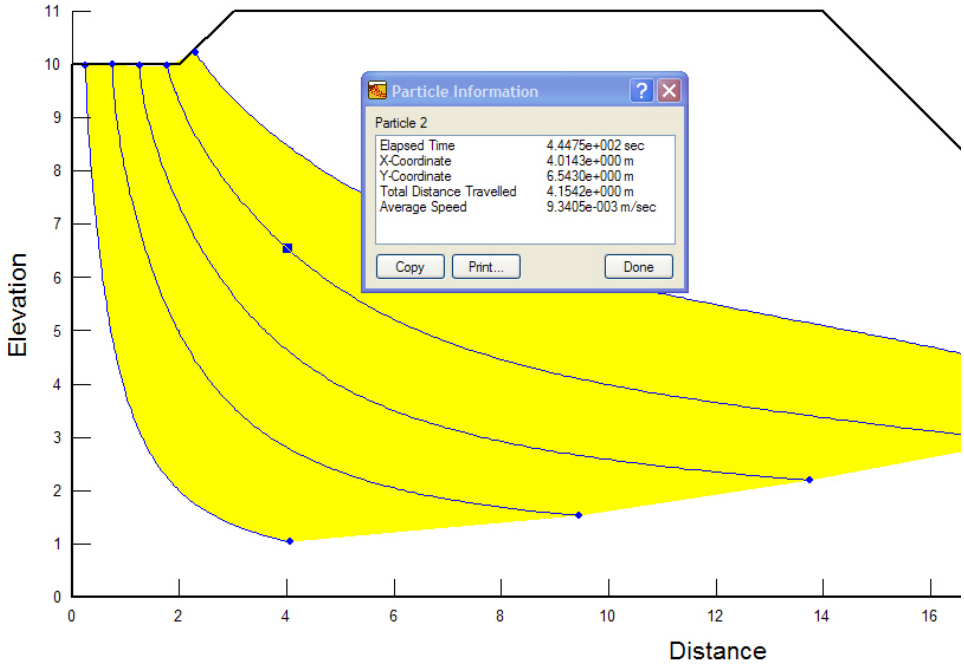


Figure 7-3 View particle information data

The position of the particles is a good indication of where the 50% concentration value will be at any given time. Consider an advection – dispersion problem where some contaminant is moving due to water flow; and some is moving ahead of the water due to molecular action, while some is retarded in progress due to molecular action in the direction opposite to flow. The "s" shape of the concentration plug illustrates this idea. Now, consider the mid-point of the "s" shape. It is a point in concentration (the 50% point) and it is moving solely due to advection. So, if we are only interested in the position of the 50% concentration point, we can simply use a particle tracking analysis and not the full advection – dispersion solution.

7.3 Mass accumulation

This feature displays accumulated mass values within selected elements. In a contaminant transport problem, it is often useful to find out the amount of mass that has accumulated in any region of the mesh. The View Mass Accumulation command allows you to select any group of elements and see the amount of mass in the elements as illustrated in Figure 7-4.

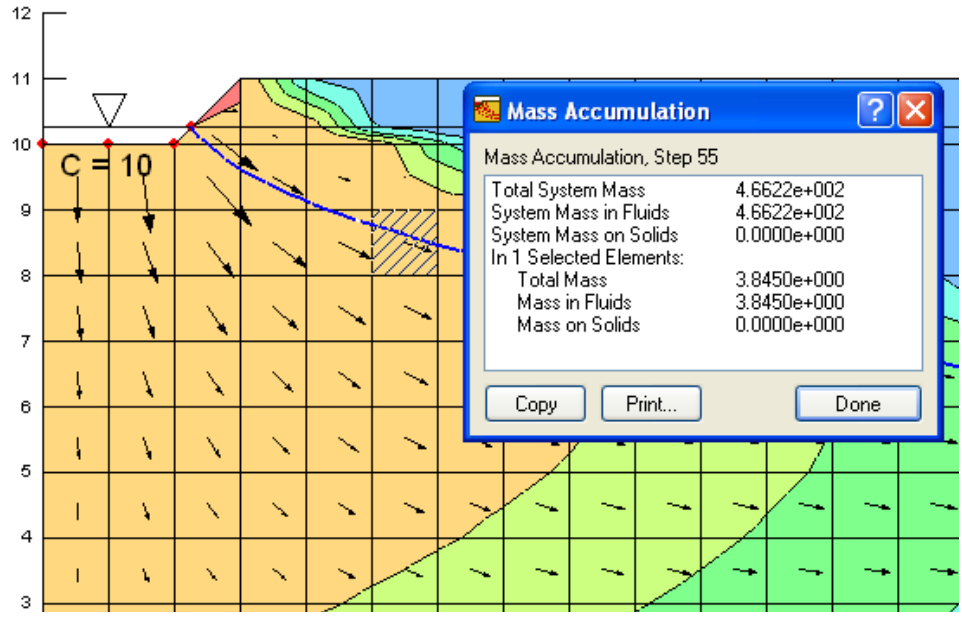


Figure 7-4 View mass accumulation data

7.4 Graphing Node and Gauss Data

The Draw Graph command allows you to plot a graph of any computed value as a function of time, position or both time and position. In past versions of GeoStudio, all graphing was based on user selected nodes. Moving forward, GeoStudio now requires the user to select graph data locations based on one or more points, a cut line, or a region of points. It is possible to select all three types of data locations within a single graph. Figure 7-5 shows a combination of all three graph data objects in a single dam cross section.

The advantage of using this type of data selection is that the location and type of data used in any graph can be named and saved. Each time you return to the graphing command, you can choose from your saved list of graphs and you do not have to re-define them. Even if you change the mesh, the model will know the new nodes nearest to your graph selections and it will draw the graph using the most recent solution.

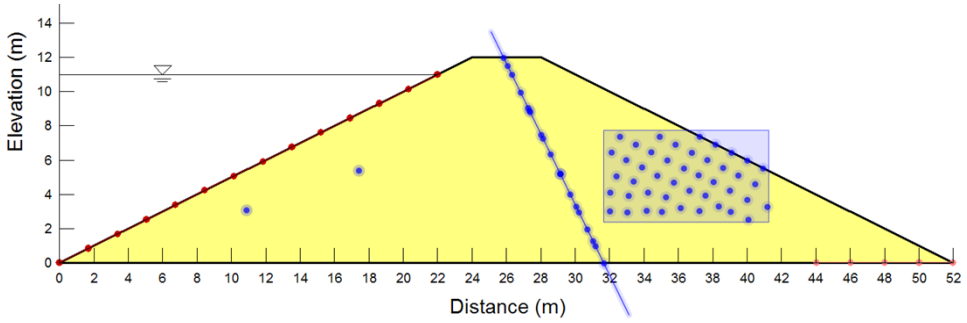


Figure 7-5 Graph data selection options (points, lines, planes)

In the previous image, the graph points were selected at any point in the domain. Sometimes it is easier to select all points along a given geometry object such as a region line or point. Consider Figure 7-6 where the entire up stream region edge line has been selected for graphing. In this case, it was easier to just

select one point along the entire edge and have the model capture all nodes along that edge. The option of selecting custom points or geometry points is totally a user preference.

Once the graph is visible there are many options to change the font, apply a legend, rotate the image, copy the image to paste it into a report, copy the data to paste to Excel or another program, or export it as a comma separated text file.

You can even hover the mouse directly on a graphed point to see the actual data as shown in Figure 7-8 below.

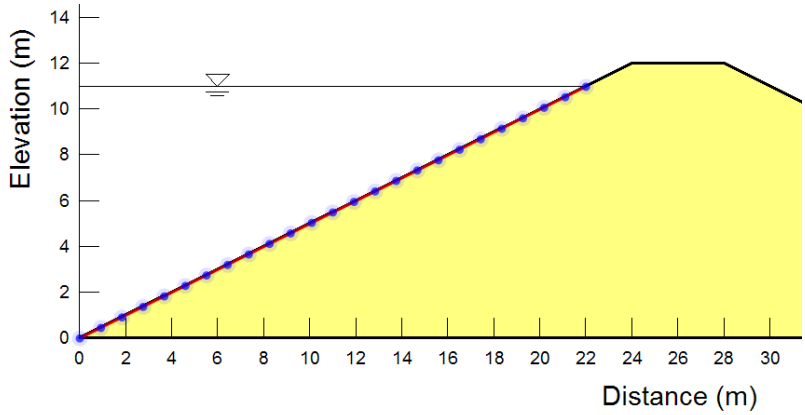


Figure 7-6 Graph selections based on geometry item (upstream region edge line)

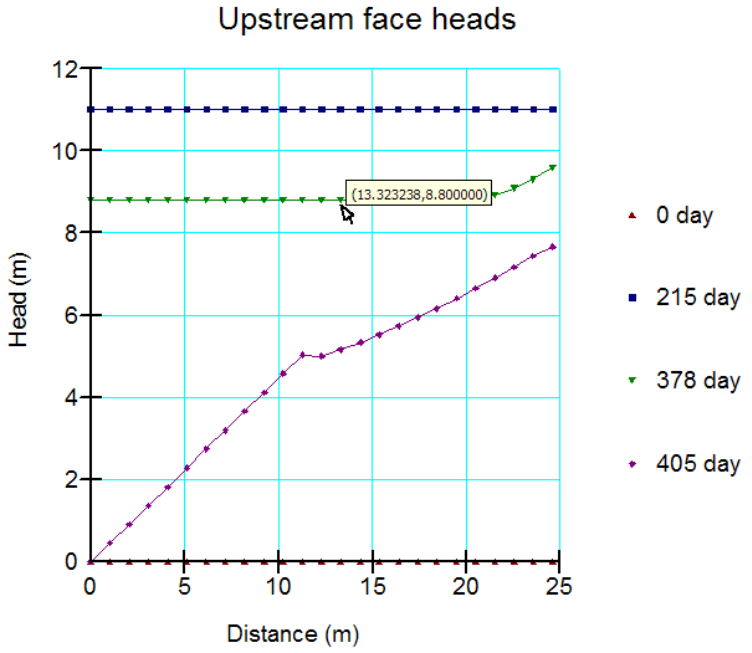


Figure 7-7 Upstream total head as a function of position for each time

The Draw Graph command allows you to plot a graph containing any of the computed parameter values. If you are viewing a concentration time increment, the following parameters can be plotted: concentration, total head, pressure, pressure head, total mass, fluid mass (portion of the mass contained in fluids), solid mass (portion of the mass on solids), adsorption, *x*-Peclet number, *y*-Peclet number, *x*-

Courant number, *y*-Courant number, *x*-velocity (log), *y*-velocity (log), *xy*-velocity (log), volumetric water content, *XX*-dispersive coefficient (log), *XY*-dispersive coefficient (log), and *YY*-dispersive coefficient (log).

If you are viewing a particle time increment, the following parameters can be plotted: total head, pressure, pressure head, *x*-velocity (log), *y*-velocity (log), and *xy*-velocity (log), volumetric water content.

The above listed parameters are the dependent variables of the graph. Any of the dependent variables can be plotted versus the following independent variables: nodal x coordinates, nodal y coordinates, and the distance between nodes (starting at the first selected node).

The independent graph variable that you choose affects how the selected nodes and time steps are used in the graph. If the graph independent variable is x coordinate, y coordinate, or distance, then the parameter value at each selected node is plotted versus the nodal coordinate or the distance between nodes. Each selected time step is plotted as a separate line on the graph. If the graph independent variable is time, then the parameter value at each selected node is plotted versus the elapsed time for each of the selected time steps. Each selected node is plotted as a separate line on the graph. These two cases are illustrated in the Figure 7-8 and Figure 7-9 where the concentration beneath the lagoon is compared versus position and time respectively. The nodes down the left edge of the above illustrated examples are chosen for plotting data in the following figures.

These illustrations show the default graph template used in the model. There is, however, the ability to customize the scales, labels, and symbols so that the plots can be used directly within your reports. In addition, the above figures were simply copied from the screen and pasted into this document using the COPY command inside CTRAN/W.

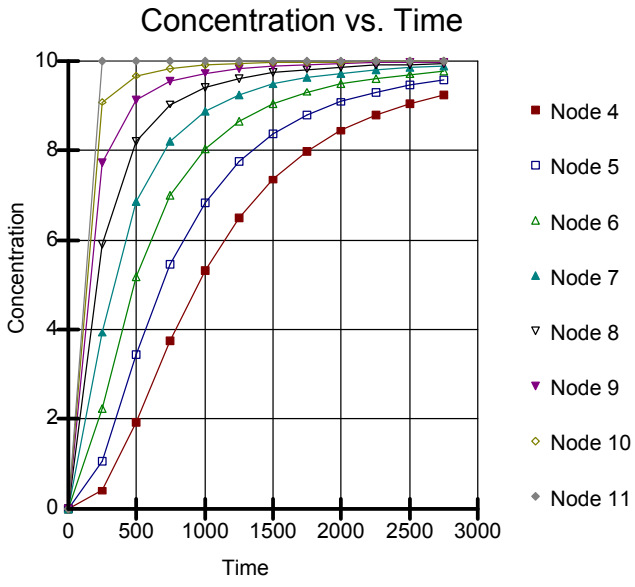


Figure 7-8 Left side node concentration as a function of time

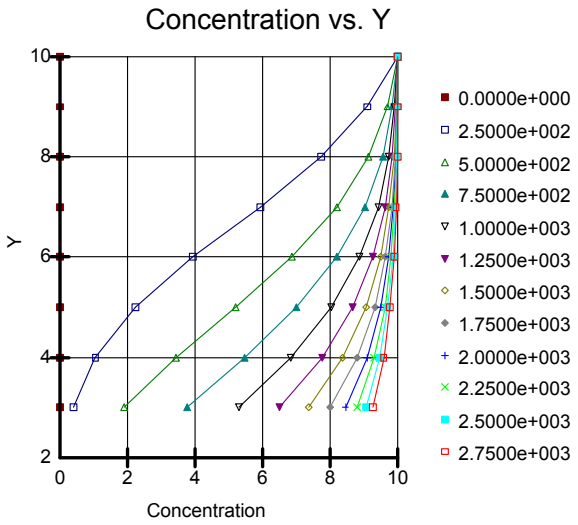


Figure 7-9 Left side node concentration as a function of y coordinate for each time

7.5 "None" values

In GeoStudio, an attempt is made to distinguish between data values that have a true value of zero, and those that are missing. A missing value is labeled as "none" in a data list or is not printed to file when you save the data for export or pasting into another program such as Excel. A missing value is simply a data type that is not relevant to the current set of analysis parameters.

"None" or missing values, are simply a way for GeoStudio to not erroneously report data values as zero (which has meaning) when they really just do not exist. Consider the following graph generated by GeoStudio of pore-water pressures in a soil as it is placed during a construction sequence. At the 0 second time, the soil surface is at 10m. At 10 seconds, 2 meters of more soil is added. At 8010 seconds, another 2 meters is added. Notice that for the two added lifts of soil, the pressure values are not graphed as zero prior to their placement time. The data is "missing" in the program so is not reported or graphed.

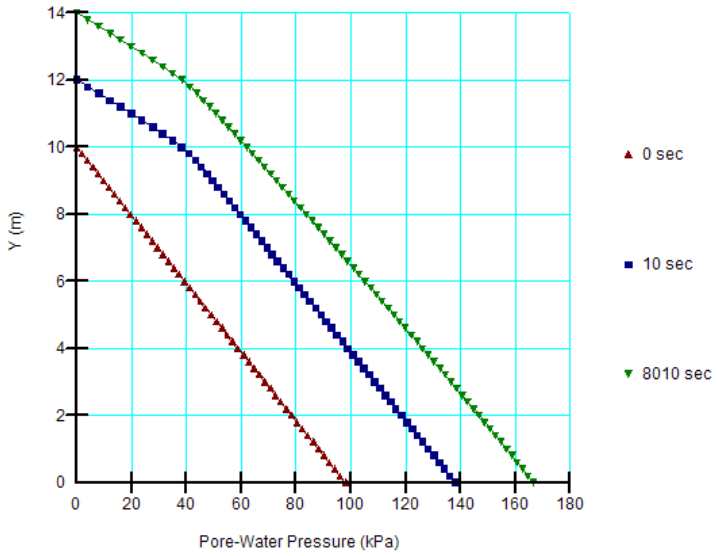


Figure 7-10 Graph showing how missing data is excluded and not printed as zero

7.6 Projecting Gauss point values to nodes

CTRAN/W performs contouring calculations based on parameter values at the nodes. Since the primary parameter, concentration, is computed at the nodes, these parameters can be contoured directly. However, secondary parameters (velocity, gradient, Peclet / Courant number, and water content etc.), are computed at the element Gauss points and must therefore be projected to the nodes for contouring purposes.

In triangular elements, the Gauss point values are projected on the basis of a plane that passes through the three Gauss points. For one-point integration, the value at the Gauss point is also taken to be the value at the nodes (i.e., the Gauss point value is constant within the element).

In quadrilateral elements, the Gauss point values are projected using the interpolating functions. (For more information about interpolating functions, see the appendix). In equation form,

$$x = \langle N \rangle \{X\}$$

where:

x	=	the projected value outside the Gauss points at a local coordinate greater than 1.0,
<N>	=	a matrix of interpolating functions, and
{X}	=	the value of Gauss point variable.

The local coordinates at the element nodes are the reciprocal of the Gauss point local coordinates when forming the element characteristic matrix. Figure 7-11 is an example of the local coordinates at the element corner nodes when projecting outwards from the four Gauss points in the element. The value of 1.7320 is the reciprocal of the Gauss point coordinate 0.57735.

This projection technique can result in some over-shoot at the corner nodes when variation in the parameter values at the Gauss points is large. For example, consider that we wish to contour water content and that in some elements the water content at the Gauss points varies over the complete range of the water content function. Projecting such a large variation to the nodes can result in projected nodal water contents beyond the range of the water content function.

Extreme changes in the parameter values at the Gauss points within an element often indicate numerical difficulties (the over-shoot at the nodes being just a symptom of the problem). This over-shoot can potentially be reduced by a finer mesh discretization. Smaller elements within the same region will result in a smaller variation of parameter values within each element, therefore lowering the potential for encountering unrealistic projections.

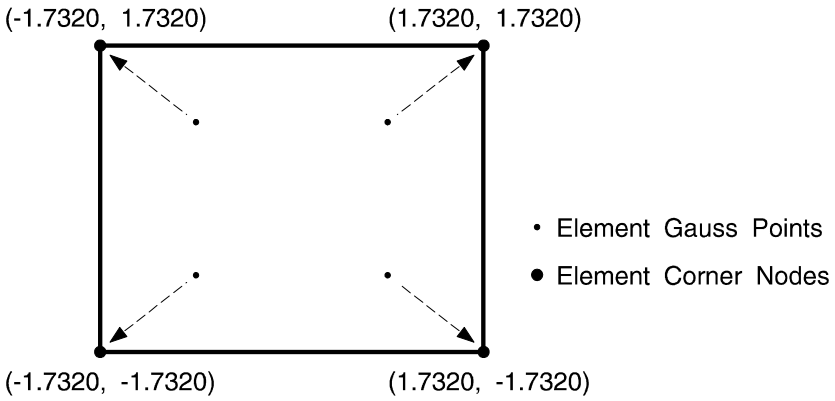


Figure 7-11 Local coordinates at the corner nodes of an element with four integration points

7.7 Contours

The power of using advanced graphical interfaces with finite element analysis is that the computer can quickly convert thousands of pieces of data into meaningful pictures. In the section above we introduced isotherms. We can use a picture of the isochlors to tell us something about what is going on in the soil. In particular, if we consider how close adjacent isochlors are to each other, we are in effect, considering how steep the concentration gradient is. If we recall that the amount of mass flow is equal to the concentration gradient multiplied by the dispersion coefficient, we then have a fast and clear picture of where the areas of high mass flow are in the domain we have modeled.

CTRAN/W is a powerful tool in that it will let you contour many different parameters such as concentration, Courant number, Peclet number, pressure, gradients, mass fluxes, water contents and more. Figure 7-12 is a contour of the X direction Courant number values for the isochlors illustrated above. We know that for an advection-dispersion type analysis, we want the Courant number to remain low. This figure shows us that it ranges between 0.05 and perhaps 0.5, which is acceptable. If this contour were to have shown us areas of high Courant or Peclet value, we would have an idea of what to adjust in order to obtain a better solution. Perhaps the mesh would need to be finer in one location or the time steps smaller.

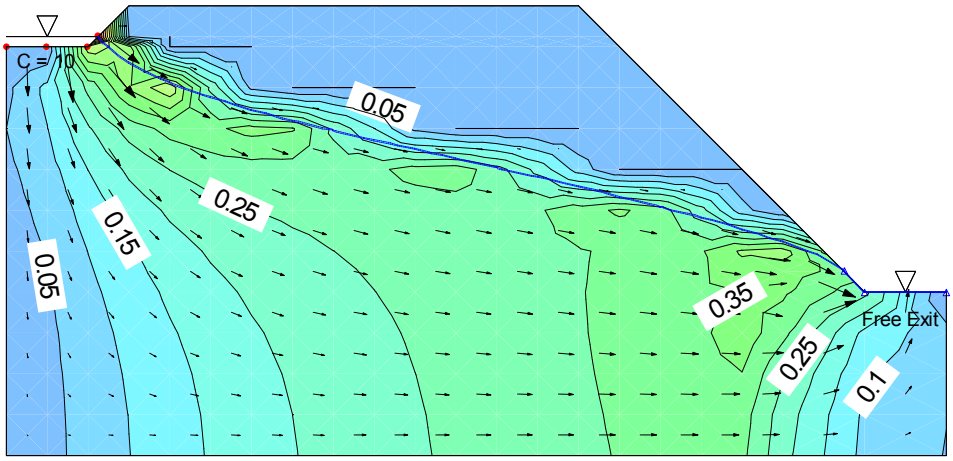


Figure 7-12 CTRAN/W computed X direction Courant numbers

7.8 Water flow vectors and flow paths

Water flow vectors and flow paths are described in detail in the SEEP/W and VADOSE/W engineering books.

7.9 Animation in GeoStudio

Movie files (*.avi) can be created in GeoStudio to illustrate a physical process in a transient analysis. The first step in creating a movie is to define the contours and specify any View Preferences that need to be visible (e.g. flux vectors or the displaced mesh). The View Animation command is selected and the time steps and viewing area are defined. After saving the movie file to the appropriate location, GeoStudio joins together all of the individual images for each time step, creating a seamless animated movie.

7.10 Flux sections

CTRAN/W has the ability to compute the instantaneous flux across a user-defined section for either a steady-state or transient analysis. The view preference command can be used to modify the flux type that is displayed on the flux section. View Preferences allows you to display total, advective, dispersive, stored, or decayed flux on the drawing. The stored flux is the rate at which mass is stored in an element. A negative stored mass means that mass is accumulating in an element (i.e., the total mass flow across the section is decreasing due to adsorption). A positive stored flux means that mass is being released from the element, thereby increasing the rate of mass flow across the section.

Flux section theory

Details of the flux section calculations are given in the Theory chapter.

Flux section application

Flux sections can be used in many ways, because they can be drawn any place across which you want to know the flux. You may want to check if an influx is equal to an out-flux such as illustrated in Figure 7-13. In this case, the values are NOT the same which is to be expected because the problem is a transient analysis and there is a change in the amount of mass storage over time.

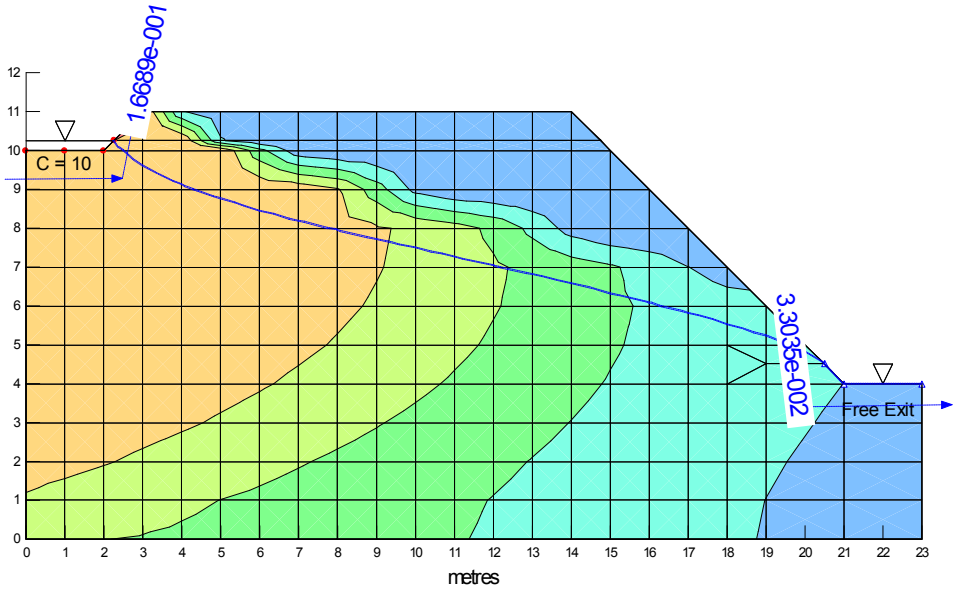


Figure 7-13 Flux section used to check balance of mass inflow and outflow

Flux sections do not have to be drawn as single straight lines. They can be made of continuous attached segments as illustrated in the figure above. When a multiple segmented flux section is drawn, the value of flux reported for the section applies to the entire section, not any individual segment.

The key point to note when defining a flux section is to make the flux section cross the sides of the elements and not the nodes of the elements. Also, if you want to check the flux around a closed loop as illustrated for the SEEP/W seepage drain nodes in Figure 7-14, make sure the end of the flux section crosses over the tail of the first segment of the flux section.

Two words of caution: flux sections MUST be defined before you solve the problem, because the program needs to calculate the values during the solution sequence, not afterward. In addition, all flux values are reported as positive, which means direction is not taken into account. This is required because the sign of the flux value will depend on which way you draw the section. To avoid any misinterpretation, all flux section values are reported as positive, and then you can plot flux vectors in order to determine the direction of flow, if it is not obvious based on your problem definition.

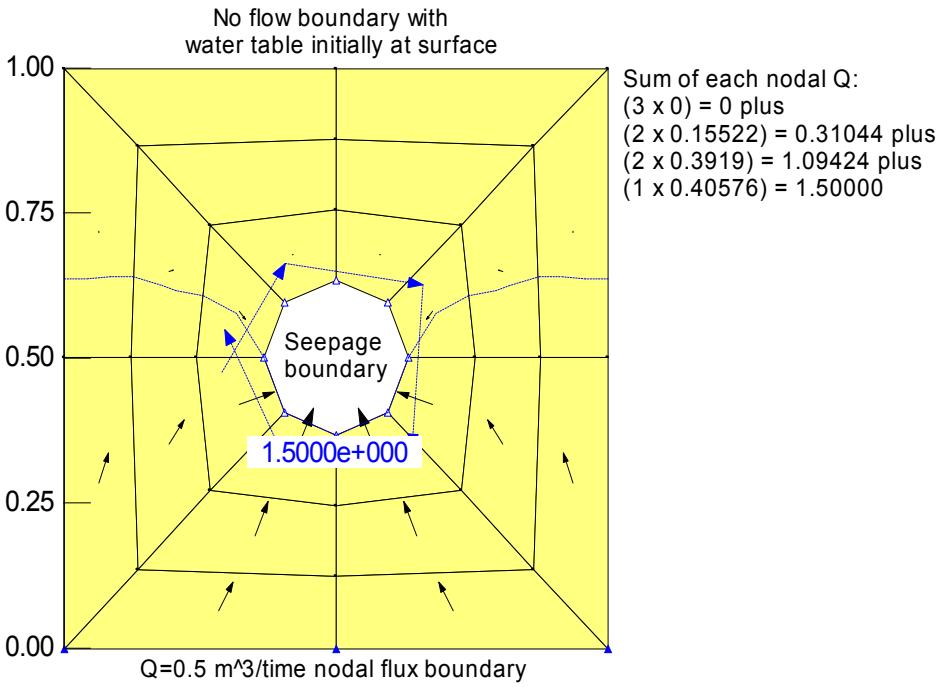


Figure 7-14 Flux section used in SEEP/W around series of drain nodes to check flow

7.11 Isolines

You can use the Draw Isolines command to choose which parameter you want the water table calculation based on. It can be water pressure concentration. You can also choose to draw an isoline contour of any other parameter at an instance in time or over multiple times. If you draw an isoline at multiple time steps then you can not also view contour shading as it only exists for any instance in time. The isolines are a way to track a single value of a parameter as it changes over time… such as a water table.

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8 Modeling Tips and Tricks

8.1 Introduction

This chapter contains many useful hints about using the software and understanding what it does. READ THIS CHAPTER!

CTRAN/W is a powerful analytical tool, but it will only provide valid solutions if the boundary conditions, material properties, and time sequence are appropriately defined. It is your responsibility to properly define the problem parameters and ensure that the results produced are valid and reasonable.

This chapter presents some general modeling guidelines. The information presented is not an exhaustive statement on the "how-to" of modeling a contaminant transport problem. Instead, it is intended to provide suggestions on how you might model various conditions, as well as to outline the implications of certain modeling specifications.

There have been many occasions where GEO-SLOPE has been contacted by clients with questions about how the model behaves in response to changes in various parameters. If we do not know the answer, we conduct a numerical experiment to test what will happen. The first few sections of this chapter illustrate a few common examples of numerical experiments. You are strongly encouraged to learn why these types of simple tests are so powerful in testing how the program computes results BUT ALSO in enhancing your understanding of how the physical mechanisms of flow through porous medium occurs.

A numerical experiment is carried out by making a very simple finite element problem. It is useful to use a mesh that is one distance unit wide and one distance unit high. This makes hand calculating flux values very simple and they can easily be checked against the computed flux values. The following discussion illustrates how some simple numerical experiments have been carried out to test some simple, yet valid, questions.

When setting up these experiments, it is a good idea to input simple soil property functions. In most cases, two data points are sufficient to define the conductivity and storage function. Just as a reminder, give both functions some slope – don’t make them horizontal!

8.2 Modeling progression

Modeling the movement of contaminants through soil is a complex type of analysis. As discussed in the Theory Chapter, the contaminant transport process is not only governed by water movement, it is also influenced by dispersion, molecular diffusion, adsorption, and radioactive decay. With so many factors involved, it can be confusing and difficult to resolve the contribution of each component in the transport process.

An important rule to follow in contaminant transport modeling is to progress from the simple to the complex. It is good practice to initially define a simplified version of the problem and then add complexity in stages. Moving from the simple to the complex makes it easier to pinpoint difficulties with the model when the results of the analysis are unrealistic.

For example, begin by analyzing a homogeneous problem with no adsorption and no decay. Then add adsorption, decay, and other materials to the analysis in separate stages. This incremental approach not only helps to evaluate the results but also provides information on the effect of the various parameters. Determining what causes unrealistic results can be difficult if all of the possible complexities are included at the start of the problem analysis.

For complex transport problems that may involve multiple sources and exit boundaries, it is useful to first do a particle tracking analysis before doing the advection-dispersion transport modeling. Particle tracking has the advantage of providing an approximate solution to the transport problem quickly with minimum input requirements. Although only the advection process (water movement) is considered in particle tracking, the solution does provide a clear picture of the approximate contaminant plume.

8.3 Problem engineering units

Any system of units can be used for a contaminant transport analysis; the only requirement is that you must be consistent with the units throughout both the CTRAN/W and the corresponding seepage analysis. Fundamentally, you must select the units for length (geometry), time, and force. Once you have selected units for these parameters, all other units must be consistent. Table 8-1 and Table 8-2 present some typical sets of consistent units.

Table 8-1 Consistent set of SI units

Parameter	Symbol	Units
Length	*L*	m
Time	*t*	s
Force	*F*	kN
Mass	*M*	g
Pressure	F/L^2	kN/m^2
Unit Weight of Water	F/L^3	kN/m^3
Hydraulic Conductivity	*L/T*	m/s
Concentration	M/L^3	g/m^3
Diffusion Coefficient	L^2/T	m^2/s
α_L and α_T (dispersivity)	*L*	m
Decay Half-Life	*T*	sec
S (adsorption)	*M/M*	g/g
Density	M/L^3	g/m^3
Mass Flux	*M/T*	g/s

Table 8-2 Consistent set of imperial units

Parameter	Symbol	Units
Length	*L*	ft
Time	*t*	hr
Force	*F*	lb_f
Mass	*M*	lb
Pressure	F/L^2	psf
Unit Weight of Water	F/L^3	pcf
Hydraulic Conductivity	*L/T*	ft/hr
Concentration	M/L^3	lb/ft^3
Diffusion Coefficient	L^2/T	ft^2/hr
α_L and α_T (dispersivity)	*L*	ft
Decay Half-Life	*T*	hr
S (adsorption)	*M/M*	lb/lb
Density	M/L^3	lb/ft^3
Mass Flux	*M/T*	lb/hr

The units of time are established once you select the units for hydraulic conductivity. The units of pressure are established once you select the unit weight of water. Generally, all units are defined by selecting the units of length for the problem geometry, units for hydraulic conductivity, and the units for the unit weight of water.

Concentration is often reported in units of milligrams per liter (One milligram per liter (mg/l) is equivalent to one part per million (ppm) and is also equivalent to one gram per cubic metre (g/m3). In equation form: mg/l = ppm = g/m^3.

Therefore, concentrations reported in mg/l or ppm can be conveniently used in a CTRAN/W analysis provided mass is defined in grams (g) and length is defined in meters (m).

In summary, the key requirement is that the system of units must be consistent.

8.4 Fracture flow simulation

CTRAN/W can be used to analyze contaminant flow through fractures by modifying the definitions for volumetric water content (Θ), adsorption (S), and the dry bulk density (ρ_d). For fracture flow, these parameters are defined as:

$$\Theta = \frac{\text{Volume of Fractures}}{\text{Total Volume}}$$

$$S = \frac{\text{Mass of Solute Adsorbed on the Fractures}}{\text{Unite Area of the Fractures}}$$

$$\rho_d = \frac{\text{Area of the Fracture Planes}}{\text{Total Volume}}$$

The adsorption terms in the finite element equation involve (ρ_d) multiplied by (S). Multiplying these two variables together results in units of mass adsorbed on the fractures per unit volume. The area of the fracture planes vanishes as far as the units are concerned.

8.5 Flux section location

Question: Does the location of a flux section within an element have any influence on the computed flux value?

Answer: No. The flux section value will be the same regardless of whether the section is drawn near the element edge or element middle. Figure 8-1 shows this to be the case and it is true for a transient and steady state solution.

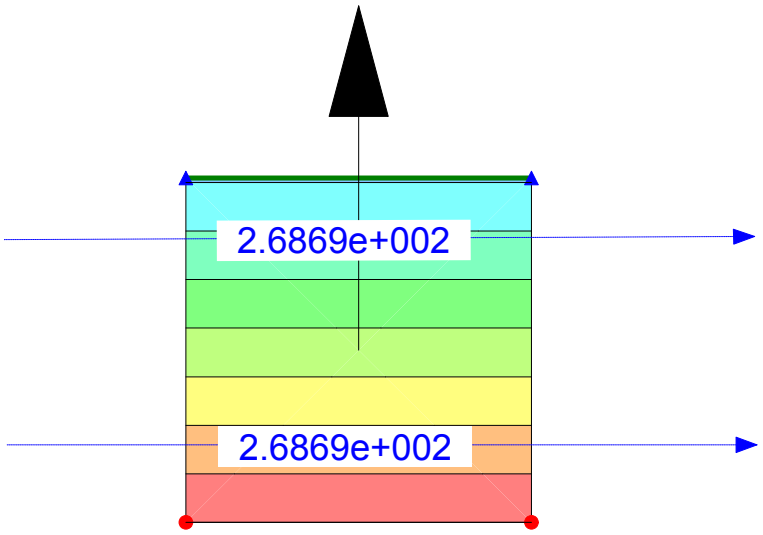

Figure 8-1 Test to check flux section locations

8.6 Unit flux versus total flux?

There are many people who are unsure of the difference between a unit flux and a total nodal flux. Do a simple test if you are unsure.

Question: How is a unit flux related to a total nodal flux in a 2D analysis?

Answer: The total nodal flux should be exactly equal to the unit flux multiplied by the total length of the element edges that contribute to that node.

In the figure below, a unit flux of -500 g / time / meter edge length has been applied to the top of the element. The top is a mass sink face which will let the contaminant out. The flux sections drawn in the element confirm that the total edge flux of -500 g / time has been converted by the solver into two equal total nodal fluxes of -250 g / time each. For such a simple mesh, it is also possible to use the View Node information option and click on each node to see the computed total flux at each node. The sum of the individual total nodal fluxes is the total flux across the element edge.

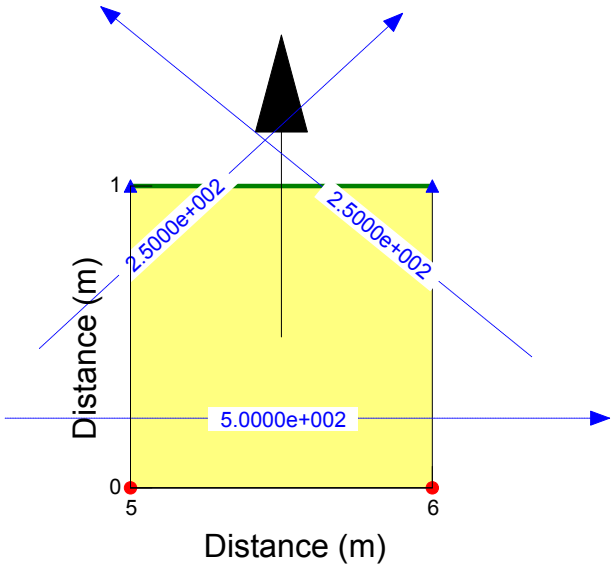

Figure 8-2 Test to compare unit flux and total flux

9 Illustrative Examples

A variety of verification and illustrative examples has been developed and are available with the software. These examples can be useful for learning how to model various problems, particularly in the selection and application of boundary conditions. Each example comes with a PDF document that provides explanations on the problem setup, comments on modeling techniques and a commentary on interpreting the results. Verification examples are discussed in terms of closed-form solutions, published information and/or laboratory measurements.

All of the examples can be downloaded and installed from GEO-SLOPE's web site (www.geo-slope.com). Once installed, it is possible to search for a particular type of analysis on the GeoStudio desktop. Conversely, the search feature is available directly on the website. It should be noted that a product-specific search is possible (e.g. search for TEMP/W or SIGMA/W).

The GeoStudio example files can be reviewed using the **free** GeoStudio Viewer license.

10 Theory

This chapter presents the methods, equations, procedures, and techniques used in the CTRAN/W formulation. It is of value to be familiar with this information in order to use the software. An understanding of these concepts will be of great benefit in applying the software, resolving difficulties, and judging the acceptability of the results.

10.1 Flow velocity

SEEP/W and VADOSE/W compute the specific discharge or D'Arcy velocity. The specific discharge is the total flux Q divided by the full cross-sectional area (voids and solids alike).

The actual cross-sectional area available for the water is less than the full area, due to the presence of the solids. Consequently, the actual rate of movement of the water is higher than the D'Arcy velocity. By definition, the porosity is the volume of voids divided by the total volume. The cross-sectional area available for the water flow is the porosity times the total cross-sectional area.

Therefore the average linear velocity of the pore fluid is: (see Freeze and Cherry, 1979)

$$v = \frac{Q}{n\,A}$$

or,

$$v = \frac{U}{n}$$

where:

U = specific discharge, or D'arcian velocity, and

n = porosity.

Under saturated conditions, the volumetric water content (Θ) is equal to the porosity. The average linear velocity then is also equal to:

$$v = \frac{U}{\Theta}$$

CTRAN/W is formulated on the assumption that the average linear velocity can be related to the volumetric water content for both saturated and unsaturated conditions. SEEP/W, being a saturated/unsaturated flow model, computes the volumetric water content. The SEEP/W specific discharge, (D'Arcy velocity), divided by the SEEP/W volumetric water content is taken in the CTRAN/W formulation as the average linear velocity.

10.2 Governing equations

The governing equation for contaminant transport is generally known as the transport equation or the advection-dispersion equation.

For ease of presentation and discussion, the governing differential equation is presented only in terms of one-dimensional transport. The actual CTRAN/W formulation is based on the corresponding two-dimensional equation.

The solute transport equation can be derived by considering the mass flux q in an elemental volume of porous material, as illustrated in Figure 10-1. The absolute net mass flux across the element is:

net mass flux $= \frac{\partial q}{\partial x}\ dx$

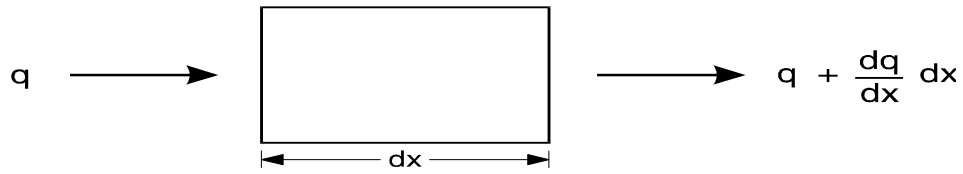

Figure 10-1 Mass balance in a one dimensional element

To conserve mass, the time rate of change of the total mass M in the element must be equal to the net mass flux. In equation form,

Equation 10-1 $$\frac{\partial M}{\partial t}\ dx\ =\ -\frac{\partial q}{\partial x}\ dx$$

By definition, the concentration C is the mass M of dissolved solute in a unit volume of water (solution). In equation form,

$$C = \frac{M}{V_w}$$

or,

$$M = CV_w$$

The volume of water per unit volume of the element is the volumetric water content Θ. The mass M per total unit volume then is:

$$M = C\Theta$$

Substituting for M in Equation 10-1 and dividing by dx leads to:

Equation 10-2 $$\Theta\frac{\partial C}{\partial t}\ =-\frac{\partial q}{\partial x}$$

The mass flux through the element arises from both advection and dispersion processes. In equation form, these two mechanisms are:

advection $= v\Theta C = UC$

and,

$$\text{dispersion} = -\Theta D \frac{\partial C}{\partial x}$$

where:

v	=	average linear velocity,
Θ	=	volumetric water content,
C	=	concentration,
D	=	hydrodynamic dispersion coefficient, and
U	=	D'Arcy velocity (specific discharge).

The negative sign in the dispersion term indicates that the direction of the mass flow is from a high concentration to a low concentration (that is, a negative gradient). Substituting the previous two terms into Equation 10-2 leads to the basic transport equation:

Equation 10-3

$$\Theta \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}\left(-\Theta D \frac{\partial C}{\partial x} + U C\right) = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x}$$

This equation can be divided by Θ, which leads to:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x}$$

where v is the average linear velocity. This is the form of the equation often seen in publications. (Freeze and Cherry, 1979). CTRAN/W uses the more general form as shown in Equation 10-3.

The hydrodynamic dispersion coefficient D is related to the dispersivity, average linear velocity and diffusion coefficient D* by:

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

For further discussion regarding this coefficient, refer to the section on the Hydrodynamic Dispersion Matrix later in this chapter.

Equation 10-3 represents the basic transport of a non-reactive and non-radioactive substance; that is, there is no loss of mass due to adsorption or radioactive decay. For general formulation, the loss of mass due to adsorption and radioactive decay must be added to the transport equation.

For the transport of a radioactive substance, mass may be lost during the transport process due to radioactive decay of ions in the pore fluid and decay of ions attached to the soil particles. The reduced concentration resulting from radioactive decay, in terms of the initial concentration, is:

Equation 10-4

$$C = C_0 e^{-\lambda t}$$

where t is the elapsed time and λ is the decay coefficient. The decay coefficient λ can be related to the half-life T of a decaying material. By definition, the half-life T is the elapsed time when the concentration of C/C0 = 1/2. Therefore,

$$\frac{C}{C_0} = \frac{1}{2} = e^{-\lambda T}$$

which can also be written as:

$$\lambda = \frac{\ln 2}{T} = \frac{0.693}{T}$$

Differentiating Equation 2-1 with respect to time leads to:

$$\frac{\partial C}{\partial t} = -\lambda C$$

The amount of radioactive mass in the pore-water Mw in an elemental unit volume is ΘC, (see above), or:

$$M_w = \Theta C = \Theta C_0 e^{-\lambda t}$$

The adsorption S is the amount of mass attached to the soil particles divided by the mass of the solids. In equation form,

$$S = \frac{\text{mass of solute attached to the solids}}{\text{mass of the solids}}$$

The mass per unit volume of the soil (solid) particles can be defined in terms of the bulk (dry) mass density ρ_d of the soil. The parameter S is then defined as:

$$S = \frac{M_s}{\rho_d}$$

or,

Equation 10-5 $$M = S\rho_d$$

where Ms is the amount of mass attached to a unit mass of soil particles.

In terms of radioactive decay,

$$M_s = S\rho_d = \rho_d S_0 e^{-\lambda t}$$

Therefore, the total radioactive mass M in both the fluid and solid phases is:

$$M = M_w + M_s$$
$$= \Theta C_0 e^{-\lambda t} + \rho_d S_0 e^{-\lambda t}$$

The rate of change of mass due to decay is then:

$$\frac{\partial \mathrm{M}}{\partial \mathrm{t}} = -\lambda \Theta \mathrm{C} - \lambda \mathrm{S} \rho_d$$

The transport equation (Equation 10-3) can now be modified to include radioactive decay. The result is:

Equation 10-6 $$\Theta \frac{\partial C}{\partial t} = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - \lambda \Theta C - \lambda S \rho_d$$

For the transport of a reactive substance, the movement of the mass is also affected by the adsorption of the solute by the soil particles. As discussed above, the amount of mass adsorbed can be defined in terms of the mass density of the soil particles. From Equation 10-5, the adsorbed mass Ms is:

$$M_s = S \rho_d$$

The rate of change of the adsorbed mass is:

$$\frac{\partial M_s}{\partial t} = \rho_d \frac{\partial S}{\partial t}$$

The adsorption S is a function of concentration C. Experimental results are usually plotted as S vs. C, as shown in Figure 10-2. The slope of the S vs. C relationship is $\partial S / \partial C$. In the case of a linear relationship, the slope is usually referred to as the distribution coefficient Kd. The previous equation can then be written as:

$$\frac{\partial M_s}{\partial t} = \rho_d \frac{\partial S}{\partial C} \frac{\partial C}{\partial t}$$

Adding the adsorption term to Equation 10-6 gives the following governing differential equation used in CTRAN/W:

$$\Theta \frac{\partial C}{\partial t} + \rho_d \frac{\partial S}{\partial C} \frac{\partial C}{\partial t} = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - \lambda \Theta C - \lambda S \rho_d$$

or,

Equation 10-7 $$\left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) \frac{\partial C}{\partial t} = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - \lambda \Theta C - \lambda S \rho_d$$

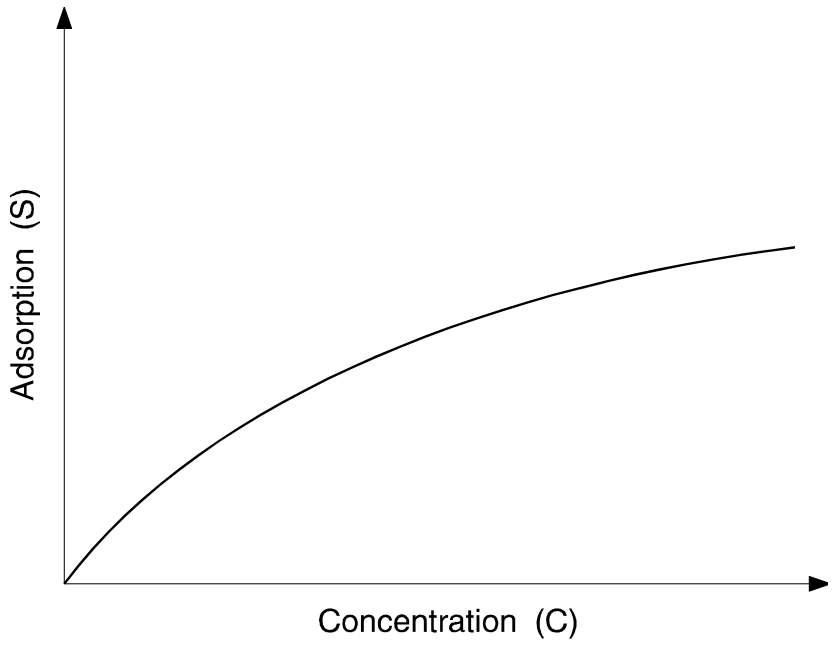

Figure 10-2 Relationship between adsorption and concentration

10.3 Finite element equations

CTRAN/W uses the same techniques as the seepage solution to develop the finite element equation. Details regarding the interpolating function, the function derivatives, the numerical integration scheme, and the implementation of the infinite elements are all presented in the SEEP/W Engineering Methodology book.

Using a Galerkin approach to deriving the finite element equation, the residual function for the governing differential equation is:

$$R(c) = \Theta D \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - \lambda \Theta C - \lambda S \rho_d - \left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) \frac{\partial C}{\partial t}$$

The concentration anywhere in the element can be expressed in terms of the nodal concentration as:

C = <N> {C}

where:

<N> = a matrix of interpolating (or shape) functions, and

{C} = the vector of nodal concentrations.

Substituting this into the prior equation leads to,

$$R(c) = \Theta D \frac{\partial^2 <N>\{C\}}{\partial x^2} - U \frac{\partial <N>\{C\}}{\partial x} - \lambda \Theta <N>\{C\} - \lambda S \rho_d - \left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) \frac{\partial < N > C}{\partial t}$$

The residual can now be multiplied by a weighting function <N>T, then integrated over the volume, and then set to zero in order to minimize the residual. The resulting equation is:

$$0 = \int_v \Theta D <N>^T \frac{\partial^2 <N>}{\partial x^2} dv \{C\}$$

$$-\int_v U <N>^T \frac{\partial <N>}{\partial x} dv \{C\}$$

$$-\lambda \int_v \Theta <N>^T <N> dv \{C\}$$

$$-\lambda \rho_d \int_v S <N>^T dv$$

$$-\int_v \left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) <N>^T <N> dv \{C\}_{,t}$$

Applying Green's theorem, the first term can be integrated by parts to give:

$$\int_v \Theta D <N>^T \frac{\partial^2 <N>}{\partial x^2} dv = \int_s \Theta D <N>^T \frac{\partial <N>}{\partial n} ds - \int_v \Theta D \frac{\partial <N>^T}{\partial x} \frac{\partial <N>}{\partial x} dv$$

where n is a direction unit vector normal to the surface.

Substituting this into the first term in the previous equation results in:

$$0 = \int_s \Theta D <N>^T \frac{\partial <N>}{\partial n} ds \{C\} - \int_v \Theta D \frac{\partial <N>^T}{\partial x} \frac{\partial <N>}{\partial x} dv \{C\}$$

$$-\int_v U <N>^T \frac{\partial <N>}{\partial x} dv \{C\}$$

$$-\lambda \int_v \Theta <N>^T <N> dv \{C\}$$

$$-\lambda \rho_d \int_v S <N>^T dv$$

$$-\int_v \left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) <N>^T <N> dv \{C\}_{,t}$$

The derivatives of the interpolating functions are designated as the gradient matrix [B]. Substituting [B] for the gradient terms and rearranging the terms leads to:

Equation 10-8 $$\int_v \Theta [B]^T [D][B] dv \{C\}$$ (Term 1)

$$+\int_v <N>^T [U][B] dv \{C\}$$ (Term 2)

$$+\lambda \int_v \Theta <N>^T <N> \, dv \, \{C\} \qquad \text{(Term 3)}$$

$$+\int_v \left(\Theta + \rho_d \frac{\partial S}{\partial C} \right) <N>^T <N> \, dv \, \{C\}_{,t} \qquad \text{(Term 4)}$$

$$= \int_s \Theta D <N>^T \frac{\partial <N>}{\partial n} \, ds \, \{C\} \qquad \text{(Term 5)}$$

$$-\lambda \rho_d \int_v S <N>^T \, dv \qquad \text{(Term 6)}$$

The surface integral on the right hand side of Term 5 represents the dispersive mass flux across the boundary, and is the natural boundary condition. However, there may also be advective mass flux across the boundary which will be equal to the specific discharge at the boundary Ub times the concentration.

A more practical boundary condition is the specification of the total mass flux across the boundary (i.e., the Cauchy type or the Third type boundary condition). This total mass flux q will be the sum of the dispersive flux and the advective flux across the boundary. In equation form,

$$q = \Theta D \frac{\partial C}{\partial n} + U_b C$$

Expressing the element concentration C in terms of the nodal concentration {C} and the shape function <N>: (See above)

Equation 10-9 $$q = \Theta D \frac{\partial <N>\{C\}}{\partial n} + U_b <N>\{C\}$$

The term, $\frac{\partial <N>\{C\}}{\partial n}$ signifies that the flow is normal (n) to the boundary.

Equation 10-7 can be rearranged as:

$$\Theta D \frac{\partial <N>\{C\}}{\partial n} = q - U_b <N>\{C\}$$

Therefore, Term 5 of Equation 10-6 can be expressed as:

$$\int_s \Theta D <N>^T \frac{\partial <N>}{\partial n} \, ds \, \{C\} = \int_s q <N>^T \, ds$$

$$- \int_s U_b <N>^T <N> \, ds \, \{C\}$$

Substituting this in Equation 10-6 leads to the general finite element equation used in the CTRAN/W formulation:

Equation 10-10 $$\int_v \Theta [B]^T [D][B] \, dv \, \{C\} \qquad \text{(Term 1)}$$

$$+\int_v <N>^T [U][B] \, dv \, \{C\} \qquad \text{(Term 2)}$$

$$+\lambda \int_v \Theta <N>^T <N>\, dv\ \{C\} \qquad \text{(Term 3)}$$

$$+\int_v \left(\Theta + \rho_d \frac{\partial S}{\partial C}\right) <N>^T <N>\, dv\ \{C\}_{,t} \qquad \text{(Term 4)}$$

$$+\int_s U_b <N>^T <N>\, ds\ \{C\} \qquad \text{(Term 5)}$$

$$= \int_s q <N>^T\, ds \qquad \text{(Term 6)}$$

$$-\lambda \rho_d \int_v S <N>^T\, dv \qquad \text{(Term 7)}$$

In abbreviated form, the finite element equation can be written as:

$$[K_1]\{C\} + [K_2]\{C\},t = \{Q\}\{K_1\}\{C\} + \{K_2\}\{C\},t = Q$$

where:

{K1} = the element characteristic matrix,
= the Dispersive Mass Flux (Term 1),
+ the Advective Mass Flux (Term 2),
+ the fluid phase Decayed Mass Flux (Term 3),
+ the boundary Advective Mass Flux (Term 5),
{K2} = the element capacitance (storage) matrix,
= the Stored Mass Flux (Term 4),
{Q} = the mass flux entering or leaving the element,
= the specified Nodal Total Mass Flux (Term 6), and
+ the solid phase Decayed Mass Flux (Term 7).

10.4 Temporal integration

The finite element solution for the transport equation is a function of time as indicated by the {C},t term in the finite element equation. The time integration can be performed by a finite difference approximation scheme. CTRAN/W uses the following general equation for the time integration:

$$\left(\omega \Delta t [K_1] + [K_2]\right)\{C_1\} = \left(\omega \Delta t \{Q_1\} + (1-\omega)\Delta t \{Q_0\}\right)$$

$$+ \left([K_2] - (1-\omega)\Delta t [K_1]\right)\{C_0\}$$

where:

Δt = time increment,

ω = a ratio between 0 and 1,

{C1} = nodal concentration at end of time increment,

{C0} = nodal concentration at start of time increment,

{Q1} = nodal mass flux at end of time increment,

{Q0} = nodal mass flux at start of time increment,

{K1} = element characteristic matrix, and

{K2} = element capacitance (storage) matrix.

CTRAN/W allows you to select between the Backward Difference Approximation Method (BDA) with ω being set to 1, and the Central Difference Approximation Method (CDA) with ω being set to 0.5. For more information about which time integration method to use, see Backward or Central Difference Time in the chapter on Numerical Issues.

As indicated by the above equation, in order to solve for the nodal concentration at the end of the time increment, it is necessary to know the nodal concentration at the start of the time increment. Stated in general, the initial conditions must be known for solving the transport equation.

When the initial conditions are not specified, CTRAN/W assumes the initial nodal concentration as zero.

10.5 Hydrodynamic dispersion matrix

For one-dimensional flow, the hydrodynamic dispersion coefficient D is defined above as:

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

where:

α = dispersivity (material property),

v = D'arcian velocity divided by volumetric water content (U/Θ), and

D* = coefficient of molecular diffusion.

Dispersion in the direction of the water flow is usually higher than dispersion perpendicular to the flow direction. Two dispersivity values are therefore required to define the spreading process. Dispersivities in the flow directions are designated as the longitudinal dispersivity α_L and the transverse dispersivity α_T.

For two-dimensional flow, as used in the CTRAN/W formulation, the hydrodynamic dispersion coefficient D can be defined in matrix form: (See Bear, 1979)

$$\begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

where:

$$D_{11} = \alpha_L \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + D^*$$

$$D_{22} = \alpha_T \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + D^*$$

$$D_{12} = D_{21} = (\alpha_L - \alpha_T) \frac{|v_x v_y|}{v}$$

$$v = \sqrt{v_x^2 + v_y^2}$$

In general, the coefficient of diffusion D* is a function of the volumetric water content, as shown in Figure 10-3. An empirical relationship between D* and Θ has been proposed by Kemper and Van Schaik, (1966) CTRAN/W allows you to define the desired values of the coefficient of diffusion function as a function of volumetric water content (i.e., the diffusion function).

The D* parameter and its dependence on water content is of significance only in unsaturated flow and when the water flow rate is very low. The value of the hydrodynamic dispersion coefficient is often governed by the water flow rate. Therefore, it is often adequate to assume that D* as independent of Θ, and to define the relationship by a constant horizontal function for a CTRAN/W analysis.

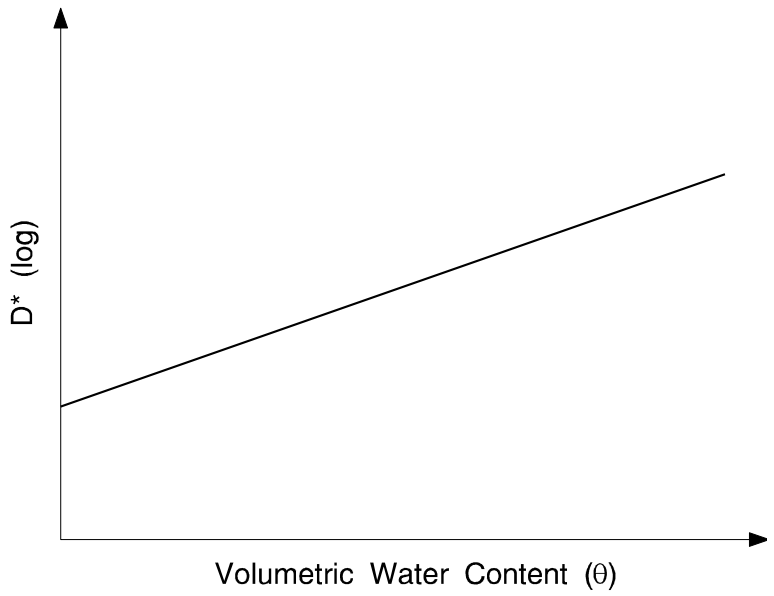

Figure 10-3 Relationship between D* and water content

10.6 Mass flux

CTRAN/W can compute the total mass flux across a user-specified section. The mass flux across a section is composed of four components; the dispersive mass flux Qdis, the advective mass flux Qadv, the stored mass flux Qsto, and the decayed mass flux Qdec. The total mass flux Q across a section is the sum of all four components, as represented by the following equation:

$$Q_{total} = Q_{dis} + Q_{adv} + Q_{sto} + Q_{dec}$$

10.7 Dispersive mass flux

The dispersive mass flux is computed in the same way as SEEP/W computes the water flux across a section. For full details see the Theory chapter of the SEEP/W Engineering Methodology book.

As described in the SEEP/W book, consider a mesh with only one element

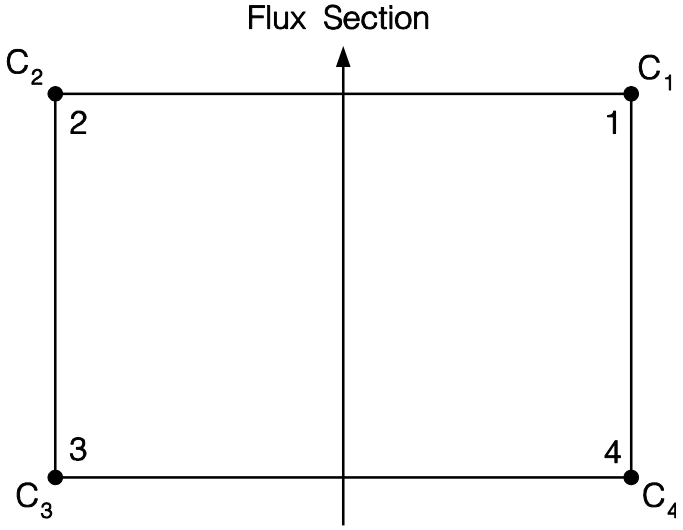

Figure 10-4 Illustration of mass flux section

The finite element equations of the dispersive mass flux term for one element can be expressed as follows:

$$\begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} \\ d_{21} & d_{22} & d_{23} & d_{24} \\ d_{31} & d_{32} & d_{33} & d_{34} \\ d_{41} & d_{42} & d_{43} & d_{44} \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{Bmatrix} = \begin{Bmatrix} Q_{dis\ 1} \\ Q_{dis\ 2} \\ Q_{dis\ 3} \\ Q_{dis\ 4} \end{Bmatrix}$$

The d coefficients in the above equation are a representation of the dispersion properties of the element. Therefore, the dispersive mass flux from Node i to Node j is:

$$Q_{dis\ ij} = d_{ij}C_i - d_{ji}C_j$$

The total dispersive mass flux through the flux section shown in Figure 10-4 is:

$$Q_{dis} = Q_{dis\ 21} + Q_{dis\ 24} + Q_{dis\ 31} + Q_{dis\ 34}$$

The imaginary flow lines from one side of the section to the other side are known as subsections. CTRAN/W identifies all subsections across a user-defined flux section, computes the mass flux along each subsection, and then sums the subsection values to obtain the total across the mass flux section.

10.8 Advective mass flux

Both the advective mass flux term and the boundary advective mass flux term are used in the advective mass flux calculations.

The finite element equations of the sum of the advective mass flux term and the boundary advective mass flux term for one element can be expressed as follows:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{Bmatrix} = \begin{Bmatrix} Q_{adv\ 1} \\ Q_{adv\ 2} \\ Q_{adv\ 3} \\ Q_{adv\ 4} \end{Bmatrix}$$

The a coefficients in the above equation are a representation of the advective properties of the element. Therefore, the advective mass flux from Node i to Node j is:

$$Q_{adv\ ij} = a_{ij}C_i - a_{ji}C_j$$

The total advective mass flux through the flux section shown in Figure 10-4 is:

$$Q_{adv} = Q_{adv\ 21} + Q_{adv\ 24} + Q_{adv\ 31} + Q_{adv\ 34}$$

10.9 Stored mass flux

The stored mass flux is computed in the same way as SEEP/W computes the stored flux across a section.

The finite element equations of the stored mass flux term for one element can be expressed as follows:

$$\frac{1}{\Delta t}\begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ s_{31} & s_{32} & s_{33} & s_{34} \\ s_{41} & s_{42} & s_{43} & s_{44} \end{bmatrix} \begin{Bmatrix} \Delta C_1 \\ \Delta C_2 \\ \Delta C_3 \\ \Delta C_4 \end{Bmatrix} = \begin{Bmatrix} Q_{sto\ 1} \\ Q_{sto\ 2} \\ Q_{sto\ 3} \\ Q_{sto\ 4} \end{Bmatrix}$$

where $\Delta C_1, \Delta C_{2,}, \Delta C_3$ and ΔC_4 are the changes of concentration at the various nodes between the start and the end of a time step. In general, the average change of concentration from Node i to Node j can be expressed as:

$$\Delta C_{ij} = \frac{\Delta C_i + \Delta C_j}{2}$$

Therefore, the stored mass flux from Node i to Node j due to a change in storage is:

$$Q_{sto\ ij} = \mathrm{s}_{ij}\frac{\Delta C_{ij}}{\Delta t}$$

The total stored mass flux through the flux section shown in Figure 10-4 is:

$$Q_{sto} = Q_{sto\ 21} + Q_{sto\ 24} + Q_{sto\ 31} + Q_{sto\ 34}$$

10.10 Decayed mass flux

Both the fluid-phase decayed mass flux term and the solid-phase decayed mass flux term are used in the decayed mass flux calculations.

For the fluid phase, the finite element equations of the decayed mass flux term for one element can be expressed as follows:

$$\begin{bmatrix} df_{11} & df_{12} & df_{13} & df_{14} \\ df_{21} & df_{22} & df_{23} & df_{24} \\ df_{31} & df_{32} & df_{33} & df_{34} \\ df_{41} & df_{42} & df_{43} & df_{44} \end{bmatrix} \begin{Bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{Bmatrix} = \begin{Bmatrix} Q_{fdec\ 1} \\ Q_{fdec\ 2} \\ Q_{fdec\ 3} \\ Q_{fdec\ 4} \end{Bmatrix}$$

The df coefficients in the above equation are a representation of the fluid phase decay properties of the element. Therefore, the fluid phase decay mass flux calculated at the mid-point of Node i and Node j is:

$$Q_{fdec\ ij} = df_{ij} \frac{(C_i + C_j)}{2}$$

As presented in the governing equation, the solid-phase decayed mass flux term is expressed in the form of nodal mass flux to be subtracted from the specified nodal total mass flux term. The nodal mass flux due to decay in the solid phase, Qsdec can be evaluated by the numerical integration of the solid phase decayed mass flux term.

Therefore, the solid-phase decayed mass flux calculated at the mid-point of Node i and Node j is:

$$Q_{sdec\ ij} = \frac{Q_{sdec\ i} + Q_{sdec\ j}}{2}$$

and, the total decayed mass flux at the mid-point of Node i and Node j is:

$$Q_{dec\ ij} = Q_{fdec\ ij} + Q_{sdec\ ij}$$

The total decayed mass flux through the flux section shown in Figure 10-4 is:

$$Q_{dec} = Q_{dec\ 21} + Q_{dec\ 24} + Q_{dec\ 31} + Q_{dec\ 34}$$

10.11 Mass quantity calculation

CTRAN/W computes the mass quantity in both the fluid phase, Mf, and the solid phase, Ms of an element by numerical integration of the following equations:

$$M_f = \int_v \Theta <N>^T <N>\, dv\ \{C\} \text{ and}$$

$$M_s = \int_v \rho_d <N>^T <N>\, dv\ \{S\}$$

In performing the numerical integration of the above equations, CTRAN/W computes the concentration at the Gauss point based on the nodal concentration and the interpolation function. The Gauss point concentration is then used to compute the Gauss point adsorption S from the adsorption function. The

volumetric water content Θ at each Gauss point is obtained from the material file generated by SEEP/W or VADOSE/W.

CTRAN/W computes the mass quantity at each Gauss point within an element. The Gauss point mass quantity is calculated based on a weighted distribution of the element mass quantity to the Gauss points. For the fluid phase, the distribution is weighted according to the product of $\Theta * C$ at each Gauss point. Similarly, for the solid phase, the distribution is weighted according to the adsorption S at each Gauss point.

The mass quantity of each element is then summed to give the total mass quantity in the flow problem.

10.12 Exit boundaries

A unique solution to the transport equation requires the specification of boundary conditions around the entire flow boundaries. In general, a boundary may be specified as a known concentration boundary or a known mass flux boundary. In certain cases, however, neither the concentration nor the mass flux is known, and, consequently, special considerations are required. This is the case at a boundary where mass leaves the flow system (i.e., an exit boundary).

Two approaches are available for dealing with exit boundaries. One is to ignore the dispersive portion of the mass flux and account only for the advective part of the flux (Qd=0). A second, more advanced alternative is to account for both dispersive and advective mass flux at the exit boundary (Qd>0).

Equation 10-10 includes the term,

$$\int_s \Theta D <N>^T \frac{\partial <N>}{\partial n} \, ds \, \{C\}$$

This term represents the dispersive mass flux across a flow boundary and is the natural boundary term derived as a result of the finite element formulation of the transport equation. The simplest option is to set this natural boundary term to zero at the exit boundary (Qd=0). This approach is sometimes referred to as a second type boundary condition. Setting the dispersive mass flux to zero has the effect of forcing the concentration gradient to zero at the exit boundary.

Frind (1988), has proposed a method whereby the natural boundary term is solved and both the dispersive and advective mass flux are accounted for at the exit boundary (Qd>0). This procedure results in what is referred to as a free exit boundary. CTRAN/W uses this method in solving for the natural boundary term.

With a free exit boundary, the nodes along the exit boundary do not behave like ordinary boundary nodes. Rather, they behave like all other internal nodes, making it possible to compute the concentration at these nodes without assuming a certain concentration of mass flux to the nodes.

The free exit approach does not force the concentration gradient to zero, as with the second type (i.e. zero dispersive mass flux) alternative. The effect of the two methods is illustrated in Figure 10-5. Note that the solutions from the two methods are the same except near the exit boundary that is specified on the right hand side of the flow problem.

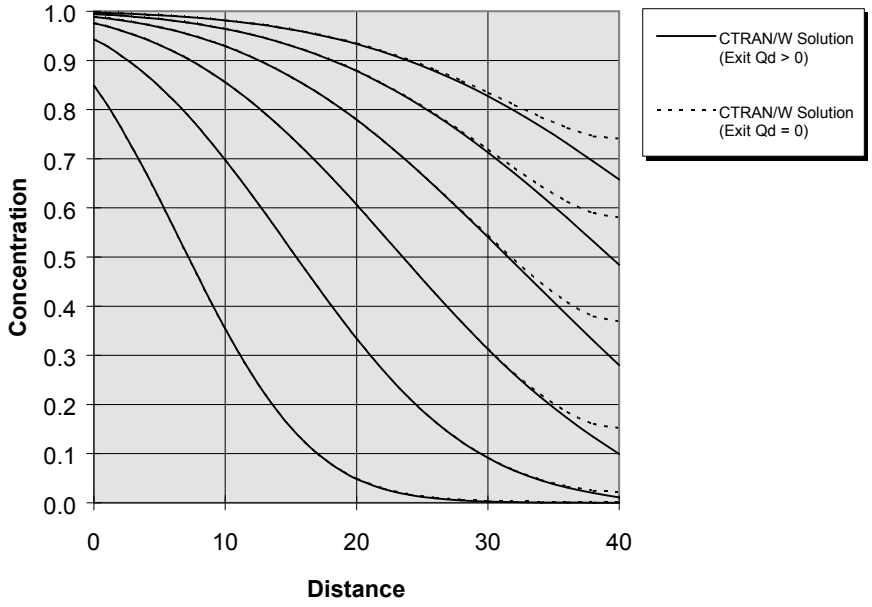

Figure 10-5 Comparison of concentration profiles computed with CTRAN/W for two exit boundary conditions

10.13 Particle tracking

It is difficult to solve the advection-dispersion finite element equation when the flow velocity is high and the dispersivity is low. In the limit when the diffusion coefficient D* and the dispersivity parameters α_L and α_T are set to zero, it is impossible to solve the advection-dispersion equation with the CTRAN/W general finite element formulation.

That said, CTRAN/W includes a separate particle tracking capability to analyze purely advective transport problems. Particles are introduced at the entrance or source boundaries. Particles are assumed to be attached to the water and to move in the direction of the water flow with the same speed as the water flow. The particle tracking feature can be used to determine where a particle of contaminant may end up and approximately how long it may take for a particle to arrive at a new position. A locus of the particle positions at all time steps depicts the migration path of the particle. It is also a means of producing a graphical representation of the migration of contaminant in a flow system with no dispersion, no adsorption and no decay.

The particle tracking process is conceptually simple and straightforward. At the start of the process, CTRAN/W locates the host element of each particle, then computes the average linear velocities vx and vy of each particle using the interpolating (or shape) functions evaluated at the coordinates of each particle. The size of the host element is also determined. The projection time step increment is determined based on the courant number criterion

For each projection time step increment, the change in position of each particle, Δ_x and Δ_y is then calculated according to the following equation:

$$\Delta x = \Delta t \; v_x$$

$$\Delta y = \Delta t \; v_y$$

where:

Δt = projection time step increment,

v_x = average linear velocity in the x direction, and

v_y = average linear velocity in the y direction.

The particle tracking process is repeated until your specified elapsed time has been reached or the particle has reached the boundary of the flow system.

CTRAN/W provides the option of tracking particles forward in the direction of water flow, or backward in the opposite direction toward the entrance or source boundaries. Backward tracking is accomplished by multiplying all linear velocities by -1.0. All computations are carried out in exactly the same way as for forward tracking. In forward tracking, particles stop at the exit boundaries, whereas in backward tracking, particles stop at the entrance or source boundaries. Therefore, forward tracking is useful in delineating the possible flow paths or contaminant plume from source boundaries, whereas the backward tracking option is useful in delineating the possible sources of contamination flowing to exit boundaries.

NOTE: Backward tracking is only possible in a steady-state flow system.

10.14 Density-dependent flow

Density-dependence refers to contaminant transport problems where the density of the contaminated water is significantly different than the density of the native groundwater. In these cases, the density contrast will affect the flow dynamics of the system. CTRAN/W allows the simulation of density-dependent transport problems by coupling with SEEP/W using an iterative procedure. VADOSE/W does not support density-dependent analysis. The density effect is accommodated by the addition of a body force term to the groundwater flow governing equation in SEEP/W. For more information about the body force term for density-dependent flow, see the Density-Dependent Flow section in the Theory chapter of the SEEP/W book.

Since the body force term is added to the seepage governing equation in SEEP/W, there is no special treatment to the finite element formulation in CTRAN/W for density-dependent flow. However, the solution procedure is different for density-dependent flow problems compared to advection-dispersion problems. For density-dependent problems, the groundwater velocities and concentrations must be solved for simultaneously at each time step because the groundwater velocities are dependent on contaminant density and the contaminant density is in turn dependent on concentration. At each time step, SEEP/W uses the contaminant concentrations to calculate the density body force term for the groundwater flow governing equation and then solves for equivalent freshwater heads and groundwater velocities. CTRAN/W then reads the groundwater velocities and solves for concentrations. Before proceeding to the next time step, the solution continues iteratively until the groundwater velocities and concentrations are compatible. The iterations are complete when either the percentage change in both the vector norm of nodal pressure head and nodal concentration are smaller than your specified convergence tolerances, or if the maximum number of your specified iterations are reached.

CTRAN/W assumes that density varies linearly with concentration. Therefore density-dependent problems require specification of the contaminant relative density, (density relative to freshwater), at some reference concentration. For example, the density of seawater is 1.025 times that of freshwater. Therefore the relative density value is specified as 1.025 at a reference concentration of 1.0. In this

particular case the reference concentration is a relative concentration representing 100% seawater. It should be noted that specification of the relative density at the reference concentration defines a linear variation of relative density with concentration. In the example given here, the relative density varies from 1.0 at a seawater concentration of zero, (freshwater), to 1.025 at a concentration of 1.0.

In order to have any density effect, there must be a density contrast between the contaminated water and freshwater. This means that the relative density of the contaminated fluid must be different (larger or smaller) than the density of freshwater. If there is no density contrast between the contaminated water and the freshwater, then the density body force term in the groundwater flow governing equation will be zero and the problem is essentially an advection-dispersion transport problem. The relative density and reference concentration values are specified in SEEP/W DEFINE under Key In Analysis Control.

10.15 Seepage solutions from SEEP/W or VADOSE/W or SIGMA/W

CTRAN/W relies on SEEP/W, VADOSE/W or SIGMA/W to provide the seepage solution in a transport analysis. You must have access to the other programs to undertake a transport analysis.

For practical purposes, CTRAN/W and the seepage model are allowed to have independent time step increments. However, depending on the type of analysis and the specified time step increments, CTRAN/W selects the appropriate seepage solution to be used in the transport analysis.

For a density-dependent flow problem, the seepage solution is computed by an iterative procedure controlled by CTRAN/W; therefore, the same time step increments must be used in both SEEP/W and CTRAN/W. To avoid redundancy, CTRAN/W makes use of the user-specified time step sequences in the CTRAN/W analysis settings.

For non-density-dependent flow problem (i.e., advection-dispersion transport and particle tracking), the seepage solutions must be computed using SEEP/W or VADOSE/W before launching CTRAN/W. In a steady-state seepage problem, CTRAN/W uses the steady-state seepage solutions for all time steps in the analysis. In a transient seepage problem with time step increments the same in both the seepage model and CTRAN/W, the seepage solution at the same time step is used in the transport analysis. However, in a transient seepage problem with different time step increments set up in analysis settings, CTRAN/W assumes that the seepage solution is constant within a time step increment. For example, assume that the seeepage elapsed times for Step 1, Step 2 and Step 3 are 50, 100 and 200 respectively. CTRAN/W uses the seepage solution of Step 1 for elapsed time between 0 and 50, the solution of Step 3 for elapsed time between 100 and 200 in the transport analysis.

CTRAN/W uses the seepage output file(s) with the highest elapsed time for all time steps that have an elapsed time greater than the highest seepage elapsed time. This allows a CTRAN/W analysis to be continued past the steady-state point in a seepage analysis.

References

Bear, J., 1979. Hydraulics of Groundwater. McGraw-Hill, London, England.

Daus, A.D., Frind, E.O., and Sudicky, E.A., 1983. Comparative Error Analysis in Finite Element Formulations of the Advection-Dispersion Equation. University of Waterloo.

Freeze, R.A., and Cherry, J.A., 1979. Groundwater. Prentice-Hall.

Frind, E.O., 1988. Solution of the Advection-Dispersion Equation with Free Exit Boundary. Numerical Methods for Partial Differential Equations. 4, John Wiley & Sons, Inc.

Frind, E.O., and Pinder, G.F., 1982. The Principal Direction Technique for Solution of the Advection-Dispersion Equation. Proceedings of 10th World Congress of the IMACS, Concordia University, Montreal, Canada.

Kemper, W.D., and Van Shaik, J.C., 1966. Diffusion of Salts in Clay-Water Systems. Soil Science of America Proceedings, Vol.30.

Lancaster, P., and Salkauskas, K., 1986. Curve and Surface Fitting: An Introduction. Academic Press.

Marsily, Ghislain de., 1986. Quantitative Hydrogeology: Groundwater Hydrology for Engineers. Academic Press.

Ogata, A., 1970. Theory of Dispersion in a Granular Medium. Fluid Movement in Earth Materials. Geological Survey Professional Paper 411-I. U.S. Government Printing Office, Washington.

Salkauskas, K., 1974. C' Splines For Interpolation of Rapidly Varying Data. Rocky Mountain Journal of Mathematics, Vol. 14, No. 1.

Segerlind, L.J., 1984. Applied Finite Element Analysis. John Wiley and Sons.

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Consistent sets of units

Parameter	Symbol	Units (SI)	Units (Imperial)
Length	*L*	m	ft
Time	*t*	s	hr
Force	*F*	kN	lb_f
Mass	*M*	g	lb
Pressure	F/L^2	kN/m^2	psf
Unit Weight of Water	F/L^3	kN/m^3	pcf
Hydraulic Conductivity	*L/T*	m/s	ft/hr
Concentration	M/L^3	g/m^3	lb/ft^3
Diffusion Coefficient	L^2/T	m^2/s	ft^2/hr
α_L and α_T (dispersivity)	*L*	m	ft
Decay Half-Life	*T*	sec	hr
S (adsorption)	*M/M*	g/g	lb/lb
Density	M/L^3	g/m^3	lb/ft^3
Mass Flux	*M/T*	g/s	lb/hr