



Vadose Zone Modeling with VADOSE/W

An Engineering Methodology

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1 Introduction

The flow of water through soil is one of the fundamental issues in geotechnical and geo-environmental engineering. In fact, if water were not present in the soil, there would not be a need for geotechnical engineering. This is a nonsensical statement: if there were no water in the soil, there would be no way to sustain an ecosystem, no humans on earth and no need for geotechnical and geo-environmental engineering. However, the statement does highlight the importance of water in working with soil and rock.

Flow quantity is often considered to be the key parameter in quantifying seepage losses from a reservoir or determining the amount of water available for domestic or industrial use. In engineering, the more important issue is the pore-water pressure. The emphasis should not be on how much water is flowing through the ground, but on the state of the pore-water pressure in the ground. The pore-water pressure, whether positive or negative, has a direct bearing on the shear strength and volume change characteristics of the soil. Research in the last few decades has shown that even the flow of moisture in the unsaturated soil near the ground surface is directly related to the soil suction (negative water pressure). So, even when flow quantities are the main interest, it is important to accurately establish the pore-water pressures.

In the past, the analyses related to groundwater have concentrated on saturated flow. As a result, flow problems were typically categorized as being confined and unconfined situations, such as confined or unconfined aquifers. Flow beneath a structure would be a confined flow problem, while flow through a homogeneous embankment would be unconfined flow. Historically speaking, unconfined flow problems were more difficult to analyze because the analysis required determining the phreatic surface. The phreatic surface was considered an upper boundary and any flow that may have existed in the capillarity zone above the phreatic line was ignored.

It is no longer acceptable to take a simplified approach and ignore unsaturated flow above the phreatic surface. Not only does it ignore an important component of moisture flow in soils, but it greatly limits the types of problems that can be analyzed. It is mandatory to deal with unsaturated flow in typical situations such as modeling infiltration of precipitation. Transient flow problems are another good example. It is nearly impossible to model a situation where a wetting front moves through an earth structure without correctly considering the unsaturated component of flow. Fortunately, it is no longer necessary to ignore the unsaturated zone. With the help of this document and the associated software, unsaturated flow can be considered in numerical modeling and the door is opened to analyzing almost any kind of seepage problem.

The term *seepage* usually refers to situations where the primary driving force is gravity controlled, such as establishing seepage losses from a reservoir, where the driving force is the total hydraulic head difference between the entrance and exit points. Another cause of water movement in soils is the existence of excess pore-water pressure due to external loading. This type of water flow is usually not referred to as seepage, but the fundamental mathematical equations describing the water movement are essentially identical. As a result, a software formulation for the analysis of seepage problems can also be used to analyze the dissipation of excess pore-water pressures resulting from changes in stress conditions. In the context of the discussions and examples in this document and in using the VADOSE/W software, the term seepage is used to describe all movement of water through soil regardless of the creation or source of the driving force or whether the flow is through saturated or unsaturated soils.

Balancing the sun's energy at the ground surface

The energy from the sun drives the physical processes that occur at the ground surface. Figure 1-1 shows a brief example of how this energy is balanced within VADOSE/W.

The sun's energy is driving the evaporation and transpiration processes. The following example describes how this energy may be distributed and accounted for in VADOSE/W.

Let us assume the sun applies an energy of 20 MJ/day/m² to the ground surface. This energy is the equivalent of approximately 8.15 mm/day of potential evaporated water (VADOSE/W will calculate the actual value based on climate data or the user can input this value if they have measured data).

If a combination of plants and bare ground exists at the surface, then this energy must be partitioned between the two. Assume the Leaf Area Index function for the plants indicates that there is significant but not total leaf coverage of the surface. Based on relationships discussed in subsequent pages of this manual, VADOSE/W determines that, for example, 6 mm/day of Potential Energy is intercepted by the plants and 2.15 mm/day is intercepted by the ground.

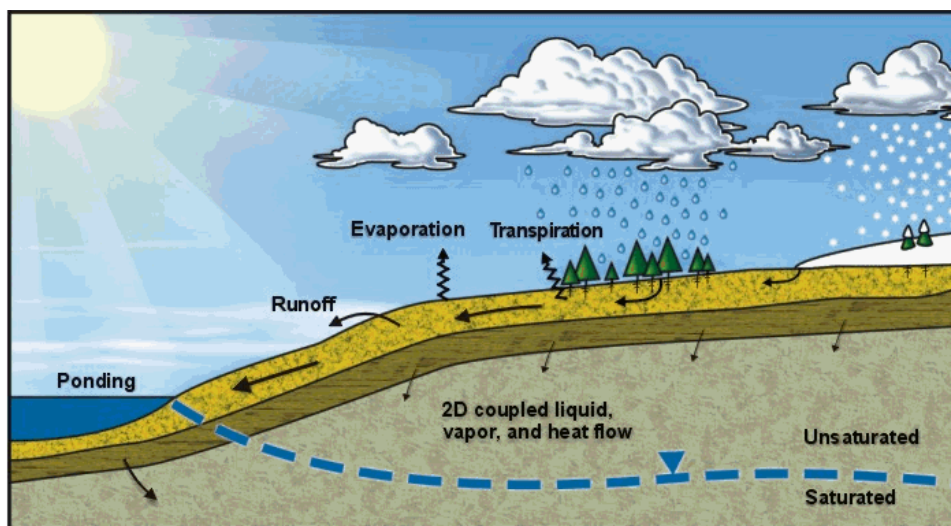


Figure 1-1 Physical processes relating to seepage

Now assume the ground is not fully saturated at the surface. Because it is not saturated, the ground can not give up water to the sun at the full potential rate. Based on the Penman-Wilson (1990, 1994) method, VADOSE/W determines that of the 2.15 mm/day Potential Evaporation, only 1.15 mm/day actually evaporates (AE).

Assuming in addition, that the ground beneath the surface is not fully saturated, the plant moisture limiting function, which deals with wilting pore pressures among other things, is used by the program to determine that the plant roots can only transpire 3 mm/day of the potential 6 mm/day intercepted by the leaves on surface.

So, we have 8.15 mm/day of potential evaporative energy (PE) being demanded at the ground surface and only 1.15 mm/day actually evaporates (AE). The plants were able to transpire 3mm/day (AT). The question that remains is; what happened to the other 4 mm/day?

Since we must balance the energy, we can not ignore this 4 mm/day. It is the extra 4 mm/day of previously unaccounted energy that results in heating of the ground surface.

VADOSE/W accounts for all of these physical processes based on first principle physics. The user is not required to make any assumptions about how the energy is partitioned or applied.

Actual evaporation

The key to geotechnical modeling of the vadose zone is the ability to accurately predict the surface boundary condition. The most significant variable to quantify is the magnitude of surface infiltration and actual evaporation, or in modeling terms, the surface unit flux boundary. VADOSE/W determines this value by coupling the moisture and heat stress states at the ground surface with climate conditions present above the ground surface. Vapor flow in the soil is mandatory and is included in VADOSE/W.

It is not acceptable to have actual evaporation (AE) computed as a function of drying time or soil water content. Actual evaporation must be computed as a function of soil surface negative water pressure; a stress state variable, and climate parameters.

Typical applications

Typical applications for VADOSE/W include:

- designing single or multi layered soil covers over mine waste and municipal landfill disposal sites;
- obtaining climate controlled soil pore pressures on natural slopes or man made covered slopes for use in stability analysis;
- determining infiltration and evaporation and plant transpiration from agricultural irrigation projects etc.

VADOSE/W can be used wherever accurate surface boundary conditions are required.

1.1 Overview of this book

Modeling the flow of water 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. Furthermore, when a soil becomes unsaturated, the coefficient of permeability or hydraulic conductivity becomes a function of the negative pore-water pressure in the soil. The pore-water pressure is the primary unknown and needs to be determined, so iterative numerical techniques are required to match the computed pore-water pressure and the material property, which makes the solution highly non-linear. These complexities make it necessary to use some form of numerical analysis to analyze seepage problems for all, but the simplest cases. A common approach is to use finite element formulations and VADOSE/W, the subject of this book, is an example of a numerical software tool.

While part of this document is about using VADOSE/W to do seepage 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 VADOSE/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 fundamental physical concepts. 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 are required to become comfortable with these aspects of numerical modeling.

A large portion of this book focuses on the general guidelines of how to conduct effective numerical modeling. Chapter 2, Numerical Modeling: What, Why and How, is devoted exclusively to discussions on this topic. The general principles discussed apply to all numerical modeling situations, but are used in the context of seepage analyses in this document.

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. Separate chapters have been devoted to each of these three key components within this document.

Part of the Analysis Settings chapter is dedicated to using VADOSE/W in a one dimensional mode. There are unique model settings that will help with the numerical solution when the mesh is a one dimensional column. There are also a few key concepts to understand regarding runoff and lateral flow that have significance in this 1D mode.

Saturated and unsaturated seepage numerical modeling is a highly non-linear problem that requires iterative techniques to obtain solutions. Numerical convergence is consequently a key issue. Also, the temporal integration scheme, which is required for a transient analysis, is affected by time step size relative to element size and material properties. These and other numerical considerations are discussed in the chapter called Numerical Issues.

One chapter is dedicated to presenting and discussing illustrative examples.

A full chapter is dedicated to theoretical issues associated with climate-ground coupling and the finite element solution of the partial differential flow equation for saturated and unsaturated heat and water flow in soils. Additional finite element numerical details regarding interpolating functions and infinite elements are given in Appendix A.

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 modelling method or to help gain confidence and develop a deeper understanding of finite element methods, VADOSE/W conventions or data results. It also contains a checklist of key vadose zone modeling issues that you can print out and use to check that you are on the right path to solving a successful model.

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

2 Numerical Modeling: What, Why and How

2.1 Introduction

The unprecedented computing power now available has resulted in advanced software products for engineering and scientific analysis. The ready availability and ease-of-use of these products makes it possible to use powerful techniques such as a finite element analysis in engineering practice. These analytical methods have now moved from being research tools to application tools. This has opened a whole new world of numerical modeling.

Software tools such as VADOSE/W do not inherently lead to good results. While the software is an extremely powerful calculator, obtaining useful and meaningful results from this useful tool depends on the guidance provided by the user. It is the user's understanding of the input and their ability to interpret the results that make it such a powerful tool. In summary, the software does not do the modeling, the user does the modeling. The software only provides the ability to do highly complex computations that are not otherwise humanly possible. In a similar manner, modern day spreadsheet software programs can be immensely powerful as well, but obtaining useful results from a spreadsheet depends on the user. It is the user's ability to guide the analysis process that makes it a powerful tool. The spreadsheet can do all the mathematics, but it is the user's ability to take advantage of the computing capability that leads to something meaningful and useful. The same is true with finite element analysis software such as VADOSE/W.

Numerical modeling is a skill that is acquired with time and experience. Simply acquiring a software product does not immediately make a person a proficient modeler. Time and practice are required to understand the techniques involved and learn how to interpret the results.

Numerical modeling as a field of practice is relatively new in geotechnical engineering and, consequently, there is a lack of understanding about what numerical modeling is, how modeling should be approached and what to expect from it. A good understanding of these basic issues is fundamental to conducting effective modeling. Basic questions such as, What is the main objective of the analysis?, What is the main engineering question that needs to be answered? and, What is the anticipated result?, need to be decided before starting to use the software. Using the software is only part of the modeling exercise. The associated mental analysis is as important as clicking the buttons in the software.

This chapter discusses the “what”, “why” and “how” of the numerical modeling process and presents guidelines on the procedures that should be followed in good numerical modeling practice.

2.2 What is a numerical model?

A numerical model is a mathematical simulation of a real physical process. SEEP/W, like VADOSE/W, is a numerical model that can mathematically simulate the real physical process of water flowing through a particulate medium. Numerical modeling is purely mathematical and in this sense is very different than scaled physical modeling in the laboratory or full-scaled field modeling.

While VADOSE/W deals with heat, mass and vapour flow, much of the discussion in this chapter focuses on seepage analysis only. This simplifies the discussion and also permits comparisons to be made with more commonly known and anticipated behaviour.

Rulon (1985) constructed a scale model of a soil slope with a less permeable layer embedded within the slope and then sprinkled water on the crest to simulate infiltration or precipitation. Instruments were inserted into the soil through the side walls to measure the pore-water pressures at various points. The

results of her experiment are shown in Figure 2-1. Modeling Rulon's laboratory experiment with SEEP/W gives the results presented in Figure 2-2, which are almost identical to the original laboratory measurements. The positions of the equipotential lines are somewhat different, but the position of the water table is the same. In both cases there are two seepage exit areas on the slope, which is the main important observation in this case.

The fact that mathematics can be used to simulate real physical processes is one of the great wonders of the universe. Perhaps physical processes follow mathematical rules, or mathematics has evolved to describe physical processes. Obviously, we do not know which came first, nor does it really matter. Regardless of how the relationship developed, the fact that we can use mathematics to simulate physical processes leads to developing a deeper understanding of physical processes. It may even allow for understanding or discovering previously unknown physical processes.

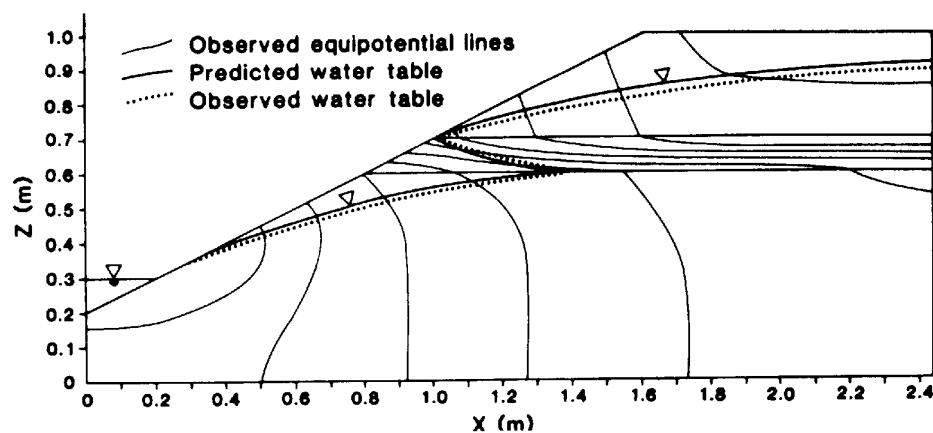


Figure 2-1 Rulon's laboratory scaled model results

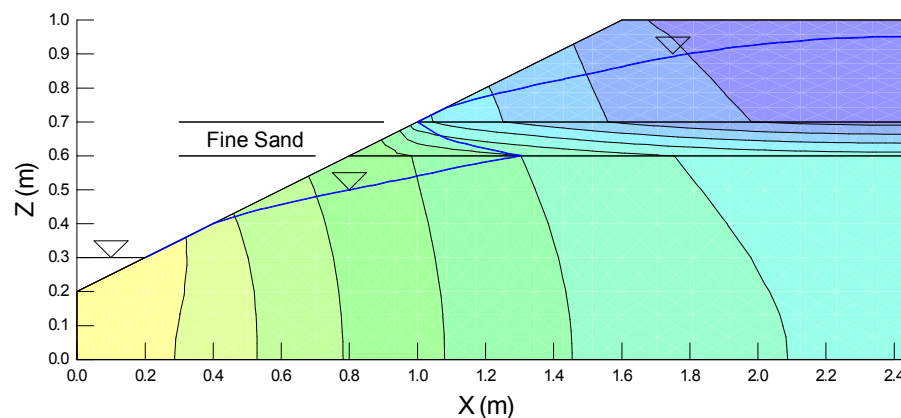


Figure 2-2 SEEP/W analysis of Rulon's laboratory model

Numerical modeling has many advantages over physical modeling. The following are some of the more obvious advantages.

Numerical models can be set up very quickly relative to physical models. Physical models may take months to construct while a numerical model can be constructed in minutes, hours or days.

A physical model is usually limited to a narrow set of conditions. A numerical model can be used to investigate a wide variety of different scenarios.

Numerical models have no difficulty accounting for gravity. Gravity cannot be scaled, which is a limitation with laboratory modeling. A centrifuge is often required to overcome this limitation.

With numerical modeling, there is no danger of physical harm to personnel. Physical modeling sometimes involves heavy equipment and worker safety is consequently a concern.

Numerical modeling provides information and results at any location within the cross-section. Physical modeling only provides external visual responses and data at discrete instrumented points.

Numerical models can accommodate a wide variety of boundary conditions, whereas physical models are often limited in the types of boundary conditions possible.

It would be wrong to think that numerical models do not have limitations. Associated with seepage flow there may also be temperature changes, volume changes and perhaps chemical changes. Including all these processes in the same formulation is not possible, as the mathematics involved simply become too complex. In addition, it is not possible to mathematically describe a constitutive relationship, due to its complexity. Some of these difficulties can and will be overcome with greater and faster computer processing power. It is important to understand that numerical modeling products will have limitations that are related to the current capability of hardware or integral to the formulation of the software, since it was developed to consider specific conditions. SEEP/W is formulated only for flow that follows Darcy's Law. Near the ground surface moisture may leave the ground as vapor. This component is not included in the SEEP/W formulation, like it is in VADOSE/W. Consequently, SEEP/W has limitations when it comes to modeling moisture leaving the system at the ground surface. VADOSE/W does not have this type of limitation.

The important point to remember is that the mathematical formulations implemented in software like VADOSE/W result in a very powerful and versatile means of simulating real physical processes.

“A mathematical model is a replica of some real-world object or system. It is an attempt to take our understanding of the process (conceptual model) and translate it into mathematical terms.” National Research Council Report (1990).

2.3 Modeling in geotechnical engineering

The role and significance of analysis and numerical modeling in geotechnical engineering has been vividly illustrated by Professor John Burland, Imperial College, London (UK). In 1987 Professor Burland presented what is known as the Nash Lecture. The title of the lecture was “The Teaching of Soil Mechanics – a Personal View”. In this lecture he advocated that geotechnical engineering consists of three fundamental components: the ground profile, the soil behavior and modeling. He represented these components as the apexes of a triangle, as illustrated in Figure 2-3. This has come to be known as the Burland triangle (Burland, 1987; Burland, 1996).

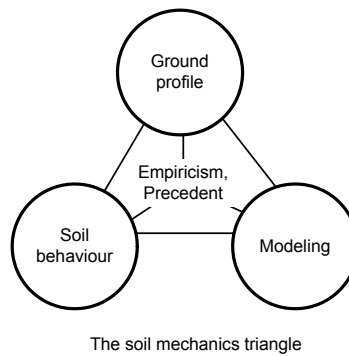


Figure 2-3 The Burland triangle (after Burland 1996)

The soil behavior component includes laboratory tests, *in situ* tests and field measurements. The ground profile component basically involves site characterization: defining and describing the site conditions. Modeling may be conceptual, analytical or physical.

Of great significance is that, in Burland's view, all three components need to be tied together by empiricism and precedent. This is the part inside the triangle.

The Burland triangle idea has been widely discussed and referred to by others since it was first presented. An article on this topic was presented in an issue of *Ground Engineering* (Anon. 1999). Morgenstern (2000) discussed this at some length in his keynote address titled "Common Ground" at the GeoEng2000 Conference in Melbourne Australia in 2000. With all the discussion, the triangle has been enhanced and broadened somewhat, as shown in Figure 2-4.

One important additional feature has been to consider all the connecting arrows between the components as pointing in both directions. This simple addition highlights the fact that each part is distinct yet related to all the other parts.

The Burland triangle vividly illustrates the importance of modeling in geotechnical engineering. Characterizing the field conditions and making measurements of behavior is not sufficient. Ultimately, it is necessary to do some analysis of the field information and soil properties to complete the triangle.

As Burland pointed out, modeling may be conceptual, analytical or physical. However, with the computing power and software tools now available, modeling often refers to numerical modeling. Accepting that modeling primarily refers to numerical modeling, the Burland triangle shows the importance that numerical modeling has in geotechnical engineering.

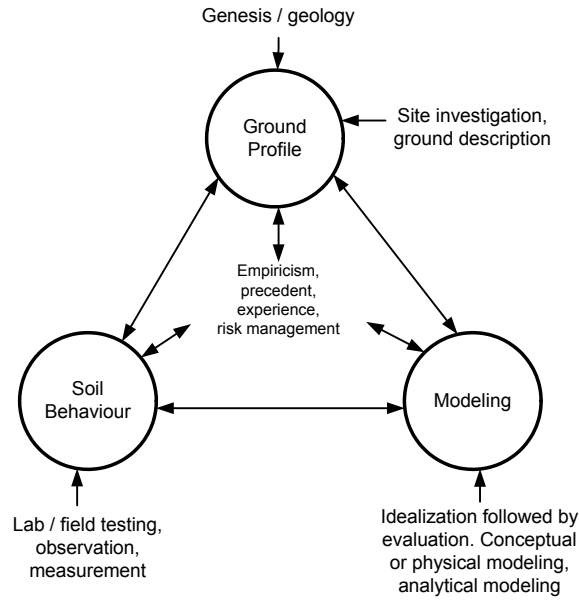


Figure 2-4 The enhanced Burland triangle (after Anon. 1999)

Making measurements and characterizing site conditions is often time consuming and expensive. This is also true with modeling, if done correctly. A common assumption is that the numerical modeling component is only a small component that should be undertaken at the end of a project, and that it can be done simply and quickly. This is somewhat erroneous. Good numerical modeling, as we will see later in the section in more detail, takes time and requires careful planning in the same manner that it takes time and planning to collect field measurements and adequately characterize site conditions.

Considering the importance of modeling that the Burland triangle suggests for geotechnical engineering, it is prudent that we do the modeling carefully and with a complete understanding of the modeling processes. This is particularly true with numerical modeling. The purpose of this book is to assist with this aspect of geotechnical engineering.

2.4 Why model?

The first reaction to the question, “why model?” seems rather obvious. The objective is to analyze the problem. Upon more thought, the answer becomes more complex. Without a clear understanding of the reason for modeling or identifying what the modeling objectives are, numerical modeling can lead to a frustrating experience and uncertain results. As we will see in more detail in the next section, it is wrong to set up the model, calculate a solution and then try to decide what the results mean. It is important to decide at the outset the reason for doing the modeling. What is the main objective and what is the question that needs to be answered?

The following points are some of the main reasons for modeling, from a broad, high level perspective. We model to:

- make quantitative predictions,
- compare alternatives,
- identify governing parameters, and
- understand processes and train our thinking.

Quantitative predictions

Most engineers, when asked why they want to do some modeling, will say that they want to make a prediction. They want to predict the seepage quantity, for example, or the time for a contaminant to travel from the source to a seepage discharge point, or the time required from first filling a reservoir until steady-state seepage conditions have been established in the embankment dam. The desire is to say something about future behavior or performance.

Making quantitative predictions is a legitimate reason for doing modeling. Unfortunately, it is also the most difficult part of modeling, since quantitative values are often directly related to the material properties. The quantity of seepage, for example, is in large part controlled by the hydraulic conductivity and, as a result, changing the hydraulic conductivity by an order of magnitude will usually change the computed seepage quantity by an order of magnitude. The accuracy of quantitative prediction is directly related to the accuracy of the hydraulic conductivity specified. Unfortunately, for a heterogeneous profile, there is not a large amount of confidence about how precisely the hydraulic conductivity can be specified. Sometimes defining the hydraulic conductivity within an order of magnitude is considered reasonable. The confidence you have defining the hydraulic conductivity depends on many factors, but the general difficulty of defining this soil parameter highlights the difficulty of undertaking modeling to make quantitative predictions.

Carter et al. (2000) presented the results of a competition conducted by the German Society for Geotechnics. Packages of information were distributed to consulting engineers and university research groups. The participants were asked to predict the lateral deflection of a tie-back shoring wall for a deep excavation in Berlin. During construction, the actual deflection was measured with inclinometers. Later the predictions were compared with the actual measurements. Figure 2-5 shows the best eleven submitted predictions. Other predictions were submitted, but were considered unreasonable and consequently not included in the summary.

There are two heavy dark lines superimposed on Figure 2-5. The dashed line on the right represents the inclinometer measurements uncorrected for any possible base movement. It is likely the base of the inclinometer moved together with the base of the wall. Assuming the inclinometer base moved about 10 mm, the solid heavy line in Figure 2-5 has been shifted to reflect the inclinometer base movement.

At first glance one might quickly conclude that the agreement between prediction and actual lateral movement is very poor, especially since there appears to be a wide scatter in the predictions. This exercise might be considered as an example of our inability to make accurate quantitative predictions.

However, a closer look at the results reveals a picture that is not so bleak. The depth of the excavation is 32 m. The maximum predicted lateral movement is just over 50 mm or 5 cm. This is an extremely small amount of movement over the length of the wall – certainly not big enough to be visually noticeable. Furthermore, the actual measurements, when corrected for base movement fall more or less in the middle of the predictions. Most important to consider are the trends presented by many of the predicted results. Many of them predict a deflected shape similar to the actual measurements. In other words, the predictions simulated the correct relative response of the wall.

Consequently, we can argue that our ability to make accurate predictions is poor, but we can also argue that the predictions are amazingly good. The predictions fall on either side of the measurements and the deflected shapes are correct. In the end, the modeling provided a correct understanding of the wall behavior, which is more than enough justification for doing the modeling, and may be the greatest benefit of numerical modeling, as we will see in more detail later.

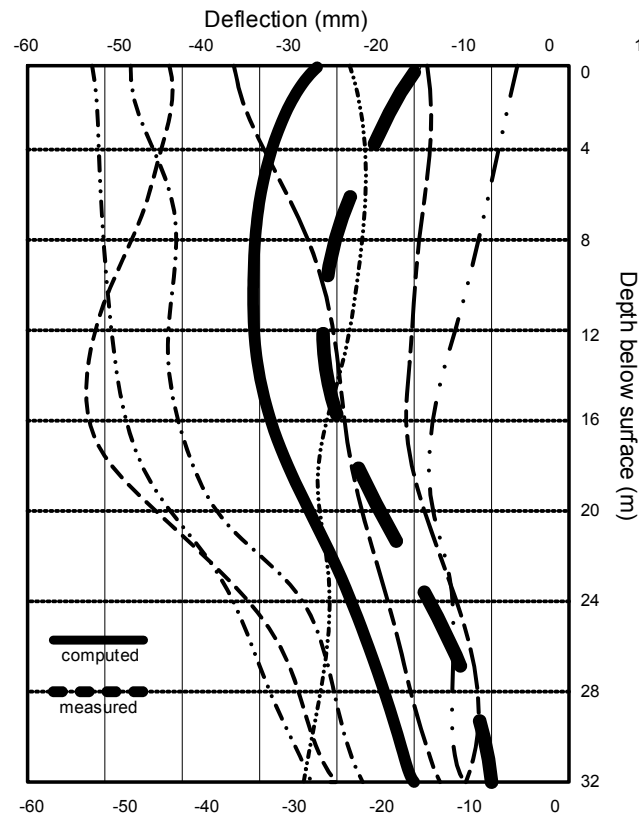


Figure 2-5 Comparison of predicted and measured lateral movements of a shoring wall (after Carter et al, 2000)

Numerical modeling is sometimes dismissed as being useless due to the difficulty with defining material properties. There are, however, other reasons for doing numerical modeling. If some of the other objectives of numerical modeling are completed first, then quantitative predictions often have more value and meaning. Once the physics and mechanisms are completely understood, quantitative predictions can be made with a great deal more confidence and are not nearly as useless as first thought, regardless of our inability to accurately define material properties.

Compare alternatives

Numerical modeling is useful for comparing alternatives. Keeping everything else the same and changing a single parameter makes it a powerful tool to evaluate the significance of individual parameters. For modeling alternatives and conducting sensitivity studies it is not all that important to accurately define some material properties. All that is of interest is the change between simulations.

Consider the example of a cut-off wall beneath a structure. With SEEP/W it is easy to examine the benefits obtained by changing the length of the cut-off. Consider two cases with different cut-off depths to assess the difference in uplift pressures underneath the structure. Figure 2-6 shows the analysis when the cutoff is 10 feet deep. The pressure drop and uplift pressure along the base are shown in the left graph in Figure 2-7. The drop across the cutoff is from 24 to 18 feet of pressure head. The results for a 20-foot cutoff are shown in Figure 2-7 on the right side. Now the drop across the cutoff is from 24 to about 15 feet of pressure head. The uplift pressures at the downstream toe are about the same.

The actual computed values are not of significance in the context of this discussion. It is an example of how a model such as SEEP/W can be used to quickly compare alternatives. Secondly, this type of analysis can be done with a rough estimate of the conductivity, since in this case the pressure distributions will be unaffected by the conductivity assumed. There would be no value in carefully defining the conductivity to compare the base pressure distributions.

We can also look at the change in flow quantities. The absolute flow quantity may not be all that accurate, but the change resulting from various cut-off depths will be of value. The total flux is $6.26 \times 10^{-3} \text{ ft}^3/\text{s}$ for the 10-foot cutoff and $5.30 \times 10^{-3} \text{ ft}^3/\text{s}$ for the 20-foot cutoff, only about a 15 percent difference.

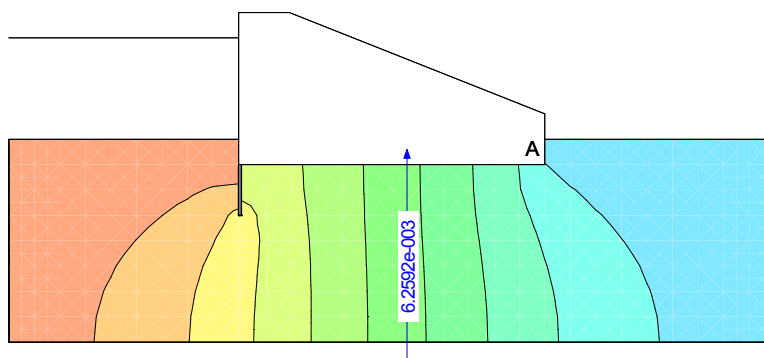


Figure 2-6 Seepage analysis with a cutoff

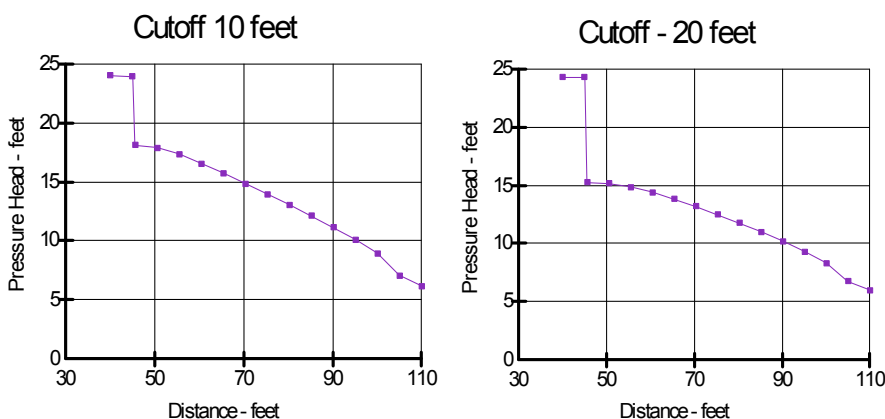


Figure 2-7 Uplift pressure distributions along base of structure

Identify governing parameters

Numerical models are useful for identifying critical parameters in a design. Consider the performance of a soil cover over waste material. What is the most important parameter governing the behavior of the cover? Is it the precipitation, the wind speed, the net solar radiation, plant type, root depth or soil type? Running a series of VADOSE/W simulations, keeping all variables constant except for one makes it possible to identify the governing parameter. The results can be presented as a tornado plot such as shown in Figure 2-8.

Once the key issues have been identified, further modeling to refine a design can concentrate on the main issues. If, for example, the vegetative growth is the main issue then efforts can be concentrated on what needs to be done to foster the plant growth.

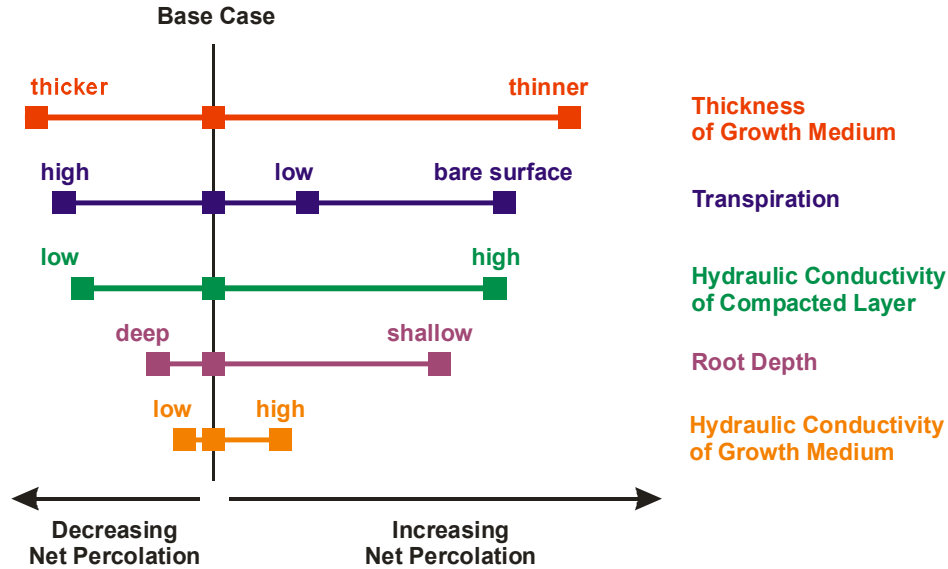


Figure 2-8 Example of a tornado plot (O'Kane, 2004)

Discover & understand physical process - train our thinking

One of the most powerful aspects of numerical modeling is that it can help us to understand physical processes in that it helps to train our thinking. A numerical model can either confirm our thinking or help us to adjust our thinking if necessary.

To illustrate this aspect of numerical modeling, consider the case of a multilayered earth cover system such as the two possible cases shown in Figure 2-9. The purpose of the cover is to reduce the infiltration into the underlying waste material. The intention is to use the earth cover layers to channel any infiltration downslope into a collection system. It is known that both a fine and a coarse soil are required to achieve this. The question is, should the coarse soil lie on top of the fine soil or should the fine soil overlay the coarse soil? Intuitively it would seem that the coarse material should be on top; after all, it has the higher conductivity. Modeling this situation with VADOSE/W, which handles unsaturated flow, can answer this question and verify if our thinking is correct.

For unsaturated flow, it is necessary to define a *hydraulic conductivity function*: a function that describes how the hydraulic conductivity varies with changes in suction (negative pore-water pressure = suction). Chapter 4, Material Properties, describes in detail the nature of the hydraulic conductivity (or permeability) functions. For this example, relative conductivity functions such as those presented in Figure 2-10 are sufficient. At low suctions (i.e., near saturation), the coarse material has a higher hydraulic conductivity than the fine material, which is intuitive. At high suctions, the coarse material has the lower conductivity, which often appears counterintuitive. For a full explanation of this relationship, refer to Chapter 4, Materials Properties. For this example, accept that at high suctions the coarse material is less conductive than the fine material.

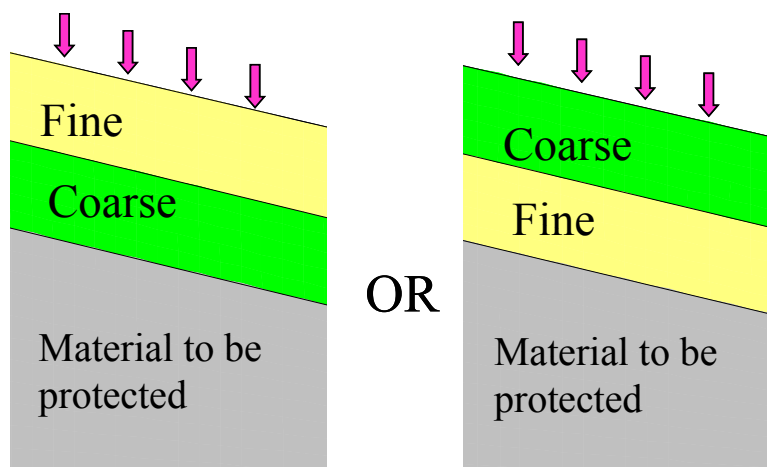


Figure 2-9 Two possible earth cover configurations

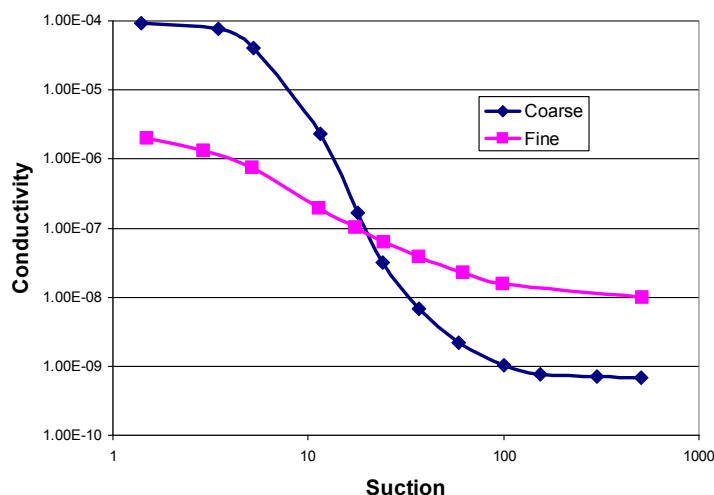


Figure 2-10 Hydraulic conductivity functions

After conducting various analyses and trial runs with varying rates of surface infiltration, it becomes evident that the behavior of the cover system is dependent on the infiltration rate. At low infiltration rates, the effect of placing the fine material over the coarse material results in infiltration being drained laterally through the fine layer, as shown in Figure 2-11. This accomplishes the design objective of the cover. If the precipitation rate becomes fairly intensive, then the infiltration drops through the fine material and drains laterally within the lower coarse material as shown in Figure 2-12. The design of fine soil over coarse soil may work, but only in arid environments. The occasional cloud burst may result in significant water infiltrating into the underlying coarse material, which may result in increased seepage into the waste. This may be a tolerable situation for short periods of time. If most of the time precipitation is modest, the infiltration will be drained laterally through the upper fine layer into a collection system.

So, for an arid site the best solution is to place the fine soil on top of the coarse soil. This is contrary to what one might expect at first. The first reaction may be that something is wrong with the software, but it may be that our understanding of the process and our general thinking that is flawed.

A closer examination of the conductivity functions provides a logical explanation. The software is correct and provides the correct response given the input parameters. Consider the functions in Figure 2-13.

When the infiltration rate is large, the negative water pressures or suctions will be small. As a result, the conductivity of the coarse material is higher than the finer material. If the infiltration rates become small, the suctions will increase (water pressure becomes more negative) and the unsaturated conductivity of the finer material becomes higher than the coarse material. Consequently, under low infiltration rates it is easier for the water to flow through the fine, upper layer soil than through the lower more coarse soil.

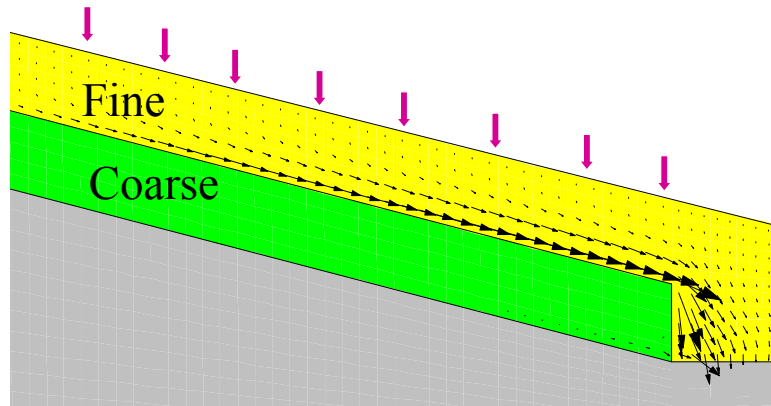


Figure 2-11 Flow diversion under low infiltration

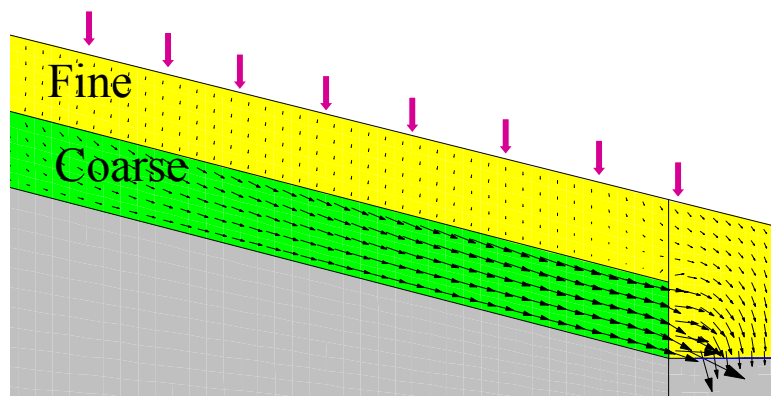


Figure 2-12 Flow diversion under high infiltration

This type of analysis is a good example where the ability to utilize a numerical model greatly assists our understanding of the physical process. The key is to think in terms of unsaturated conductivity as opposed to saturated conductivities.

Numerical modeling can be crucial in leading us to the discovery and understanding of real physical processes. In the end the model either has to conform to our mental image and understanding or our understanding has to be adjusted.

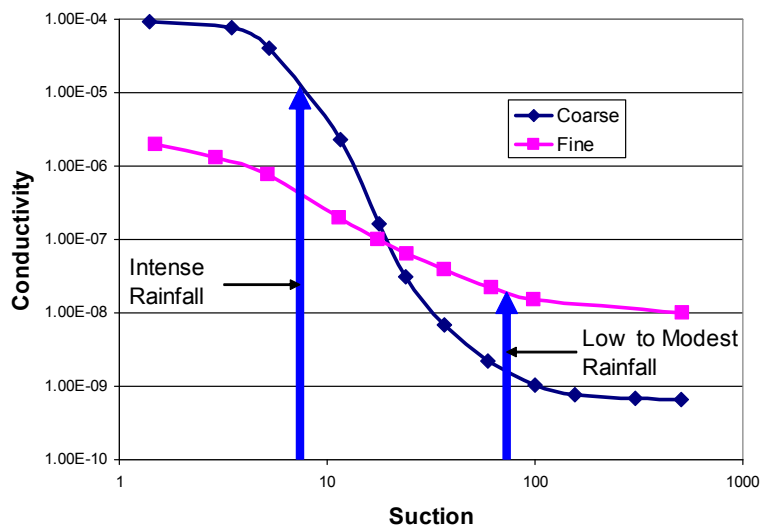


Figure 2-13 Conductivities under low and intense infiltration

This is a critical lesson in modeling and the use of numerical models in particular. The key advantage of modeling, and in particular the use of computer modeling tools, is the capability it has to enhance engineering judgment, not the ability to enhance our predictive capabilities. While it is true that sophisticated computer tools greatly elevated our predictive capabilities relative to hand calculations, graphical techniques, and closed-form analytical solutions, still, prediction is not the most important advantage these modern tools provide. Numerical modeling is primarily about ‘process’ - not about prediction.

“The attraction of ... modeling is that it combines the subtlety of human judgment with the power of the digital computer.” Anderson and Woessner (1992).

2.5 How to model

Numerical modeling involves more than just acquiring a software product. Running and using the software is an essential ingredient, but it is a small part of numerical modeling. This section talks about important concepts in numerical modeling and highlights important components in good modeling practice.

Make a guess

Generally, careful planning is involved when undertaking a site characterization or making measurements of observed behavior. The same careful planning is required for modeling. It is inappropriate to acquire a software product, input some parameters, obtain some results, and then decide what to do with the results or struggle to decide what the results mean. This approach usually leads to an unhappy experience and is often a meaningless exercise.

Good modeling practice starts with some planning. If at all possible, you should form a mental picture of what you think the results will look like. Stated another way, we should make a rough guess at the solution before starting to use the software. Figure 2-14 shows a very quick hand sketch of a flow net. It is very rough, but it gives us an idea of what the solution should look like.

From the rough sketch of a flow net, we can also get an estimate of the flow quantity. The amount of flow can be approximated by the ratio of flow channels to equipotential drops multiplied by the conductivity and the total head drop. For the sketch in Figure 2-14 the number of flow channels is 3, the number of equipotential drops is 9 and the total head drop is 5 m. Assume a hydraulic conductivity of $K = 0.1$ m/day. A rough estimate of the flow quantity then is $(5 \times 0.1 \times 3) / 9$, which is between 0.1 and 0.2 m³ / day. The VADOSE/W computed flow is 0.1427 m³/day and the equipotential lines are as shown in Figure 2-15.

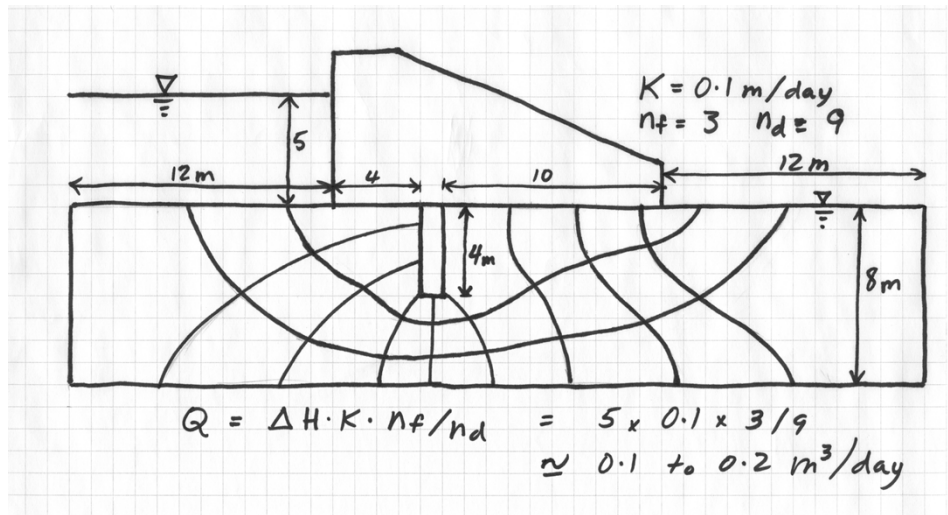


Figure 2-14 Hand sketch of flow net for cutoff below dam

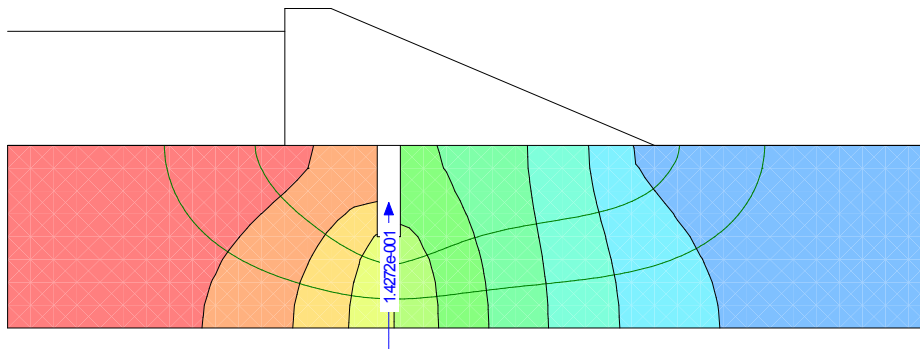


Figure 2-15 Computed results compared to hand sketch estimate

The rough flow net together with the estimated flow quantity can now be used to judge the model results. If there is no resemblance between what is expected and what is computed with the model then either the preliminary mental picture of the situation was not right or something has been inappropriately specified in the numerical model. Perhaps the boundary conditions are not correct or the material properties specified are different than intended. The difference ultimately needs to be resolved in order for you to have any confidence in your modeling. If you had never made a preliminary guess at the solution then it would be very difficult to judge the validity of the numerical modeling results.

Another extremely important part of modeling is to clearly define at the outset, the primary question to be answered by the modeling process. Is the main question the pore-water pressure distribution or is the quantity of flow. If your main objective is to determine the pressure distribution, there is no need to spend a lot of time on establishing the hydraulic conductivity – any reasonable estimate of conductivity is

adequate. If on the other hand your main objective is to estimate flow quantities, then a greater effort is needed in determining the conductivity.

Sometimes modelers say “I have no idea what the solution should look like - that is why I am doing the modeling”. The question then arises, why can you not form a mental picture of what the solution should resemble? Maybe it is a lack of understanding of the fundamental processes or physics, maybe it is a lack of experience, or maybe the system is too complex. A lack of understanding of the fundamentals can possibly be overcome by discussing the problem with more experienced engineers or scientists, or by conducting a study of published literature. If the system is too complex to make a preliminary estimate then it is good practice to simplify the problem so you can make a guess and then add complexity in stages so that at each modeling interval you can understand the significance of the increased complexity. If you were dealing with a very heterogenic system, you could start by defining a homogenous cross-section, obtaining a reasonable solution and then adding heterogeneity in stages. This approach is discussed in further detail in a subsequent section.

If you cannot form a mental picture of what the solution should look like prior to using the software, then you may need to discover or learn about a new physical process as discussed in the previous section.

Effective numerical modeling starts with making a guess of what the solution should look like.

Other prominent engineers support this concept. Carter (2000) in his keynote address at the GeoEng2000 Conference in Melbourne, Australia when talking about rules for modeling stated verbally that modeling should “start with an estimate.” Prof. John Burland made a presentation at the same conference on his work with righting the Leaning Tower of Pisa. Part of the presentation was on the modeling that was done to evaluate alternatives and while talking about modeling he too stressed the need to “start with a guess”.

Simplify geometry

Numerical models need to be a simplified abstraction of the actual field conditions. In the field the stratigraphy may be fairly complex and boundaries may be irregular. In a numerical model the boundaries need to become straight lines and the stratigraphy needs to be simplified so that it is possible to obtain an understandable solution. Remember, it is a “model”, not the actual conditions. Generally, a numerical model cannot and should not include all the details that exist in the field. If attempts are made at including all the minute details, the model can become so complex that it is difficult and sometimes even impossible to interpret or even obtain results.

Figure 2-16 shows a stratigraphic cross section (National Research Council Report 1990). A suitable numerical model for simulating the flow regime between the groundwater divides is something like the one shown in Figure 2-17. The stratigraphic boundaries are considerably simplified for the finite element analysis.

As a general rule, a model should be designed to answer specific questions. You need to constantly ask yourself while designing a model, if this feature will significantly affects the results? If you have doubts, you should not include it in the model, at least not in the early stages of analysis. Always, start with the simplest model.

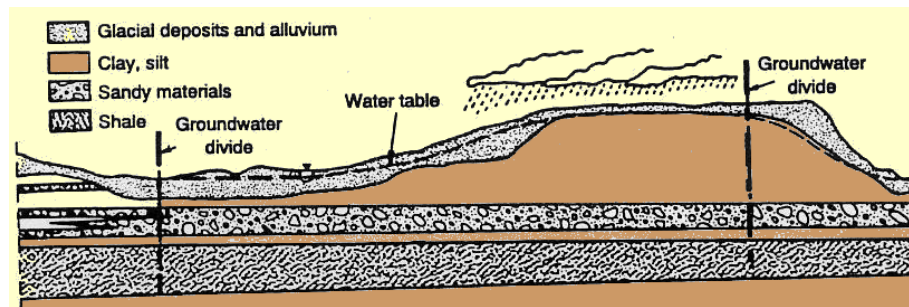


Figure 2-16 Example of a stratigraphic cross section
(from National Research Report 1990)

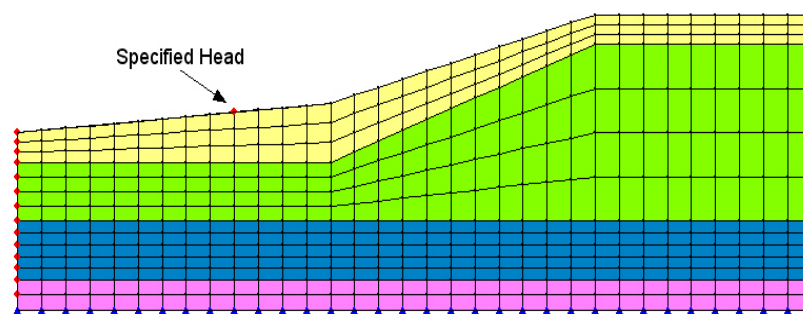


Figure 2-17 Finite element model of stratigraphic section

The tendency of novice modelers is to make the geometry too complex. The thinking is that everything needs to be included to get the best answer possible. In numerical modeling this is not always true. Increased complexity does not always lead to a better and more accurate solution. Geometric details can, for example, even create numerical difficulties that can mask the real solution.

Start simple

One of the most common mistakes in numerical modeling is to start with a model that is too complex. When a model is too complex, it is very difficult to judge and interpret the results. Often the result may look totally unreasonable. Then the next question asked is - what is causing the problem? Is it the geometry, is it the material properties, is it the boundary conditions, or is it the time step size or something else? The only way to resolve the issue is to make the model simpler and simpler until the difficulty can be isolated. This happens on almost all projects. It is much more efficient to start simple and build complexity into the model in stages, than to start complex, then take the model apart and have to rebuild it back up again.

A good start may be to take a homogeneous section and then add geometric complexity in stages. For the homogeneous section it is likely easier to judge the validity of the results. This allows you to gain confidence in the boundary conditions and material properties specified. Once you have reached a point where the results make sense, you can add different materials and increase the complexity of your geometry.

Another approach may be to start with a steady-state analysis even though you are ultimately interested in a transient process. A steady-state analysis gives you an idea as to where the transient analysis should end

up; to define the end point. Using this approach you can then answer the question of how does the process migrate with time until a steady-state system has been achieved.

It is unrealistic to dump all your information into a numerical model at the start of an analysis project and magically obtain beautiful, logical and reasonable solutions. It is vitally important to not start with this expectation. You will likely have a very unhappy modeling experience if you follow this approach.

Do numerical experiments

Interpreting the results of numerical models sometimes requires doing numerical experiments. This is particularly true if you are uncertain as to whether the results are reasonable. This approach also helps with understanding and learning how a particular feature operates. The idea is to set up a simple problem for which you can create a hand calculated solution.

Consider the following example. You are uncertain about the results from a flux section or the meaning of a computed boundary flux. To help satisfy this lack of understanding, you could do a numerical experiment on a simple 1D case as shown in Figure 2-18. The total head difference is 1 m and the conductivity is 1 m/day. The gradient under steady state conditions is the head difference divided by the length, making the gradient 0.1. The resulting total flow through the system is the cross sectional area times the gradient which should be 0.3 m³/day. The flux section that goes through the entire section confirms this result. There are flux sections through Elements 16 and 18. The flow through each element is 0.1 m³/day, which is correct since each element represents one-third of the area.

Another way to check the computed results is to look at the node information. When a head is specified, VADOSE/W computes the corresponding nodal flux. In VADOSE/W these are referred to as boundary flux values. The computed boundary nodal flux for the same experiment shown in Figure 2-18 on the left at the top and bottom nodes is 0.05. For the two intermediate nodes, the nodal boundary flux is 0.1 per node. The total is 0.3, the same as computed by the flux section. Also, the quantities are positive, indicating flow into the system.

The nodal boundary values on the right are the same as on the left, but negative. The negative sign means flow out of the system.

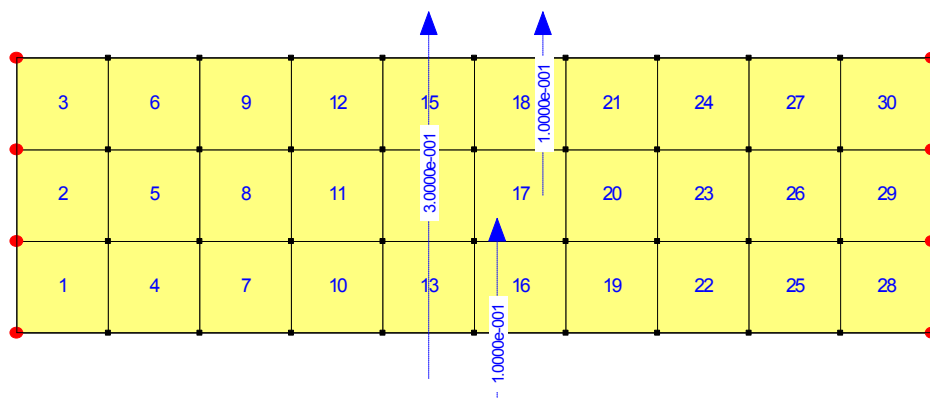


Figure 2-18 Horizontal flow through three element section

A simple numerical experiment takes only minutes to set up and run, but can be invaluable in confirming to you how the software works and in helping you interpret the results. There are many benefits; the most obvious is that it demonstrates the software is functioning properly. You can also see the difference between a flux section that goes through the entire problem versus a flux section that goes through a single element. You can see how the boundary nodal fluxes are related to the flux sections. It verifies for

you the meaning of the sign on the boundary nodal fluxes. Fully understanding and comprehending the results of a simple example like this greatly helps increase your confidence in the interpretation of results from more complex problems.

Conducting simple numerical experiments is a useful exercise for both novice and experienced modelers. For novice modelers it is an effective way to understand fundamental principles, learning how the software functions, and gaining confidence in interpreting results. For the experienced modeler it is an effective means of refreshing and confirming ideas. It is sometimes faster and more effective than trying to find appropriate documentation and then having to rely on the documentation. At the very least it may enhance and clarify the intent of the documentation.

Model only essential components

One of the powerful and attractive features of numerical modeling is the ability to simplify the geometry and not to have to include the entire physical structure in the model. A very common problem is the seepage flow under a concrete structure with a cut-off as shown in Figure 2-19. To analyze the seepage through the foundation it is not necessary to include the dam itself or the cut-off as these features are constructed of concrete and assumed impermeable.

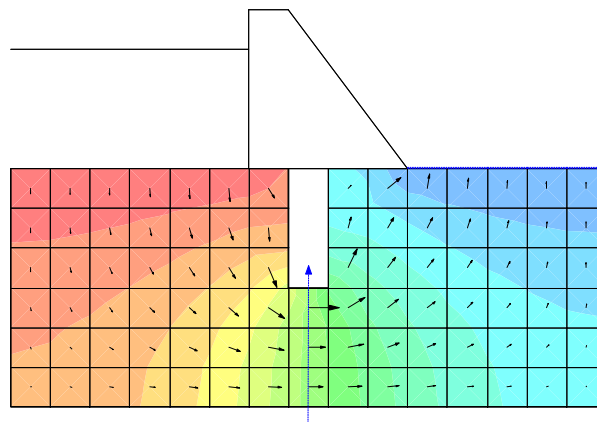


Figure 2-19 Simple flow beneath a cutoff

Another common example is the downstream toe drain or horizontal under drain in an embankment (Figure 2-20). The drain is so permeable relative to the embankment material that the drain does not contribute to the dissipation of the head (potential energy) loss through the structure. Physically, the drain needs to exist in the embankment, but it does not need to be present in a numerical model. If the drain becomes clogged with fines so that it begins to impede the seepage flow, then the situation is different and the drain would need to be included in the numerical model. With any material, the need to include it in the analysis should be decided in the context of whether it contributes to the head loss.

Another example is the downstream shell of a zoned dam as illustrated in Figure 2-21. Often the core is constructed of fine-grained soil while the shells are highly permeable coarse granular material. If there is a significant difference between core and shell conductivities then seepage that flows through the core will drip along the downstream side of the core (usually in granular transition zones) down to an under drain. If this is the case, the downstream shell does not need to be included in the seepage analysis, since the shell is not physically involved in the dissipation of the head loss. Once again the shell needs to exist physically, but does not need to be included in the numerical seepage model.

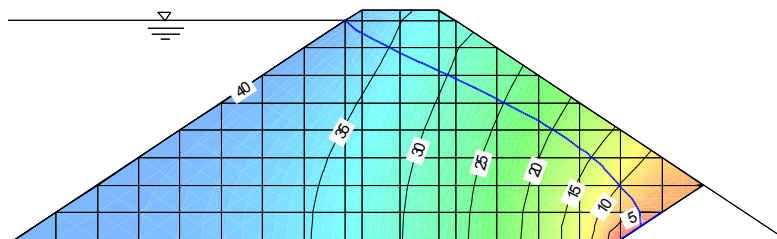


Figure 2-20 Flow through a dam with coarse toe drain

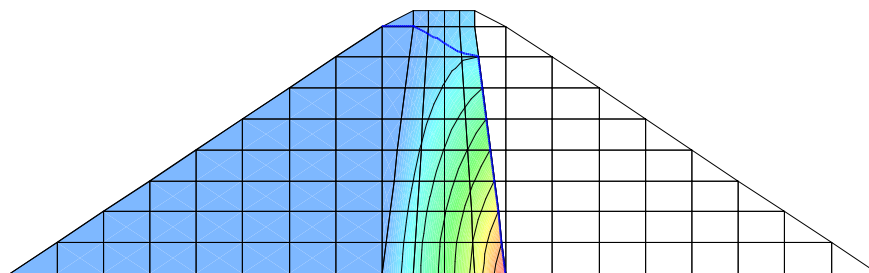


Figure 2-21 Head loss through dam core with downstream shell

Including unnecessary features and trying to model adjacent materials with extreme contrasts in material properties create numerical difficulties. The conductivity difference between the core and shell of a dam may be many, many orders of magnitude. The situation may be further complicated if unsaturated flow is present and the conductivity function is very steep, making the solution highly non-linear. In this type of situation it can be extremely difficult if not impossible to obtain a good solution with the current technology.

The numerical difficulties can be eased by eliminating non-essential segments from the numerical model. If the primary interest is the seepage through the core, then why include the downstream shell and complicate the analysis? Omitting non-essential features from the analysis is a very useful technique, particularly during the early stages of an analysis. During the early stages, you are simply trying to gain an understanding of the flow regime and trying to decide what is important and what is not important.

While deliberately leaving components out of the analysis may at first seem like a rather strange concept, it is a very important concept to accept if you want to be an effective numerical modeler.

Start with estimated material properties

In the early stages of a numerical modeling project it is often good practice to start with estimates of material properties. Simple estimates of material properties and simple property functions are more than adequate for gaining an understanding of the flow regime for checking that the model has been set up properly or to verify that the boundary conditions have been properly defined. Estimated properties are usually more than adequate for determining the importance of the various properties for the situation being modeled.

The temptation exists when you have laboratory data in hand that the data needs to be used in its entirety and cannot be manipulated in any way. There seems to be an inflexible view of laboratory data which can sometimes create difficulties when using the data in a numerical model. A common statement is; "I measured it in the lab and I have full confidence in my numbers". There can be a large reality gap that exists between laboratory determined results and actual insitu soil behavior. Some of the limitations arise

because of how the material was collected, how it was sampled and ultimately quantified in the lab. Was the sample collected by the shovelful, by collecting cuttings or by utilizing a core sampler? What was the size and number of samples collected and can they be considered representative of the entire profile? Was the sample oven-dried, sieved and then slurried prior to the test being performed? Were the large particles removed so the sample could be trimmed into the measuring device? Some of these common laboratory techniques can result in unrealistic property functions. Perhaps the amount of data collected in the laboratory is more than is actually required in the model. Because money has been spent collecting and measuring the data, it makes modelers reticent to experiment with making changes to the data to see what effect it has on the analysis.

It is good modeling practice to first obtain understandable and reasonable solutions using estimate material properties and then later refine the analysis once you know what the critical properties are going to be. It can even be more cost effective to determine ahead of time what material properties control the analysis and decide where it is appropriate to spend money obtaining laboratory data.

Interrogate the results

Powerful numerical models such as VADOSE/W need very careful guidance from the user. It is easy to inadvertently and unintentionally specify inappropriate boundary conditions or incorrect material properties. Consequently, it is vitally important to conduct spot checks on the results to ensure the constraints and material properties are consistent with what you intended to define and the results make sense. It is important to check, for example that the boundary condition that appears in the results is the same as what you thought was specified defining the model. Is the intended property function being applied to the correct soil? Or, are the initial conditions as you assumed?

VADOSE/W has many tools to inspect or interrogate the results. You can view node or element details and there are a wide range of parameters that can be graphed for the purpose of spot checking the results.

Inspecting and spot checking your results is an important and vital component in numerical modeling. It greatly helps to increase your confidence in a solution that is understandable and definable.

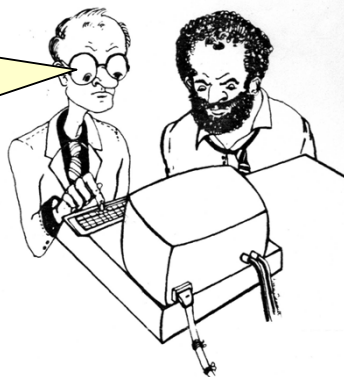
Evaluate results in the context of expected results

The fundamental question that should be asked during modeling is; “Do the results conform to the initial mental picture?” If they do not, then your mental picture needs to be fixed, there is something wrong with the model or both the model and your concept of the problem need to be adjusted until they agree. The numerical modeling process needs to be repeated over and over until the solution makes perfect sense and you are able to look at the results and feel confident that you understand the processes involved.

Remember the real world

While doing numerical modeling it is important to occasionally ask yourself how much you really know about the input compared to the complexity of the analysis. The following cartoon portrays an extreme situation, but underscores a problem that exists when uneducated or inexperienced users try to use powerful software tools.

“If we can incorporate boundary elements rather than simple finite elephants, enhance the statistical evaluation of parameter generation and stick with the fuzzy sets, I am confident that accuracy will be increased to at least the fourth decimal place.”



“Put another shovel full in Pat! It is full-cores they’re wanting!”

Note: origins of this figure are unknown at time of printing.

2.6 *How not to model*

As mentioned earlier in this chapter, it is completely unrealistic to expect to set up a complex model at the start of a project and immediately obtain realistic, understandable and meaningful results. There are far too many parameters and issues which can influence the results, so if this is your expectation, then modeling is going to lead to major disappointments.

For novice modelers; the initial reaction when faced with incomprehensible results is that something must be wrong with the software. It must be a limitation of the software that the solution is inappropriate or completely senseless. It is important to remember that the software is very powerful; it can keep track of millions of pieces of information and do repetitive computations which are far beyond the capability of the human mind. Without the software it would not be possible to make these types of analyses. The software by itself is extremely powerful numerically speaking, but essentially unintelligent. Conversely, the human mind has the capability of logic and reasoning, but has significant limitations retaining large amounts of digital data. It is the combination of the human mind together with the capability of a computer that makes numerical modeling so immensely powerful. Neither can do the task in isolation. The software can only be used effectively under the careful guidance and direction of the modeler.

Sometimes it is suggested that due to a time limitation, it is not possible to start simple and then progress slowly to a more complex analysis. A solution is needed quickly and since the budget is limited, it is necessary to immediately start with the ultimate simulation. This approach is seldom, if ever, successful. Usually this leads to a lot of frustration and the need to retreat to a simpler model until the solution is understandable and then build it up again in stages. Not following the above “how to” modeling procedures generally leads to requiring more time and financial resources than if you follow the recommended modeling concepts.

Remember, the software is only as good as your ability to guide and direct it. The intention of this document is to assist you in providing this guidance and direction so that you can take full advantages of the power the software can offer.

2.7 *Closing remarks*

As noted in the introduction, numerical modeling is a relatively new area of practice. Most university educational curricula do not include courses on how to approach numerical modeling and, consequently, the skill is often self-taught. As software tools such as VADOSE/W become increasingly available at educational institutions and educators become comfortable with these types of tools, classes and instruction should improve with respect to numerical modeling.

When the numerical analysis software tool, VADOSE/W, is effectively utilized as it was intended to be used, it becomes an immensely powerful tool, making it possible to do highly complex analyses. It can even lead to new understandings about actual physical process.

The process of modeling is a journey of discovery, a way of learning something new about the complex behavior of our physical world. It is a process that can help us understand highly complex, real physical process so that we can exercise our engineering judgment with increased confidence.

3 Geometry and Meshing

3.1 Introduction

Finite element numerical methods are based on the concept of subdividing a continuum into small pieces, describing the behavior or actions of the individual pieces and then reconnecting all the pieces to represent the behavior of the continuum as a whole. This process of subdividing the continuum into smaller pieces is known as *discretization* or *meshing*. The pieces are known as *finite elements*.

In GeoStudio, the geometry of a model is defined in its entirety prior to consideration of the discretization or meshing. Automatic mesh generation algorithms have now advanced sufficiently to enable a well behaved, numerically robust default discretization often with no additional effort required by the user. Of course, it is still wise to view the default generated mesh but any required changes can easily be made by changing a single global element size parameter, by changing the number of mesh divisions along a geometry line object, or by setting a required mesh element edge size.

Figure 3-1 shows the fully defined model for a soil excavation project. The entire model was built using various geometry items.

- Soil regions were specified;
- Geometry lines were drawn at the locations of tie-back anchors and cutoff wall;
- Soil material models were created and assigned onto the geometry objects; and
- Pre-defined boundary conditions were drawn on the region edges.

As a final step before solving, the mesh properties were viewed and adjustments made. In this case, the global element size was specified as 1.0 meter. In addition, the geometry line representing the grouted section of the anchors was discretized. The pre-stressed length of the anchors was intentionally left non-discretized. The final model is shown in Figure 3-2.

Now that you have a basic introduction to the concept of building your model using geometry objects, we can discuss each type of object in more detail. We must also have a discussion about the finite elements themselves, as these are the backbone to the entire finite element method.

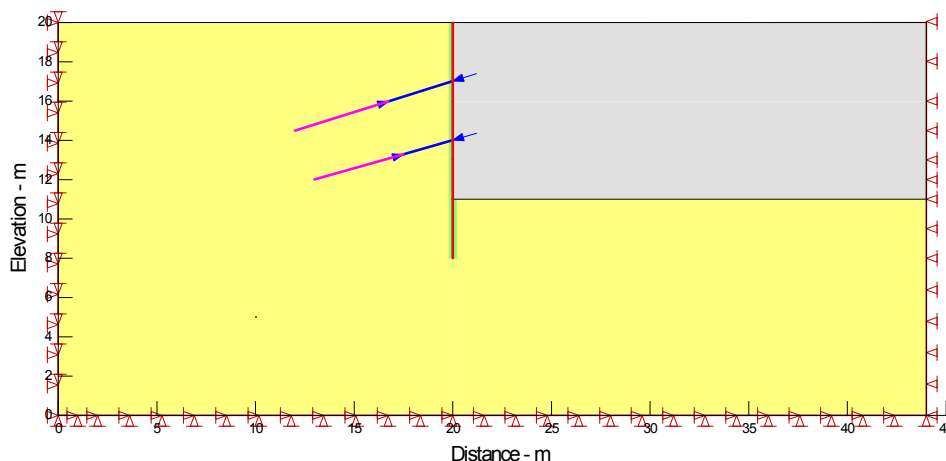


Figure 3-1 Fully defined geometry for soil excavation model

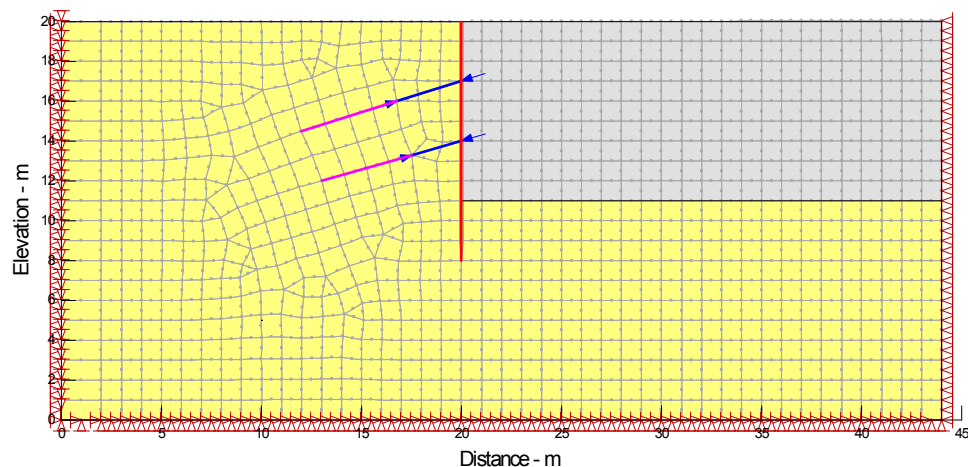


Figure 3-2 Default element discretization for model using 1m global element size constraint

3.2 Geometry Objects in GeoStudio

The entire model is defined as a series of geometry objects. These objects can be soil regions, circular openings line objects, surface regions, and point objects. These objects are shown in the images below – as defined and then with the mesh applied.

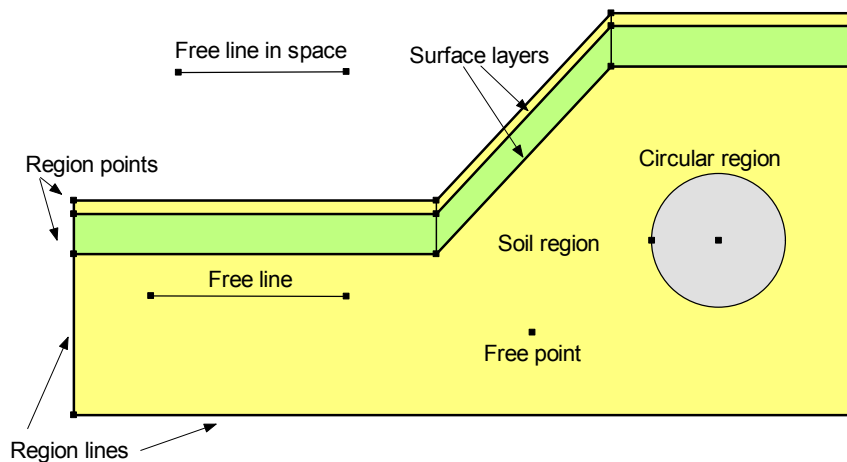


Figure 3-3 Available geometry objects

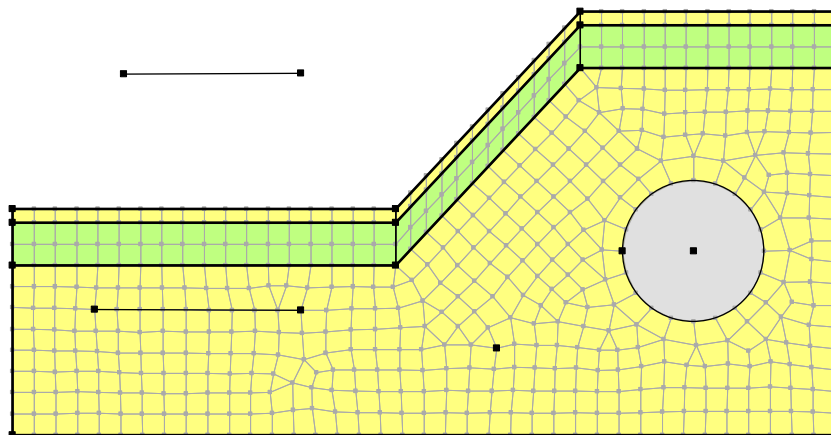


Figure 3-4 Mesh pattern for example model

Each of these geometry objects can have additional objects assigned to them such as material or boundary conditions objects. They can also have special properties, such as mesh element type, size and integration order.

Let us consider each in turn.

Regions, Points and Lines

GeoStudio uses the concept of regions and points to define the geometry of a problem and to facilitate discretization of the problem. The attraction of using regions is that they replicate what we intuitively do as engineers and scientists to illustrate concepts and draw components of a system. To draw a stratigraphic section, for example, we intuitively draw the different soil types as individual regions.

The use of regions offers all the advantages of dividing a large domain into smaller pieces, working and analyzing the smaller pieces, and then connecting the smaller pieces together to obtain the behavior of the whole domain, exactly like the concept of finite elements. Generally, all physical systems have to be broken down into pieces to create, manage and control the whole body.

A collection of highly adaptive individual pieces that can be joined together makes it possible to describe and define almost any complex domain or physical system. Such an approach is more powerful and can be applied to a wider range of problems than any system that attempts to describe the whole domain as a single object.

Regions may be simple straight-sided shapes like quadrilaterals or triangles or a free form, multi-sided polygon. Figure 3-5 illustrates a domain constructed using one quadrilateral and two triangular regions. Also shown in this figure are the region points and the region lines. Each segment of a region edge between any two adjacent points is called a line. Both points and lines can have special properties as discussed in the next sections. In this figure the lines and points are not “free” as they belong to a region. They do, however have similar behavior to free points and lines.

Figure 3-6 shows a multi-sided polygonal region defined using 10 points. There is no restriction on the number of points in a region. However, the rule of thumb to keep things simple is always encouraged.

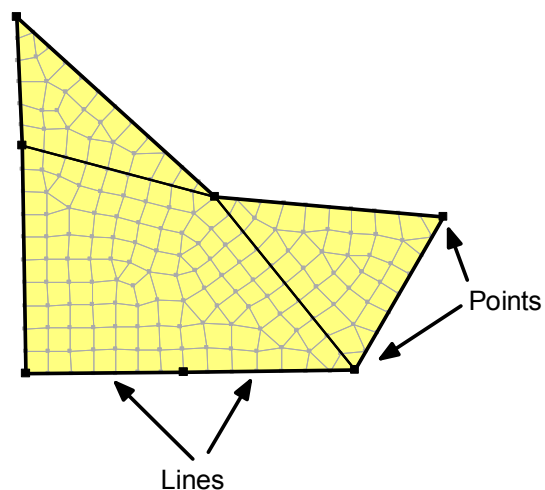


Figure 3-5 Illustration of a region's lines and points

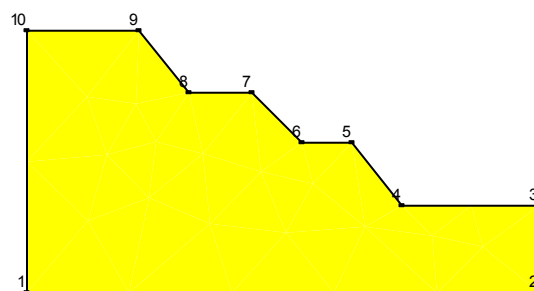


Figure 3-6 A multi-side polygonal region

Points can be selected and moved to modify the shape and position of regions, which provides for great flexibility in making adjustments and alterations to a problem definition.

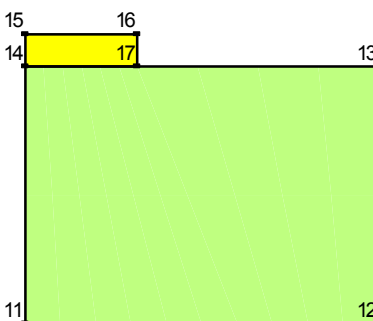


Figure 3-7 Regions of different size

Points are also required in order to join regions of different sizes and to control the meshing for specific purposes. Figure 3-7 shows a homogeneous soil region with a concrete footing region. The foundation region is made up of Points 11, 12, 13, 17 and 14. The footing region is made up of Points 14, 17, 16, and 15. Points 14 and 17 are common to both regions and therefore the two regions are properly joined and connected along this edge. In addition, Point 17 ensures that an element node will be created and will exist at the edge of the footing, which is required for proper meshing. It also breaks up the region edge between points 13 and 14 so that a unique boundary condition may be placed along the edge sub-section.

When a region is defined, it is restricted to having:

- One type of material,
- One type of element meshing pattern (or no mesh),
- One order of elements; either first- or second-order, and
- One integration order.

More information on finite elements is provided later in this chapter.

Free Points

As seen in the illustrations above, regions are made up of a series of points. It is also possible for a point to exist within a region or outside of a region on its own. By default, a finite element “node” must exist at the location of all points, whether region corner points or free points. The advantage of this is that by placing a “free point” you can ensure that a boundary condition is applied at the desired location.

All boundary conditions must be applied directly to region lines, region (or free) points or geometry lines. The power of this approach will be readily evident to the user who decides to change the default generated mesh. In the past, changing the mesh required that all boundary conditions and soil properties (in some cases) were lost or attempted to be re-applied. Now, because properties and boundary condition exist as objects on geometry items, the mesh can be changed with no threat of having to re-do parts of the model set up.

Free Lines

A free line is a line object that does not make up any part of a region. They can be very useful for applying anchors to a model or for specifying a geo-fabric or insulation layer. They can also be used for creating structural components that are partially in the soil and partially outside the soil. Here are some examples...

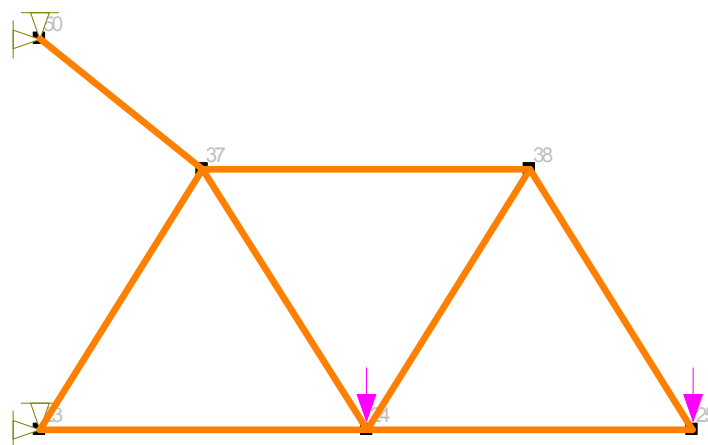


Figure 3-8 Truss loading model

In Figure 3-8 structural bar properties have been applied to a pattern of free lines in order to determine displacements under loading for the truss system.

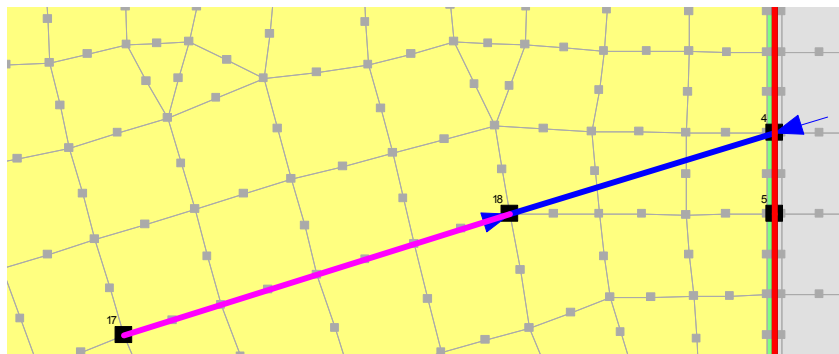


Figure 3-9 Anchors on lines (line is partially meshed)

Figure 3-9 shows two key aspects of free lines. A free line in two segments has been drawn to model a tie back anchor. The upper length of the free line was left un-discretized (i.e., independent of the finite element mesh) while the lower length is incorporated into the mesh. The lower end represents a beam structural member which requires that it is aligned with the surrounding soil elements. The upper length represents a structural bar element which only acts in tension or compression and only has an active force and stiffness at its end points which do coincide with nodal locations. It does not interact with the soil so does not need to share a mesh with the soil except at its end points.

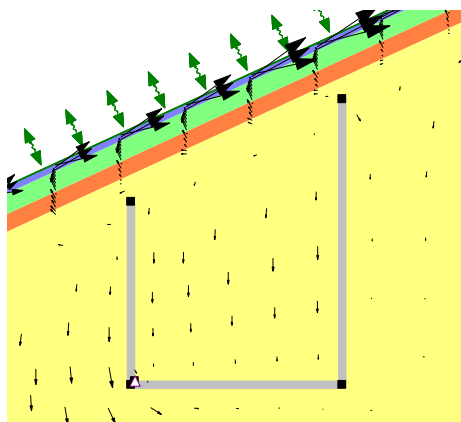


Figure 3-10 Lines with material model “none” (no flow) assigned to simulate lysimeter collection basin in waste beneath an engineered soil cover

Figure 3-10 shows the use of free lines to construct a lysimeter collection basin beneath an engineered soil cover system. The line was assigned a material model of “none” to simulate a no flow condition (i.e., a null material). This is a key point to understand, that the line was assigned a material model. When this is done, the line inherits the behavioral properties of the material assigned and a special interface element is added to the line mesh. The interface behavior depends on the application being solved. In this example, the interface has “no flow” across it. In a stress-deformation model, the interface on the line may be assigned soil – structure friction/slippage properties. Interface elements are discussed in more detail in the next section.

Interface Elements on Lines

In the previous section the concept of applying a material model to a single line was introduced. The actual material models that can be used are dependent on the analysis being solved. For example, in SEEP/W an interface model may be used to represent a geo-fabric or a null material to represent a barrier to flow. In TEMP/W it may be a thin insulation layer. In SIGMA/W, the material model may describe

the friction properties between soils, or a soil and a structure such as a cutoff wall. You can read about all of these models in the respective engineering books.

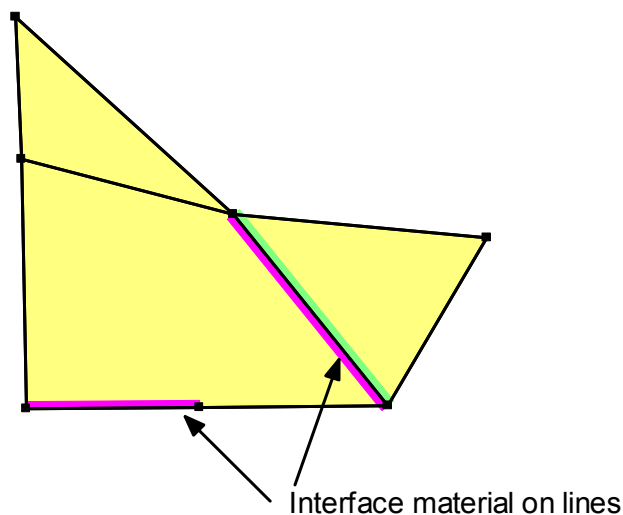


Figure 3-11 Illustration of "interface elements" on geometry lines

The discussion now will focus on how to apply an interface region to a line object. There are two ways to do this. There is a Draw Line Material Properties command in which you can choose a material model you have defined and apply it to a line by clicking just next to a line as shown in Figure 3-12. You can assign a different property to either side of a line. If you use this option, you are specifying the material as well as creating special thin "interface" elements. You can then go back and change the element thickness from its default value using the Draw Mesh Properties command and choosing the line.

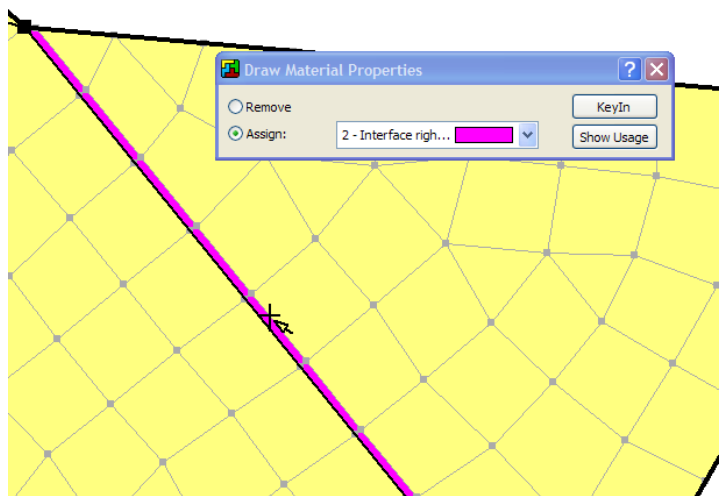


Figure 3-12 Using the Draw Line Material command to assign an interface model to a line

The second option for specifying an interface model on a line is to first create the thin elements and then assign the material to the line. You can use the Draw Mesh Properties command, select the line, choose the Generate Interface Elements option and specify an interface element thickness. This process is illustrated in Figure 3-13.

The actual thickness of the interface elements may or may not have physical meaning but the material model assigned to them will hold some meaning. If, for example, the interface represents an insulation layer in TEMP/W, then the thickness is relevant. However, if the interface describes the frictional behavior between two sliding blocks, then the thickness specified is not factored in the solution and it can be specified only to satisfy your presentation needs.

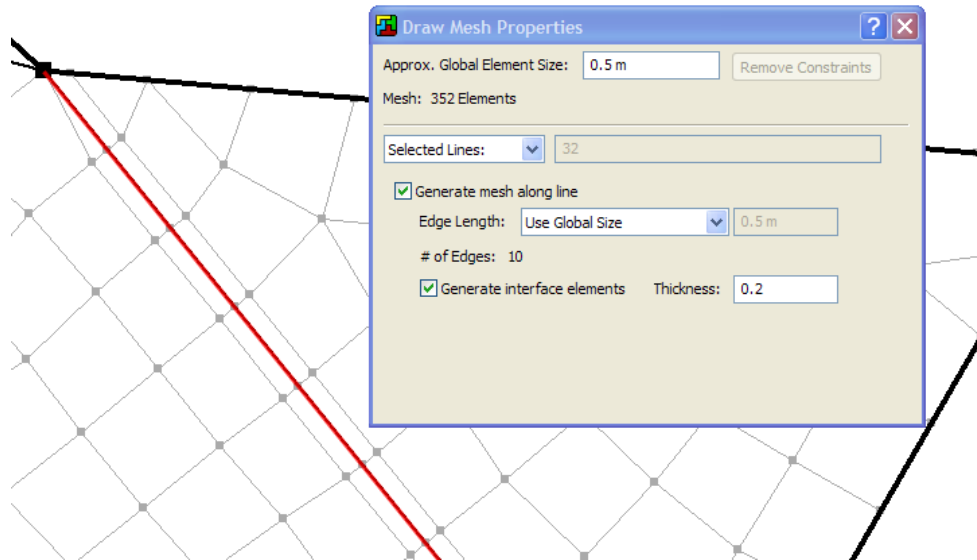


Figure 3-13 Using Draw Mesh Properties to create interface elements on selected line

Circular Openings

A circular opening is a type of region that “floats” over top of another soil region. It is created using a Draw command and is defined by its center point and one point on its circumference. The region can be dragged to a different location or its circumference point can be moved to change the size of the opening. Like all other regions, it can have a mesh assigned to it; it can have material properties assigned to its edge (such as a tunnel liner interface material); and it can have boundary conditions assigned to its edge or center point.

Figure 3-14 shows a circular opening region that was placed on top of an existing soil region. The circular region was applied by clicking on the desired center point and then dragging the radius point to a desired location. Once defined, the region can be designated to be a mesh opening or an un-meshed opening or hole. A mesh may be necessary to obtain in-situ stresses prior to excavation. A hole may be necessary to simulate a pipe or culvert. In the opening presented in the figure, interface elements have been added to the tunnel face. This will make it possible to apply a structural beam to the face with a soil-structure interaction model applied between the beam and soil.

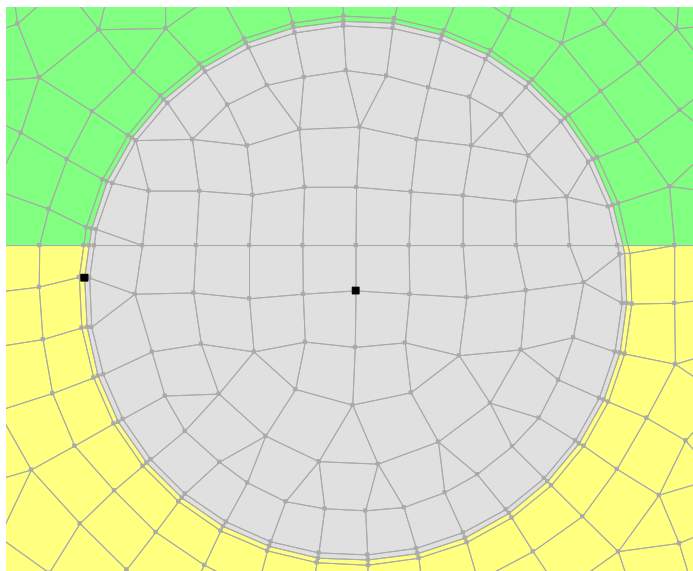


Figure 3-14 Circular region with defined center point, radius point and interface elements

3.3 Mesh Generation

In GeoStudio all meshing is now fully automatic. There is no longer the ability to draw individual “finite elements.” In addition, there is no worry whether the mesh will be compatible across different regions or whether your material properties or boundary conditions will disappear if you change the mesh.

When a geometry region or line is initially drawn it is by default un-meshed. A default mesh is generated for the soil regions when you first use the Draw Mesh Properties command, which you may accept or modify. You may alter the size of the elements at a global level for the entire mesh, within any one or more regions, or along a line or around a point. You may specify mesh density as a real length unit, as a ratio of the global mesh size, or as the number of divisions along a line edge. Generally, however, it is recommended that you limit altering the mesh to changing the global density and then, if necessary, at a few limited locations where finer or coarser density is needed.

Meshing options and available patterns are shown in the image below.

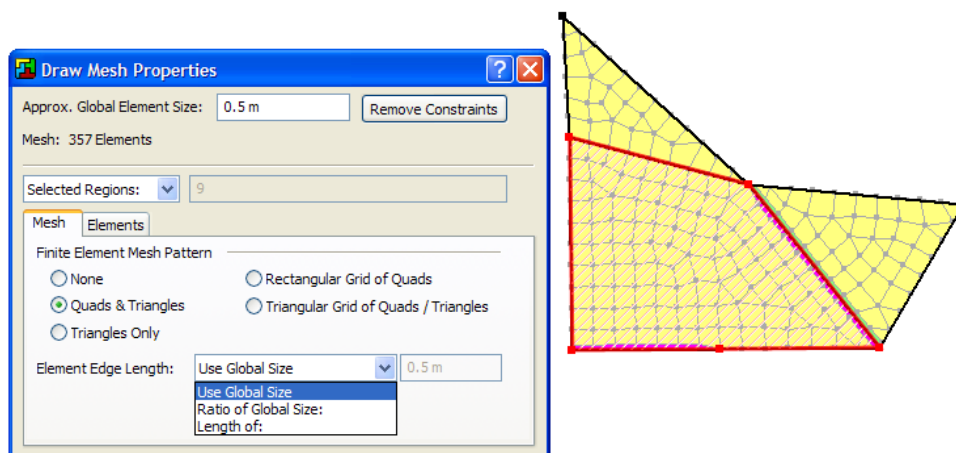


Figure 3-15 Draw Mesh Properties options

Structured mesh

Figure 3-16 presents what is known as a structured mesh because the elements are ordered in a consistent pattern and are of only two shapes and sizes. A structured mesh for a non-symmetrical geometry shape requires that several soil regions are created and the meshing is controlled within each region. This is likely more work to accomplish and will not yield a significant improvement in results. More efficient, automatic meshing options with good numerical performance are available and will be discussed in the next section. A structured mesh is created using either a rectangular grid of quads or a triangular grid of quads/triangles.

Unstructured quad and triangle mesh

The fully structured mesh shown in Figure 3-16 may require several regions to be defined so that you can control the meshing at a detailed level in order to maintain structure. A new meshing pattern is available that will automatically generate a well behaved unstructured pattern of quadrilateral and triangular elements as shown in Figure 3-17. In our opinion, this mesh option should be the first one you choose as it will meet your needs in most cases.

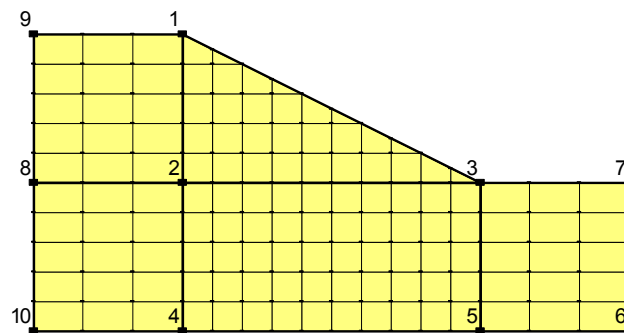


Figure 3-16 Structured mesh

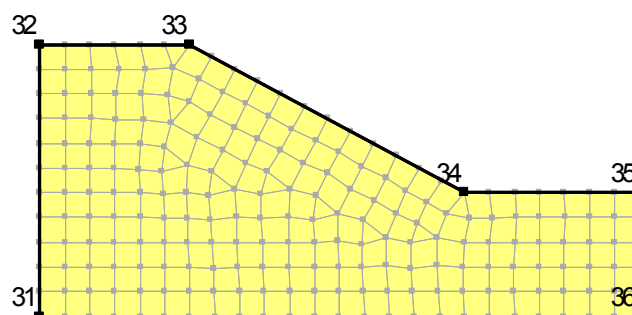


Figure 3-17 Mixed quad and triangle unstructured mesh

Unstructured triangular mesh

The diagram in Figure 3-18 shows the same section as in Figure 3-16, but this time with an unstructured triangular mesh. In this case the mesh is automatically created using Delaunay triangulation techniques. One of the great attractions of unstructured meshing is that almost any odd-shaped region can be meshed.

This meshing simplicity however has some numerical and interpretation consequences as discussed in more detail in the Structured versus Unstructured Section below.

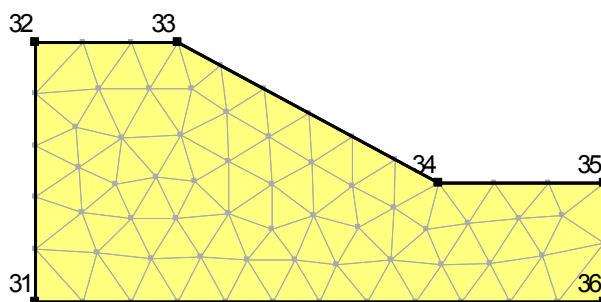


Figure 3-18 Unstructured triangular mesh

Triangular grid regions

GeoStudio has a special structured pattern for triangular regions called a triangular grid of quads/triangles. The next figure (Figure 3-19) shows a typical triangular region with the resulting structured mesh. The elements are a mixture of squares, rectangles, trapezoids and triangles. The use of this pattern is fairly general, but it does have some limitations and restrictions.

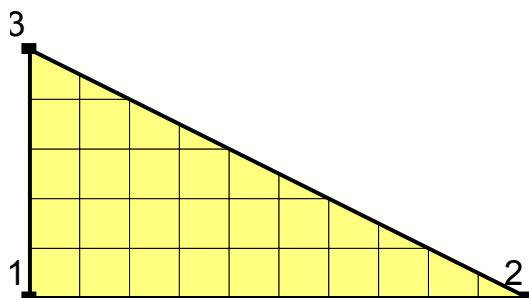


Figure 3-19 Triangular grid region

It is useful to think of the region as having three sides: a short side, an intermediate length side and a long side. The algorithm attempts to sort the edges so that the sides go from the shortest to the longest in a counter-clockwise direction. In this example, the shortest side is 3-1, the intermediate 1-2 and the longest 2-3.

The meshing algorithm works best when the number of divisions is controlled on the shortest and intermediate sides. To retain the even pattern shown in Figure 3-19, the number of divisions should be defined on the shortest side first and then on the intermediate side. The number of divisions on the intermediate side can be an even multiple of the number on the shortest side. In the above example, the shortest side has 5 divisions and the intermediate side can have 10, or 2 times that of the shortest side. The algorithm works best and gives the best structured mesh if the numbers of divisions on the longest side are left undefined allowing the algorithm to compute the appropriate number of divisions.

If a triangular region is mixed in with other more general regions, GeoStudio will attempt to ensure mesh compatibility. Sometimes however it may not be possible to adhere to the requirements for generating a structured mesh in a triangular region and then GeoStudio will substitute an unstructured mesh.

Rectangular grid of quads

Figure 3-20 shows the same region geometry meshed with the rectangular grid of quads pattern. This is a structured mesh but has the potential to be more difficult to control. The mesh pattern on the left side is very nice but near the base of the slope the quad shape is starting to distort. This distortion could be controlled by adding more region points along the bottom edge but this will still result in a mesh with large elements on the left and thinner elements on the right. This mesh pattern is ideally suited for four sided regions only.

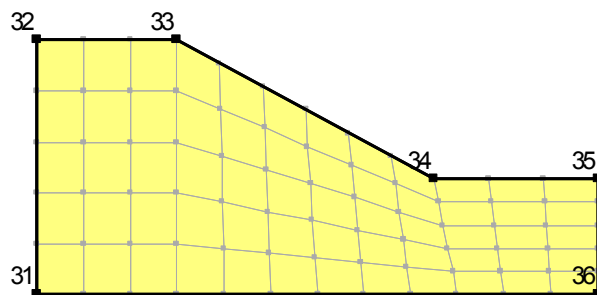


Figure 3-20 Rectangular grid of quad elements

3.4 Surface layers

At the ground surface conditions change in response to the climate and climatic conditions can change dramatically over short periods of time. For example, the ground maybe highly desiccated near the surface on a hot day before a thunderstorm. In a short period of time, the soil changes from being very dry to being saturated. Another example may be penetration of frost from the ground surface. To numerically deal with rapid and dramatic boundary changes it is necessary to have fine discretization near the ground surface. GeoStudio has a special procedure for constructing a surface layer that can be finely discretized. Figure 3-21 illustrates a surface layer placed over the surface of a larger region. The surface layer capability is also invaluable for discretizing features such as engineered soil covers over waste material, which may consist of several relatively thin layers of soil which also require fine discretization.

The ability to construct a surface layer is available in VADOSE/W, SEEP/W and TEMP/W. In SEEP/W the surface layer is used to tell the solver that it should track seepage face flows and infiltration events for any unit flux boundary condition. As a result, water that does not immediately infiltrate the ground is not considered lost from the analysis, but is allowed to pond and build up a positive pressure head in any user-defined low points along the surface. The other GeoStudio modules cannot be used to construct a surface layer, but once the surface mesh has been created it will exist in all the other modules. Consequently, if a layer has been created for a SEEP/W analysis, the surface layer will also be part of a SLOPE/W analysis, since GeoStudio uses only one geometry definition within a single data file.

Once the main soil profile has been meshed, a special Draw Surface Layer command can be used to build up a single or multi layer region along all or part of a ground surface. Parameters such as the soil type and individual layer geometry are defined and a quadrilateral element mesh with vertically oriented nodes is automatically built on top of the existing ground region. The structure of the mesh will ensure optimum numerical stability during the solution.

Quadrilateral elements are much better for modeling ground surface processes because the primary unknown gradients are usually steeper in a direction perpendicular to the surface. The presence of triangular elements in thin layers near the surface causes excessive fluctuation in the computed results

relative to the orientation of the triangular elements. Also, dealing with plant root zones in the VADOSE/W model necessitates that element nodes in the surface layer all fall on vertical lines. Moreover, using quadrilaterals greatly reduces the number of elements required, an important consideration when dealing with situations that will be very computationally intensive.

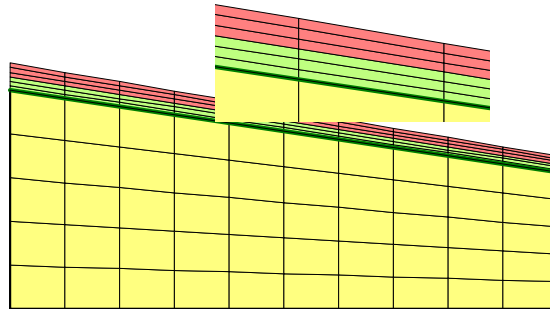


Figure 3-21 Illustration of a surface layer mesh

Surface layers have special viewing options. Consider the two meshes illustrated in Figure 3-22. The left diagram shows a surface layer without all the cluttering details as illustrated on the right. When many thin elements are located in a close proximity to each other, they can appear indistinguishable when viewed from a far away scale. By optionally turning off the surface mesh details a clearer image of the structure of the near surface soil layers can be viewed.

Figure 3-23 is another illustration of this optional viewing concept. The left diagram in the figure shows the detailed mesh and soil layers across the 0.75m thick surface region and the right diagram leaves the details out, but still shows the layer colors. A couple of additional key points can be made in regards to the figure. Notice that bottom two elements of the left diagram are the same soil type as the main underlying soil. This is a good mesh design strategy – that being to have the bottom most layer of the surface mesh be made of the same soil as the existing ground. Consider if the bottom layer of the surface soil was VERY different from the underlying soil. If a finely spaced mesh was placed directly on top of the different underlying soil then the numerical integration of material properties at the common mesh node between the two soils would be less accurate because of the influence of the large element area from the material below the common nodal point. By having the bottom layer of the surface layer be the same as the underlying soil, the element shapes are very similar in size and aspect at the common nodal point between the two very contrasting soils.

The second point to note from Figure 3-23 is that in the right diagram the nodes that are located at the interface between two soils are still viewable even though the main mesh details are not. This is intentional so that you can easily see and graph data at nodes that are used for automatic tracking of interlayer fluxes in the VADOSE/W model.

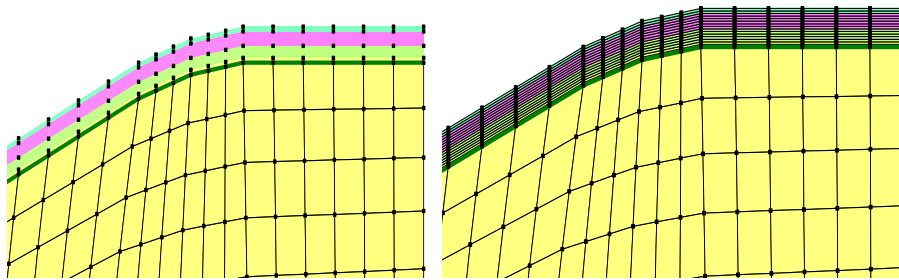


Figure 3-22 Surface region mesh with details off (left) and on (right)

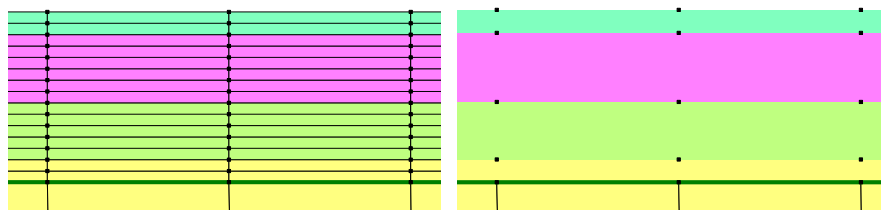


Figure 3-23 Close up of surface details on and off (note inter-layer nodes still visible in figure on right)

Boundary flux modeling with rainfall infiltration, runoff, snow melt etc. can be very numerically demanding from a convergence perspective. Potential problems can be made worse if the shape of the surface mesh is not “realistic.” Consider the two meshes illustrated in Figure 3-24 and Figure 3-25. In the first figure, the ground profile has rounded corners which are much more natural and much more numerically friendly. In the second figure, changes in slope angle are represented by a sharp break. This sharp break is not only unnatural, but the shape of the individual elements right at the transition points creates numerical problems if there are large changes in boundary condition type at different nodes within the same element. This would be the case when the corner node at the bottom of the slope becomes a seepage face point while the next node up slope is still an infiltration node. Basically, it is better to build the mesh to look somewhat natural.

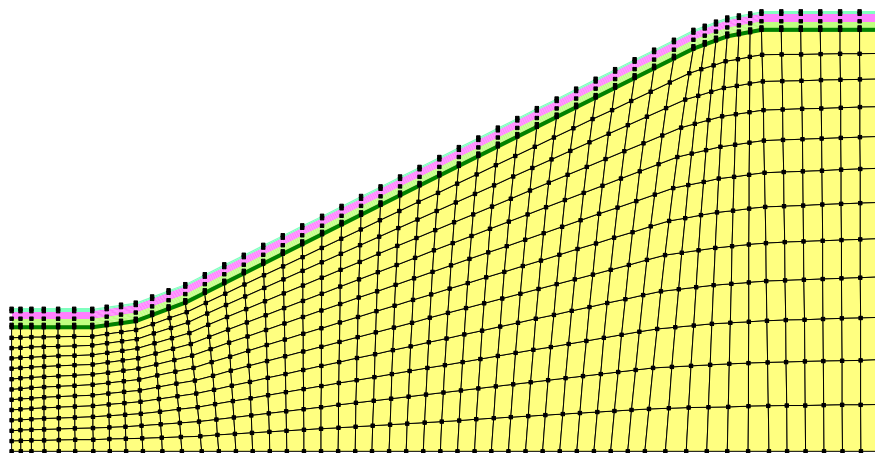


Figure 3-24 Mesh showing rounded surface slope breaks

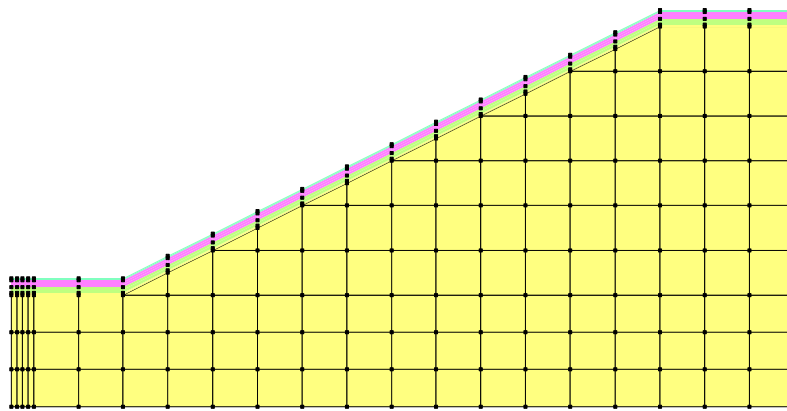


Figure 3-25 Mesh showing angular surface slope breaks

In order to create a surface mesh with more rounded features it is necessary to build the underlying soil mesh with the same rounded profile. This is easily accomplished in GeoStudio by adding additional region points near a slope break such that the region points can be moved slightly to create a rounded profile. This is the case in Figure 3-26 below where three region points are used at both the toe and crest of the slope. Also notice that three region points are used on the bottom of the mesh beneath the toe and crest location. This is a useful tip to remember. When you want to have more control over the trans-finite element mesh you should add region points on opposite sides of the mesh from where you need the detail. As a final note, adding region points can be done at any time – even after the surface layer is created. When the region beneath a surface layer is changed, the surface layer above it will be automatically regenerated to ensure mesh compatibility with the region below.

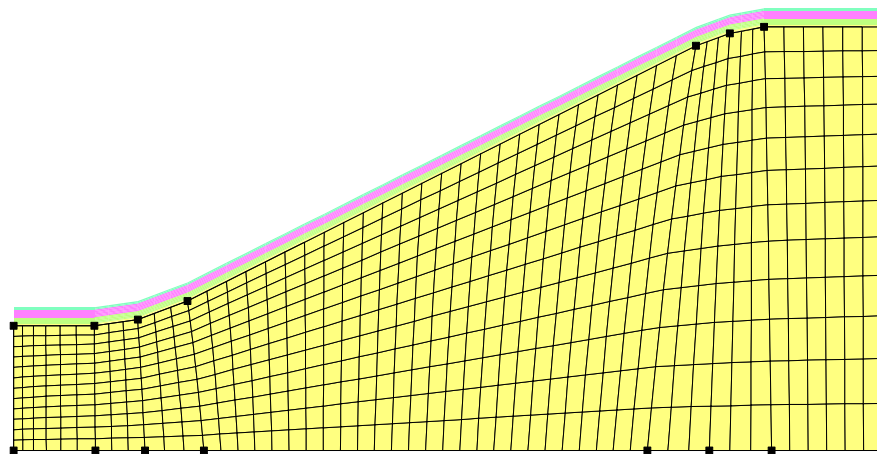


Figure 3-26 Region mesh with region corner points viewed and surface details not viewed

3.5 Joining regions

Compatibility must be maintained between regions to ensure the regions are connected. Regions must be joined at the region points and points must be common to adjoining regions for the regions to be properly connected. GeoStudio has a number of features to assist in achieving region compatibility.

The following are some of the main characteristics:

If the cross-hair symbol moves close to an existing point, the symbol will snap to the existing point.

A new point will be created if the cursor is on the perimeter of an existing region. The new point will then be common to the new region and to the existing region.

Points in between selected points are automatically selected along an existing region edge unless the Ctrl key is held down.

Consider the diagram in Figure 3-27. Region 1 is drawn first and Region 2 can be drawn by clicking on Points 7, 3, 8 and 9. Points 4, 5 and 6 are automatically added to Region 2.

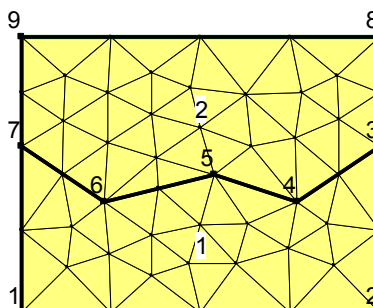


Figure 3-27 Regions joined along jagged line

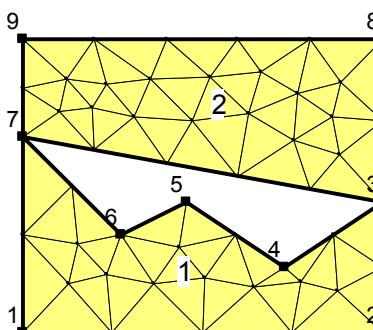


Figure 3-28 Adjoining regions with an open space

Sometimes it may be desirable to create an open area in a mesh and then it is necessary to hold down the Ctrl key when going from Point 7 to 3 or 3 to 7. Doing this results in a mesh as shown in Figure 3-28. In this case the Ctrl key was held down after clicking on Point 7, but before clicking on Point 3.

Additional details on joining regions are presented in the on-line help.

3.6 Meshing for transient analyses

Modeling transient processes requires a procedure to march forward in time increments. The time increments are referred to in GeoStudio as time steps. Selecting and controlling the time step sequence is a topic in itself and will be dealt with later. Obtaining acceptable transient solutions is not only influenced by the time steps, but also by the element size. In a contaminant transport advection-dispersion analysis (CTTRAN/W) it is necessary to have a time step sufficiently large to allow an imaginary contaminant

particle to move a significant distance relative to the element size, while at the same time not have the time step size be so large as to allow the particle to jump across several elements. The particle should, so to speak, make at least one stop in each element. In CTRAN/W this is controlled by the Peclet and Courant criteria.

In a simulation of consolidation, the time step size for the first time step needs to be sufficiently large so that the element next to the drainage face consolidates by at least 50 percent. Achieving this is related to the element size; the larger the element the greater the required initial time step. If the time step size is too small, the computed pore-water pressures may be unrealistic.

The important point in this section on meshing is to realize that meshing, more particularly element sizes, comes into play in a transient analysis. Rules and guidelines for selecting appropriate time stepping are discussed elsewhere with reference to particular types of analysis.

3.7 *Finite Elements*

Discretization or meshing is one of the three fundamental aspects of finite element modeling. The other two are defining material properties and boundary conditions. Discretization involves defining geometry, distance, area, and volume. It is the component that deals with the physical dimensions of the domain.

A numerical book-keeping scheme is required to keep track of all the elements and to know how all the elements are interconnected. This requires an ordered numbering scheme. When finite element methods were first developed, creating the mesh numbering was very laborious. However, many computer algorithms are now available to develop the mesh and assign the element numbering. Developing these algorithms is in some respects more complex than solving the main finite element equations. GeoStudio has its own system and algorithms for meshing, which are designed specifically for the analysis of geotechnical and geo-environmental problems.

Some human guidance is required to develop a good finite element mesh in addition to using the powerful automatic meshing algorithms available. One of the issues, for example, is mesh size. Computers, particularly desktop or personal computers, have limited processing capability and therefore the size of the mesh needs to be limited. Variable mesh density is sometimes required to obtain a balance between computer processing time and solution requirements. Ensuring that all the elements are connected properly is another issue. Much of this can be done with the meshing algorithm, but it is necessary for the user to follow some fundamental principles. In finite element terminology this is referred to as ensuring mesh compatibility. GeoStudio ensures mesh compatibility within a region and for the most part ensures mesh compatibility across adjacent regions, but it is still possible to create a situation whereby mesh incompatibility exists. The user needs to provide some guidance in ensuring compatibility between regions.

The purpose of this chapter is to introduce some of the basic concepts inherent in meshing and outline some procedures which must be followed when developing a mesh. An understanding of these fundamentals is vital to proper discretization.

Much of this chapter is devoted to describing the meshing systems and the features and capabilities available in GeoStudio. In addition, there are also discussions on the selection, behavior and use of various element types, sizes, shapes and patterns. A summary of practical guidelines for good meshing practice are also outlined.

3.8 Element fundamentals

Element nodes

One of the main features of a finite element are the nodes. Nodes exist at the corners of the elements or along the edges of the elements. Figure 3-29 and Figure 3-30 show the nodes, represented as black dots.

The nodes are required and used for the following purposes:

- The positions of the nodes in a coordinate system are used to compute the geometric characteristics of the element – such as length, area or volume.
- The nodes are used to describe the distribution of the primary unknowns within the element. In the SEEP/W formulation, the primary field variable is the hydraulic head or pore-water pressure.
- The nodes are used to connect or join all the elements within a domain. All elements with a common node are connected at that node. It is the common nodes between elements that ensure compatibility, which is discussed in further detail below.
- All finite element equations are formed at the nodes. All elements common to a single node contribute to the characteristics and coefficients that exist in the equation at that node, but it is the equation at the node that is used to compute the primary unknown at that node. In other words, the seepage equation is developed for each node and the material properties which are used within the equations are contributed from the surrounding elements.

There can be multiple finite element equations developed at each node depending on the degrees of freedom. In seepage analysis there is only one degree of freedom at each node, which is the head or pore-water pressure. The number of finite element equations to be solved is equal to the number of nodes used to define the mesh. In a 2D stress-deformation analysis, there are two degrees of freedom at each node – displacement x and displacement y . Consequently, the number of equations for the whole domain is equal to two times the number of nodes. In a coupled consolidation analysis there are three degrees of freedom at each node – displacement x , displacement y and pore-water pressure. For a coupled consolidation analysis the total number of equations required to solve the problem is three times the number of nodes.

Since the number of finite element equations is related to the number of nodes, the number of nodes in a problem is one of the main factors in the computing time required to solve for the primary unknowns.

Field variable distribution

In a finite element formulation it is necessary to adopt a model describing the distribution of the primary variable within the element (e.g., total head). The distribution could be linear or curved.

For a linear distribution of the primary unknown, nodes are required only at the element corners. The two nodes (points) along an edge are sufficient to form a linear equation. Figure 3-29 illustrates this situation. Elements with nodes existing at the corners are referred to as first-order elements.

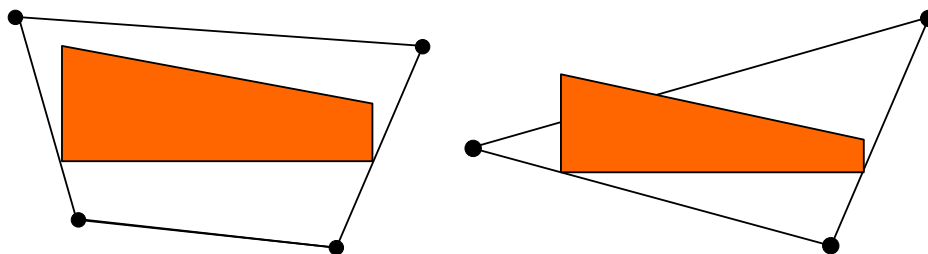


Figure 3-29 Primary field variable distribution in first-order elements

The derivative of the primary unknown with respect to distance is the gradient. For a linear distribution the gradient is consequently a constant. In the context of a seepage formulation the primary unknown is the hydraulic head. The derivative of head with respect to distance is the seepage gradient and the gradient is therefore constant within a first order element.

With three nodes defined along an edge, we can write a quadratic equation describing the distribution of the primary unknown within the element. Consequently the distribution of the primary unknown can be curved as shown in Figure 3-30. The derivative of the quadratic head distribution results in a linear gradient distribution. Elements with three or more nodes along an edge are referred to as higher order elements. More specifically, an element with three nodes along an edge is known as a second-order element.

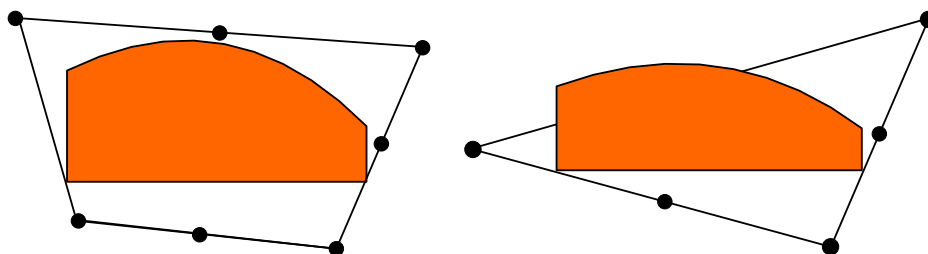


Figure 3-30 Primary field variable distribution in higher-order elements

Higher order elements are more suited to problems where the primary unknowns are vectors as in a stress-deformation analysis (deformation x and y). When the primary unknown is a scalar value as in a seepage formulation, there is often little to be gained by using higher-order elements. Smaller first-order elements can be as effective as larger higher-order elements. This is discussed in more detail in the meshing guidelines at the end of this chapter.

Element and mesh compatibility

Element and mesh compatibility are fundamental to proper meshing. Elements must have common nodes in order to be considered connected, and the distribution of the primary unknown along an element edge must be the same for an edge common to two elements.

Consider the illustration in Figure 3-31. Element numbers are shown in the middle of the element and node numbers are presented beside the nodes. Even though elements 4, 5 and 6 appear to be connected to elements 7, 8 and 9, they are actually not connected. Physically, the elements would behave the same as the two element groups shown with a physical separation on the right side of Figure 3-31. Common nodes are required to connect the elements as shown in Figure 3-32. Node 11, for example, is common to Elements 5, 6, 8 and 9.

Mixing elements of a different order can also create incompatibility. Figure 3-33 shows 4-noded quadrilateral elements connected to 8-noded elements. Elements 1 and 2 are 8-noded elements while

Elements 3 to 10 are 4-noded first-order elements. The field variable distribution in Element 1 along edge 9 to 11 could be curved. In Elements 3 and 4 the field variable distribution between 9 and 10 and between 10 and 11 will be linear. This means the field variable distributions between Elements 1 and 2 are incompatible with the field variable distributions in Elements 3 to 6.

The meshing algorithms in GeoStudio ensure element compatibility within regions. A special integer-based algorithm is also included to check the compatibility between regions. This algorithm ensures that common edges between regions have the same number of elements and nodes. Even though the software is very powerful and seeks to ensure mesh compatibility, the user nonetheless needs to be careful about creating adjoining regions. The illustration in Figure 3-31 can also potentially exist at the region level. At the region level, region points need to be common to adjoining regions to ensure compatibility.

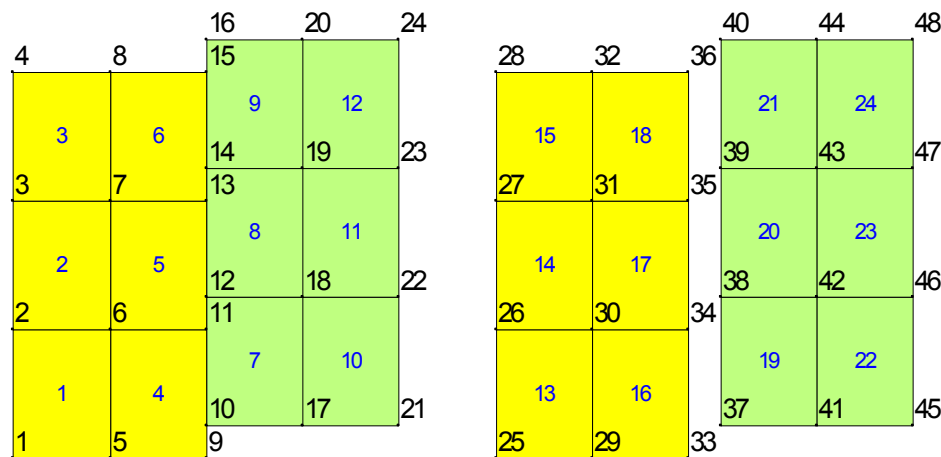


Figure 3-31 Disconnected elements – lack of compatibility



Figure 3-32 Connected elements – compatibility satisfied

5	8	13	18	23
4	2	12 6	17 10	22
3	7	11 5	16 9	21
2	1	10 4	15 8	20
1	6	9 3	14 7	19

Figure 3-33 Element incompatibility

The integer programming algorithm in GeoStudio seeks to ensure that the same number of element divisions exist between points along a region edge. The number of element divisions are automatically adjusted in each region until this condition is satisfied. It is for this reason that you will often notice that the number of divisions along a region edge is higher than what was specified. The algorithm computes the number of divisions required to achieve region compatibility.

Numerical integration

In a finite element formulation there are many integrals to be determined, as shown in the Theory chapter. For example, the integral to form the element characteristic matrix is:

$$\int [B]^T [C] [B] dv$$

For simple element shapes like 3-noded or 4-noded brick (rectangular) elements, it is possible to develop closed-form solutions to obtain the integrals, but for higher-order and more complex shapes it is necessary to use numerical integration. GeoStudio uses the Gauss quadrature scheme. Basically, this scheme involves sampling the element characteristics at specific points known as Gauss points and then adding up the sampled information. Specific details of the numerical integration in GeoStudio are presented in the Theory Chapter.

Generally, it is not necessary for most users to have a comprehensive understanding of the Gauss integration method, but it is necessary to understand some of the fundamentals since there are several options in the software related to this issue and some results are presented at the Gauss sampling points.

The following table shows the options available. Use of the defaults is recommended except for users who are intimately familiar with numerical integration and understand the significance of the various options. The integration point options are part of the meshing operations in GeoStudio.

Element Type	Integration Points	Comments
4-noded quadrilateral	4	Default
8-noded quadrilateral	4 or 9	4 is the default
3-noded triangle	1 or 3	3 is the default
6-noded triangle	3	Default

Some finite element results are computed at the Gauss sampling points. GeoStudio presents the results for a Gauss region, but the associated data is actually computed at the exact Gauss integration sampling point. Even though a Gauss region is displayed, the data is not necessarily constant within the region.

With the View Object Information command, you can click inside a region and the geometry and material information is displayed together. By expanding the mesh folder, you can review the mesh information that has been assigned to the region. The number of Gauss regions within an element is equal to the number of Gauss integration points used in the analysis.

It is important to be cognizant of the impact of Gauss points on computing time and data storage. Nine-point integration in a quadrilateral element, for example, means that the element properties need to be sampled nine times to form the element characteristic matrix and element data is computed and stored at nine points. This requires more than twice the computing time and disk storage than for four-point integration. Sometimes nine-point integration is necessary, but the option needs to be used selectively.

Secondary variables

Earlier it was noted that finite element equations are formed at the nodes and the primary unknowns are computed at the nodes. Again, in a seepage formulation the primary unknowns are the total heads at the nodes. Once the primary unknowns have been computed, other variables of interest can be computed such as the seepage gradients within the element. Since these parameters are computed after the primary values are known, they are called secondary variables.

Secondary quantities are computed at the Gauss integration points. GeoStudio displays a Gauss region, but the associated values are strictly correct only at the Gauss integration point.

For contouring and graphing, the secondary values are projected and then averaged at the nodes. This can sometimes result in unrealistic values if the parameter variations are excessive between Gauss points. The procedure and consequence of the projection from Gauss points to the nodes is discussed further in the Visualization of Results Chapter. The important point is to be aware of the fact that secondary parameters are computed at Gauss integration points.

3.9 General guidelines for meshing

Meshing, like numerical modeling, is an acquired skill. It takes practice and experience to create the ideal mesh. Experience leads to an understanding as to how the mesh is related to the solution and vice versa. It is when you can anticipate an approximation of the solution that you will be more proficient at meshing.

The attraction of the GeoStudio system is that a mesh can quickly be created with relative ease and later modified with relative ease. This makes it convenient to try various configurations and observe how the meshing influences the results.

An appropriate finite element mesh is problem-dependent and, consequently, there are no hard and fast rules for how to create a mesh. In addition, the type of mesh created for a particular problem will depend on the experience and creativity of the user. However, there are some broad guidelines that are useful to follow. They are as follows:

- Use as few elements as possible at the start of an analysis. Seldom is it necessary to use more than 1000 elements to verify concepts and get a first approximate solution.

- All elements should be visible to the naked eye when the mesh is printed at a zoom factor of 100 % and when the horizontal and vertical scales are the same. The exception to this guideline are the elements found in a surface layer.

- The mesh should be designed to answer a specific question, and it should do not include features that do not significantly influence the system behavior.

The mesh should represent a simplified abstraction of the actual complex geometric field configuration.

Number of elements

Based on many years of responding to GEO-SLOPE user support questions, most users start with a mesh that is too complex, containing too many elements for the objective of the analysis. The thinking when users first start doing finite element analyses seems to be the more elements, the better; that a large number of elements will somehow improve the accuracy of the solution. This is not necessarily true. If the mesh is too large, the time required to obtain a solution can become unattainable. Sometimes it also becomes very difficult to interpret the results, particularly if the solutions appear to be unreasonable. The effort required to determine the reason for an unreasonable solution increases dramatically with mesh size.

We highly recommend that you try and create a mesh with less than 1000 elements, particularly at the start of an analysis. Our experience is that most geotechnical problems can be modeled with 1000 elements or less. Obviously there are exceptions, but this number is a good goal to strive for. Later, once you have a good first understanding of the critical mechanisms in your problem, you can increase the mesh density to refine the analysis.

Effect of drawing scale

Another good guideline is that all elements should be visible to the naked eye when the mesh is printed or viewed at a 100% zoom factor. Groups of elements that appear as a solid or nearly solid black smudge on the drawing are too small. This means a suitable element size is related to the drawing scale. A drawing at a scale of 1:100 can have much smaller elements than a drawing at a scale of 1:2000. In other words, if it is necessary to zoom in on an area of the drawing to distinguish the elements, the elements may be unnecessarily small.

All elements should be readily distinguishable when a drawing is viewed when the vertical scale is equal to the horizontal scale. It is possible to draw a nice looking mesh at a vertical exaggerated scale, but when viewed at a true vertical scale the mesh appears as a wide black line. This effect is illustrated in Figure 3-34. The top part of the figure shows a nice mesh at 10V:100H, a 10 times vertical exaggeration. The same mesh at a scale of 100V:100H appears at the bottom of Figure 3-34. At an exaggerated scale the elements appear suitable, but at a true scale they are not appropriate.

It is important to remember that the main processor which solves the finite element equations sees the elements only at the true scale. The vertical exaggeration is used only in DEFINE and CONTOUR for presentation purposes.

A good rule to follow is to always view the mesh at a true scale before solving the problem to check that the mesh is reasonable for the purpose of the analysis.

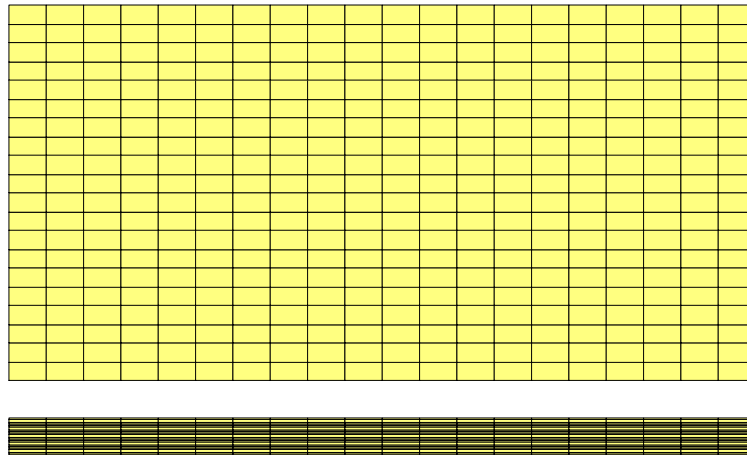


Figure 3-34 Mesh at an exaggerated scale (upper) and at a true scale (lower)

Mesh purpose

The “How To” modeling chapter notes that in good numerical modeling practice it is important to form a mental image of what the solution may possibly look like and to clearly define the purpose of the model before trying to create a model. Meshing is closely tied to this guideline. The mesh should be designed to answer specific questions. Trying to include all possible details in a mesh makes meshing unnecessarily time consuming and can sometimes make it difficult to interpret the results.

Let us assume that we are interested in estimating the seepage through the clay core of a zoned dam with rock shells. Figure 3-35 shows a typical case. The rock shells are considered to be many orders of magnitude more permeable than the core. In addition, the granular drain filter layers between the clay and the rock are clean and can easily handle any seepage through the core without impeding the drainage. In other words, the granular filter layers and rock shells make no contribution to dissipating the hydraulic head on the upstream side of the core. If this consideration is true, then there is nothing to be gained by including the highly permeable materials in the analysis. A mesh such as in Figure 3-35 is adequate to analyze the seepage through the core.

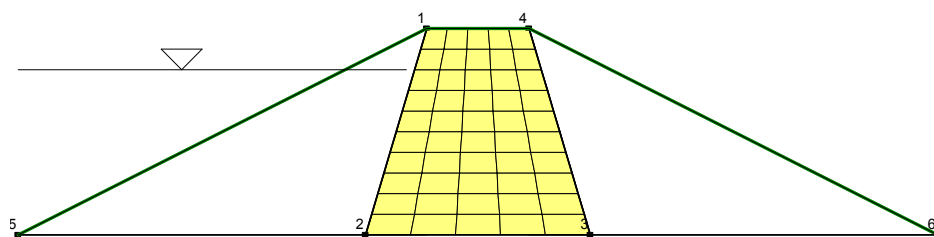


Figure 3-35 Modeling core of zoned dam

Figure 3-36 shows the total head contours (equipotential lines) in the core. From this the seepage quantities through the core can be computed.

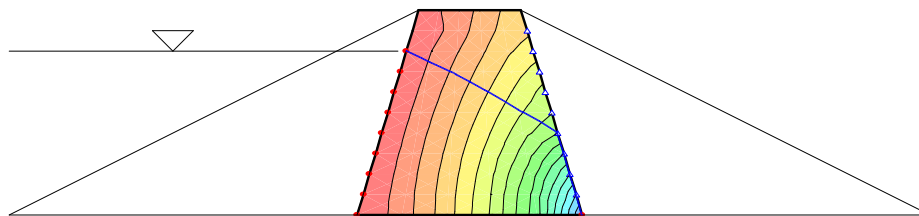


Figure 3-36 Equipotential lines in core of dam

Sometimes a mesh may be required to include the shells in the analysis for other reasons, such as a stress-deformation analysis. In such a case, the mesh can exist, but does not need to be included in the analysis. This is accomplished using null elements as shown in Figure 3-37. Elements in GeoStudio can be null (not active) by leaving a key material property undefined. In SEEP/W the elements are null if there is no specified conductivity function for the material. In the example in Figure 3-37 the rock shells have no conductivity function assigned to the material.

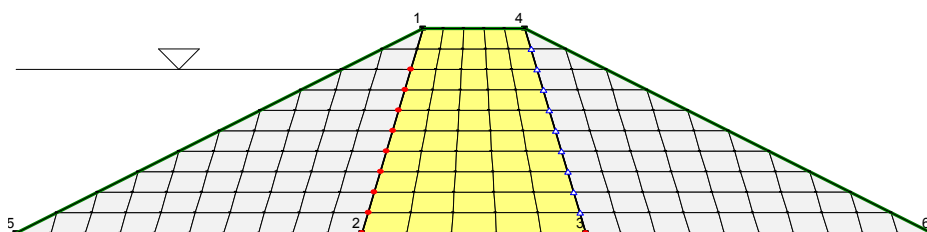


Figure 3-37 Mesh with null elements in shells of dam

One of the attractions inherent to numerical modeling is that the geometry and finite element mesh do not necessarily have to conform strictly to the physical conditions. As in Figure 3-35, the core can be analyzed in isolation. This would not be possible in physical modeling. The dam with a toe drain in Figure 3-38 is another good example. The toe drain does not have to be included in the numerical analysis. This, of course, would not be possible in a physical model.

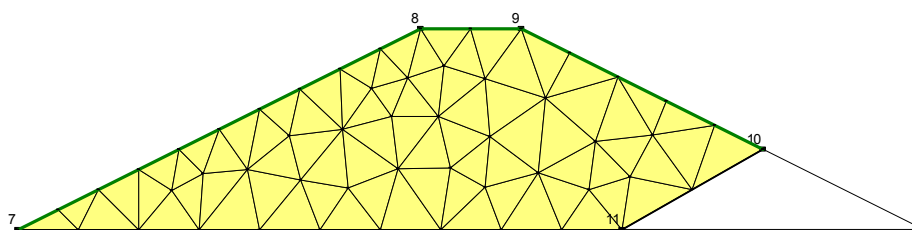


Figure 3-38 Dam with a toe drain

Simplified geometry

A numerical model needs to be a simplified abstraction of the actual field conditions. This is particularly true when it comes to the geometry. Including all surface irregularities is unnecessary in most situations. Geometric irregularities can cause numerical irregularities in the results, which distract from the main overall solution. The main message can be lost in the numerical noise.

Simplifying the geometry as much as possible is particularly important at the start of an analysis. Later, once the main processes involved are clear, the geometry can be altered to determine if the geometric details are important to the main conclusions.

The situation is different if the main objective of the analysis is to study the effects of surface irregularities. Then the irregularities of course need to be included. So, once again, the degree of geometric complexity depends on the objectives of the analysis.

Also, the level of geometric detail that needs to be included in the problem must be evaluated in light of the certainty with which other factors such as the boundary conditions and material properties are known. There is little to be gained by defining a very detailed geometry if the material properties are just a rough estimate. A simplified geometry is more than adequate if the material properties are rough estimates. There needs to be a balance in complexity between all the aspects of a finite element analysis, including the geometry.

Over-complicating the geometry is a tendency when users first get into numerical modeling. Then as modelers gain more experience they tend to use more simple geometries. This obviously comes from understanding how the mesh can influence the results and what level of complexity is required. The situation should be the reverse. It is the modelers with limited experience who should use simplified geometries.

The main message to remember when starting to model is to keep the problem as simple as possible until the main engineering issues are well understood.

4 Material Properties

4.1 Soil behavior models

This chapter describes the various soil material models and related soil properties that are required in the solution of the VADOSE/W partial differential equations. 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.

There are four different material models to choose from when using VADOSE/W with the main difference between them being related to simplifying assumptions about the thermal properties. A summary of these models and the required soil properties are given below. A discussion of the individual parameters and function are provided in the next section.

Material models in VADOSE/W

- None (used to removed part of a model in an analysis)

- Full thermal model

 - Water conductivity function, ratio and direction

 - Water content function

 - Thermal conductivity vs water content function

 - Volumetric specific heat function

 - Gas decay (half life)

- Simplified thermal model

 - Water conductivity function, ratio and direction

 - Water content function

 - Frozen and unfrozen volumetric heat capacities

 - Frozen and unfrozen thermal conductivity

 - Gas decay (half life)

- Interface model

 - Water normal and tangent conductivity

 - Thermal conductivity

The Simplified Thermal soil model is very useful for quickly defining thermal properties of a model in which you are not so concerned about the temperature influence on water flow and evaporation. If there is any doubt about which model to choose for a soil region (as opposed to an interface region), you should select the Full Thermal model.

The Interface soil model is to be used in conjunction with “interface elements” that are added to the mesh to represent geo-membranes, wick drains, or cut off walls. In these cases, you can specify a different tangent and normal conductivity – which would be the case in a wick drain where the smearing effect caused during installation results in a lower conductivity in the normal flow direction than in the tangent direction.

4.1 Soil water storage – water content function

It is important to understand the relationship between pore-water pressure, pore-air pressure and water content in a VADOSE/W analysis. Soil consists of a collection of solid particles and interstitial voids. The pore spaces or voids can be filled either with water or air, or with a combination of both. In a saturated soil, all the voids are filled with water and the volumetric water content of the soil is equal to the porosity of the soil according to:

$$\Theta_w = nS$$

where:

- Θ_w = the volumetric water content,
- n = the porosity of the soil, and
- S = the degree of saturation (in saturated soil equal to 1.0 or 100%).

The porosity, n , is related to the void ratio, e , by:

$$e = \frac{n}{1-n} = \frac{wG_s}{S}$$

where:

- w = the gravimetric water content, and
- G_s = the particle specific gravity.

In an unsaturated soil, the volume of water stored within the voids will vary depending on the matric suction within the pore-water, where matric suction is defined as the difference between the air and water pressure as follows: $U_a - U_w$.

There is no fixed water content in time and space and so a function is required to describe how the water contents change with different pressures in the soil.

The volumetric water content function describes the capability of the soil to store water under changes in matric pressures. A typical function for a drying soil is shown in Figure 4-1 where the function was measured for an air pressure of zero.

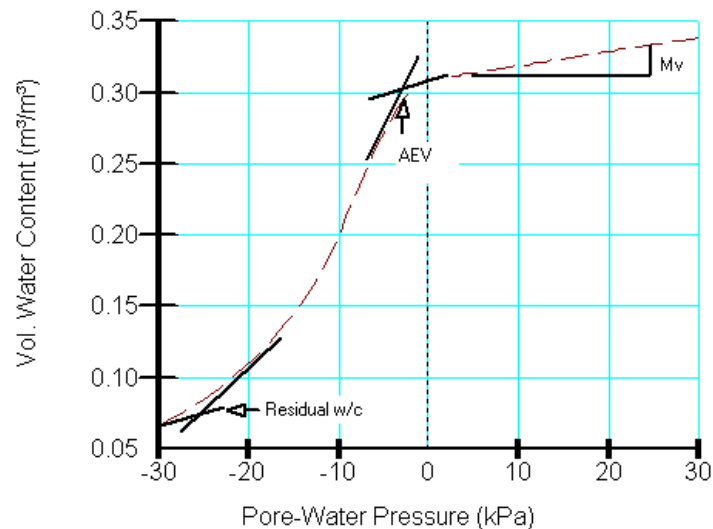


Figure 4-1 Volumetric water content (storage) function

The volumetric water content function describes what portion or volume of the voids remains water-filled as the soil drains. The three main features that characterize the volumetric water content function are the air-entry value, (AEV), the slope of the function for both the positive and negative pore-water pressure ranges (designated as m_w), and the residual water content or saturation, (θ_r or S_r). The air-entry value (AEV) corresponds to the value of negative pore-water pressure when the largest voids or pores begin to drain freely. It is a function of the maximum pore size in a soil and is also influenced by the pore-size distribution within a soil. Soils with large, uniformly shaped pores have relatively low AEV's.

Adequately representing the slope of the water content function, in both the positive and negative pore-water pressure regions, can be very important in a seepage analysis, since water can be released from the soil in two ways. Water can be released by draining the water-filled voids and desaturating the soil profile by gravitation forces, or by compressing the soil skeleton and reducing the size of the voids, effectively squeezing water out of a saturated system. In the positive pore-water pressure region, m_w becomes equivalent to m_v , the coefficient of compressibility for one-dimensional consolidation. The slope of the volumetric water content function in the negative pore-water pressure range represents the rate at which the volume of water stored within the soil changes as the pressure changes, over a range of values from the AEV to the pressure at the residual water content.

Another key feature of the volumetric water content function is the residual volumetric water content, which represents the volumetric water content of a soil where a further increase in negative pore-water pressure does not produce significant changes in water content. This point can also be expressed in terms of the degree of saturation by dividing the residual volumetric water content by the porosity of the soil. It is possible to remove water to a state less than the residual water content value, but this process is controlled by evaporation and / or osmotic forces. Evaporative drying is excluded from SEEP/W, but is included in VADOSE/W by considering simultaneous coupled heat, mass and vapor flow.

Water can be released by draining the water-filled voids and desaturating the soil profile by gravitation force; by compressing the soil skeleton and reducing the size of the voids, effectively squeezing water out of a saturated system; or by applying evaporative demand.

Factors affecting the volumetric water content

The three main features of the volumetric water content function as described above are most strongly influenced by the size of the individual soil particles and the distribution of particle sizes in the soil. By way of example, consider the differences between the volumetric water content functions for sand, silt and clay shown in Figure 4-2

There are several factors that influence the shape of the volumetric water content function. As mentioned earlier, the air-entry value (AEV) reflects how much negative pore-water pressure can be applied to the pore-water before the largest pores or voids start to drain.

Consider the uniform sand function. Since the particles are relatively large and approximately the same size, water can easily be removed under relatively small negative pore-water pressures and the resulting air entry value is smaller than that for the silt or clay. The uniform nature of the pores means that all the pores drain over a small range of negative pore-water pressures, which makes the slope of the function steeper than the others.

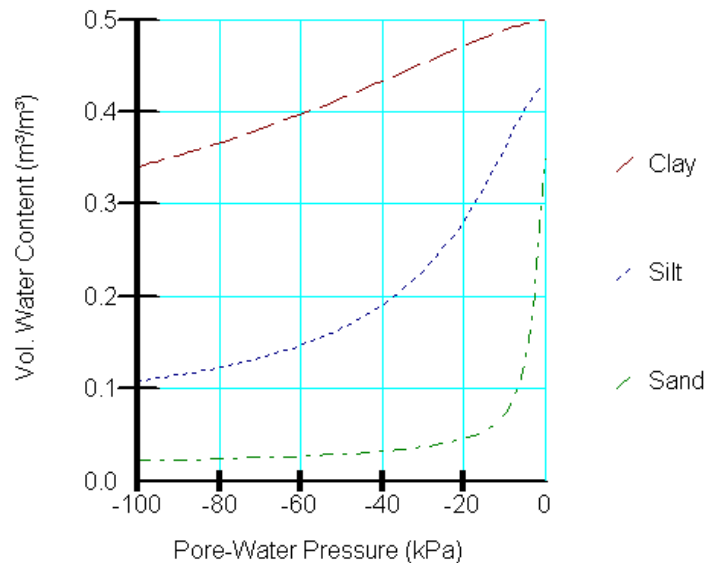


Figure 4-2 Typical storage functions for 3 soil types

The silt has a wider distribution of pore sizes. Some of the pores between the larger sand particles are filled with silt particles, making the largest pores sizes smaller than those of uniform sand. Consequently, a more negative pore-water pressure must be applied before drainage begins, thereby increasing the AEV. In addition, the pore sizes are not as uniform and the slope of the function is less steep.

The pores between the individual clay particles in the clay are small. It is often difficult to identify a specific air-entry value for clay, as consolidation and changes to the structure of the clay can release water from the system over a significant range before air actually enters the pores. Since clay tends to be compressible, the slope of the function in the positive pore-water pressure region tends to be steeper and becomes a significant parameter to consider in saturated seepage analyses.

4.2 Storage function types and estimation methods

It is not especially difficult to obtain a direct measurement of a volumetric water content function in a laboratory, but it does require time and it requires finding a geotechnical laboratory that performs the service. It is, however, standard practice to obtain a grain-size distribution curve and many companies

have the capability and facilities to develop their own curves. The development of the grain-size distribution curve is inexpensive and can be quickly accomplished.

One of the required input parameters for a transient analysis is the volumetric water content function. Since it can sometimes be difficult or time consuming to obtain a volumetric water content function, it may be of benefit to be able to develop an estimation of the volumetric water content function using either a closed-form solution that requires user-specified curve-fitting parameters, or to use a predictive method that uses a measured grain-size distribution curve. VADOSE/W has four methods available to develop a volumetric water content function. One is a predictive methods based on grain size, one is to base your function of a sample set of functions built into the software, and two are closed form equations based on known curve fit parameters.

Estimation method 1 (grain size - Modified Kovacs)

Aubertin et al (2003) presented a method to predict the volumetric water content function which is modified from the method proposed by Kovacs (1981). The modifications were made to Kovac's method to better represent materials such as tailings from hard-rock mines. A further modification extended the method for clay type soils. The Aubertin et al. method predicts the volumetric water content function using basic material properties which can be useful, particularly for preliminary analysis. It should be cautioned that, especially for clay type materials, it is critical to base final design on measured material properties.

The function is initially determined as a degree of saturation function and then is later converted to a volumetric water content function. The function is developed by defining the degree of saturation for two main components. The first component contributes to the amount of water that is stored in a soil by capillary forces that exist at relatively small negative pore-water pressures. The second component contributes to the volumetric water content function at large negative pore-water pressures where the amount of water that exists in the soil is primarily a function of adhesion. Both of these components can be evaluated from the negative pore-water pressure and material property information such as particle-size, the shape of the particles and the porosity.

The degree of saturation as determined based on the capillary and adhesive components is as follows:

$$S_r = \frac{\Theta_w}{n} = S_c + S_a^*(1 - S_c)$$

where:

S_r = the degree of saturation,

Θ_w = the volumetric water content,

n = the porosity,

S_c = the degree of saturation due to capillary forces, and

S_a^* = the bounded degree of saturation due to adhesion (S_a).

where:

$$S_a^* = \langle 1 - S_a \rangle + 1$$

The adhesive component is a bounded value since it is possible at low suctions for the value S_a to be greater than 1. The bounded value ensures that for a S_a greater or equal to 1, $S_a^* = 1$ and if S_a is less than 1, then $S_a^* = S_a$.

The adhesion component is associated with the thin film of water that covers the surface of the soil grain and depends on basic material properties such as the negative pore-water pressure in the soil and the particle-size, shape coefficient and porosity of the soil. It is determined by the following equation:

$$S_a = aC_\Psi \frac{\left(\frac{h_{co}}{\Psi_n}\right)^{2/3}}{e^{1/3} \left(\frac{\Psi}{\Psi_n}\right)^{1/6}}$$

where:

- a = a curve fitting parameter,
- Ψ = the suction,
- Ψ_n = a suction term introduced to ensure dimensionless component,
- e = the void ratio,
- h_{co} = the mean capillary rise (cm) determined for capillary soils by:

$$h_{co} = \frac{b(cm^2)}{eD_{10}(cm)}$$

or

$$h_{co} = \frac{\xi w_L^{1.75}}{e}$$

for cohesion type soils where:

- D_{10} = the particle diameter (cm) corresponding to 10% passing on a grain-size curve,

$b(cm^2)$ = is given by:

$$b(cm^2) = \frac{0.75}{1.17 \log C_u + 1}$$

where:

- C_u = the coefficient of uniformity,
- w_L = the liquid limit (%),
- ξ = a constant approximately equal to 402.2 cm^2 ,
- C_Ψ = a correction coefficient that allows a progressive decrease in water content at high suctions, forcing the function through a water content of zero at one million kPa suction as initially proposed by Fredlund and Xing (1994) and described by:

$$C_{\Psi} = 1 - \frac{\ln\left(1 + \frac{\Psi}{\Psi_r}\right)}{\ln\left(1 + \frac{\Psi_o}{\Psi_r}\right)}$$

where:

Ψ_r = the suction corresponding to the residual water content at which point an increase in suction will not effectively remove more liquid water from the soil and given by:

$$\Psi_r = 0.86 \left(\frac{\xi}{e} \right)^{1.2} w_L^{1.74}$$

The capillary saturation, which depends essentially on the pore diameter and the pore size distribution, is given by:

$$S_c = 1 - \left[\left(\frac{h_{co}}{\Psi} \right)^2 + 1 \right]^m \exp \left[-m \left(\frac{h_{co}}{\Psi} \right)^2 \right]$$

where:

m = a fitting parameter that takes into account the pore size distribution and controls the shape and position of the volumetric water content function in the capillary zone.

For plastic-cohesive soils considered here, both the value of parameters m and a can be taken as constants with $m=3 \times 10^{-5}$ and $a=7 \times 10^{-4}$ in the predictive applications. For the capillary based soils, m and a can be taken as 1 and 0.01 respectively.

Estimation method 2 (sample functions)

GeoStudio provide several “typical” water content functions for different types of soils. In using these sample functions, it is up to you to specify the saturated water content and the residual water content (if any) based on your understanding of field conditions. These functions are provided as a means to letting you set up some test models quickly, change functions easily, decide how sensitive your results are to function shape, and ultimately to have you decide if you need to spend more time and money obtaining more accurate data. In the past, our list of “real” functions ended up being used as final design material properties with little thought about their relevance. This is not good modeling practice.

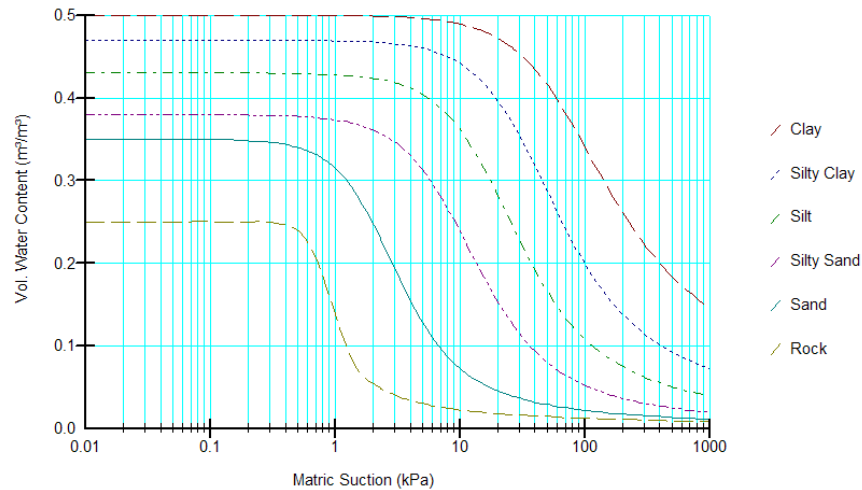


Figure 4-3 Sample Functions in GeoStudio

Closed form option 1 (Fredlund and Xing, 1994)

The Fredlund and Xing (1994) method is a closed-form solution that can be used to develop the volumetric water content function for all possible negative pressures between zero and minus one million kPa based on the user's knowledge of a group of three parameters. The governing equation is as follows:

$$\Theta_w = C_\psi \frac{\Theta_s}{\left\{ \ln \left[e + \left(\frac{\Psi}{a} \right)^n \right] \right\}^m}$$

where:

- Θ_w = the volumetric water content,
- C_ψ = the correction function described above,
- Θ_s = the saturated volumetric water content,
- e = the natural number (2.71828),
- Ψ = the negative pore-water pressure, and
- a, n, m = curve fitting parameters.

The 'a' parameter, which has units of kPa, is the inflection point of the volumetric water content function. It is generally slightly larger than the air-entry value. The parameter n controls the slope of the volumetric water content function and the m parameter controls the residual water content. The three parameters a, n, and m are determined as follows:

$$a = \Psi_i$$

$$m = 3.67 \ln \left(\frac{\Theta_s}{\Theta_i} \right)$$

$$n = \frac{1.31^{m+1}}{m\Theta_s} 3.72s\Psi_i$$

where:

Ψ_i = the suction pressure corresponding to the water content occurring at the inflection point of the curve, and
 s = the slope of the line tangent to the function that passes through the inflection point.

The Fredlund and Xing, 1994 method is only functional if you know values of a , n and m . In general, the a , n and m values can be determined using a fitting algorithm and applying it to measured data points. VADOSE/W has this ability.

It is important to understand that this method is not intended to predict a volumetric water content function from grain-size curves, but was developed to obtain a smooth function over the complete range of negative pore-water pressure values (0 to one Million kPa).

Closed form option 2 (Van Genuchten, 1980)

In 1980, van Genuchten proposed a four-parameter equation as a closed form solution for predicting the volumetric water content function. The governing equation is as follows:

$$\Theta_w = \Theta_r + \frac{\Theta_s - \Theta_r}{\left[1 + \left(\frac{\Psi}{a} \right)^n \right]^m}$$

where:

Θ_w = the volumetric water content,
 Θ_s = the saturated volumetric water content,
 Ψ = the negative pore-water pressure, and
 a, n, m = curve fitting parameters (note: “ a ” has units of pressure, not 1/pressure head as in some formulations of this equation)

Although the terminology of the a , n and m parameters are similar to those of Fredlund and Xing (1994), the definitions are slightly different. The a parameter in particular cannot be estimated by the air-entry value, but instead is a pivot point about which the n parameter changes the slope of the function. The parameter m affects the sharpness of the sloping portion of the curve as it enters the lower plateau. The van Genuchten closed form method can only be used then the curve fit parameters are known, but there are some references to these values in the literature that can be applied in the model.

CAUTION: the units of the “ a ” value should be checked to make sure they are consistent between your data source and VADOSE/W, which requires the units be in terms of pressure and not 1/pressure.

4.3 Coefficient of volume compressibility

The coefficient of volume compressibility m_v is the slope of the volumetric water content function in the positive pore pressure range. The coefficient characterizes the volume of water stored or released from the soil when the pore-water pressure changes. More fundamentally, the coefficient of volume compressibility embodies the compressibility of the soil structure and water. The coefficient of volume compressibility can be calculated from specific storage, which is given by:

$$S_s = \rho g (\alpha + n\beta) = \rho g (m_v)$$

where:

ρ	=	the water density,
g	=	the gravitational constant,
α	=	the compressibility of the soil structure,
n	=	the soil porosity, and
β	=	the compressibility of the water.

Water can be assumed incompressible for most geotechnical applications. The coefficient of volume compressibility is often assumed equivalent to the coefficient obtained from a 1D compression test; however, this assumption is not strictly valid unless a constrained flow system is being simulated. In that case, or as an approximation, the coefficient of volume change can be calculated as:

$$m_v = \frac{1}{M} = \frac{a_v}{1 + e_0}$$

where:

M	=	the modulus of elasticity in confined compression. It is also given by:
a_v	=	the coefficient of compressibility, and
e_0	=	the initial void ratio.

The metric units for the coefficient of volume compressibility are 1/kPa and the value generally ranges from 1e-6 1/kPa to 1e-3 1/kPa for most soils.

4.4 Hydraulic conductivity

The ability of a soil to transport or conduct water under both saturated and unsaturated conditions is reflected by the hydraulic conductivity function. In a saturated soil, all the pore spaces between the solid particles are filled with water. Once the air-entry value is exceeded, air enters the largest pores and the air-filled pores become non-conductive conduits to flow and increase the tortuosity of the flow path as shown schematically in Figure 4-4. As a result, the ability of the soil to transport water (the hydraulic conductivity) decreases. As pore-water pressures become increasingly more negative, more pores become air-filled and the hydraulic conductivity decreases further. By this description, it is clear that the ability of water to flow through a soil profile depends on how much water is present in the soil, which is represented by the volumetric water content function. Actually measuring the hydraulic conductivity function is a time-consuming and expensive procedure, but the function can be readily developed using

one of several predictive methods that utilize either a grain-size distribution curve or a measured volumetric water content function and the saturated hydraulic conductivity. VADOSE/W has built-in predictive methods that can be used to estimate the hydraulic conductivity function once the volumetric water content function and a K_{sat} value have been specified.

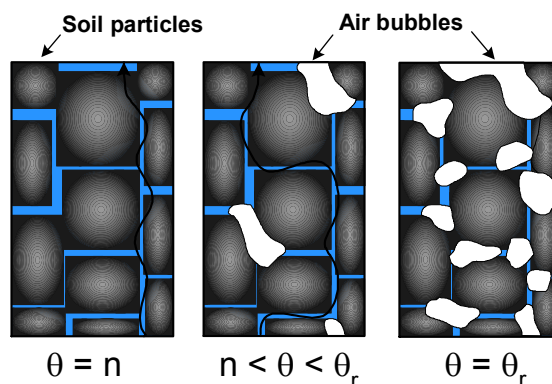


Figure 4-4 Availability of water filled flow paths from saturation to residual

A hydraulic conductivity function should be specified for all materials in a problem that will have an unsaturated zone. Even if the hydraulic conductivity function is an estimate, the results will be more realistic than if the function is omitted or entered as a flat horizontal line. In a unsaturated seepage analysis with negative surface fluxes (such as evaporation) where negative pressures can become extreme, the conductivity function should be defined over a pressure range that exceeds several hundred thousand kPa (or equivalent) of negative pressure. If the function is not defined over the full range, the lowest specified value will be used for any increasingly negative pressures.

Adopting a perfectly flat hydraulic conductivity function (i.e., a constant conductivity) for an unsaturated soil can lead to unrealistic results. The phreatic surface may end up at an unrealistic position, and the proportion of flow through the unsaturated zone may be too high. This occurs because with a horizontal conductivity function, water can flow through the unsaturated zone with the same ease as through the saturated zone. In other words, for a given constant head differential, the volume of flow is the same in the unsaturated zone as in the saturated zone when the hydraulic conductivities in the two zones are the same. In general, water cannot flow through unsaturated soil with the same ease as through saturated soil, because the unsaturated hydraulic conductivity is lower than that of a saturated soil.

To illustrate the effect of assuming that hydraulic conductivity is independent of negative pore-water pressure (i.e., a perfectly flat conductivity function), consider the example of seepage flow through a rectangular screened box, as shown in Figure 4-5. Initially, the box is filled with clay. The phreatic surface will have the form of a hyperbolic curve (top of figure). In the bottom of the figure, the box is enlarged, the upstream half is filled with clay, and the downstream half is filled with sand. The sand is assigned a perfectly flat hydraulic conductivity function. In this case, the phreatic surface in the clay will be at a lower position. The reason for this is that a significant portion of the flow passes through the unsaturated sand. Since the resistance to flow is the same in the unsaturated sand as in the saturated sand, there is no reason for the sand to be saturated in order to conduct the water. Intuition alone reveals that this is not the case. The phreatic surface in the clay should be approximately the same in both configurations, and the seepage that arrives at the clay-sand contact should flow vertically down the contact and then horizontally along the bottom of the box to the exit point at the lower right corner.

To model the clay-sand configuration, the sand needs to be assigned a very steep function, such that as soon as the sand desaturates, the hydraulic conductivity drops dramatically. This ensures that there is no significant flow in the unsaturated sand. However, a nearly vertical function may cause convergence

difficulties. A compromise would be to use a moderately steep hydraulic conductivity function, which would eliminate the majority of the flow in the unsaturated sand and yet produce a reasonable result. It would certainly be closer to the correct solution than for the first case where the sand has a perfectly flat hydraulic conductivity function.

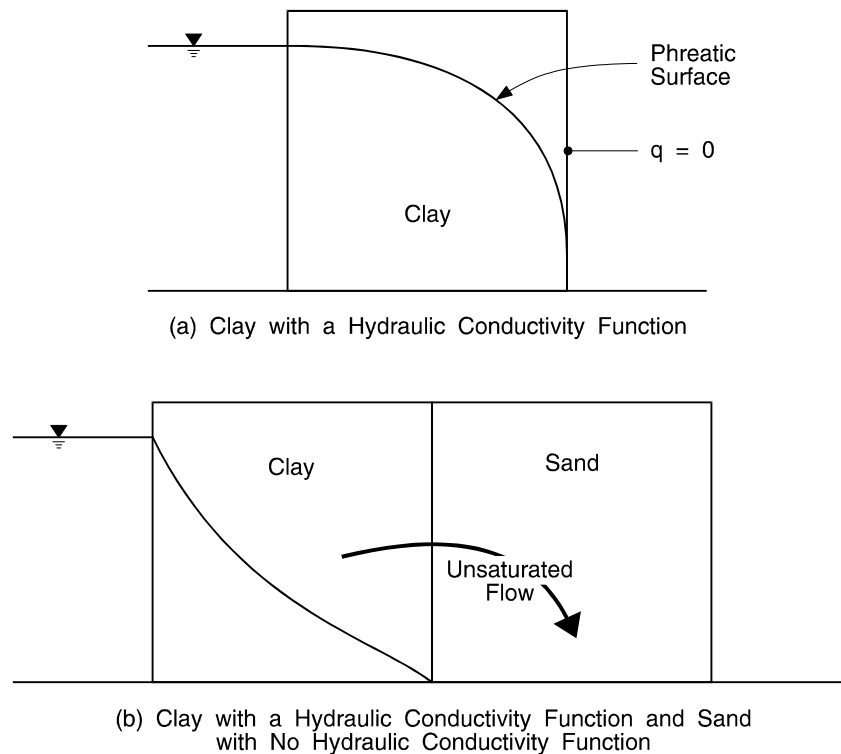


Figure 4-5 Comparison of flow with and without a K function

Coarse granular materials essentially have an infinitely steep (vertical) hydraulic conductivity function when unsaturated. The soil desaturates completely when the pore-water pressure is zero or negative; consequently, no flow passes through such a soil when it is unsaturated. As a result, the hydraulic conductivity in the unsaturated zone should be infinitely low.

Whenever a problem contains a coarse granular soil that ideally has a near vertical hydraulic conductivity function when unsaturated, it is necessary to ask the question, "Does the material contribute to the dissipation of the head?" If it does not, then consideration should be given to excluding the material from the analysis. In the clay-sand box example, the sand may not contribute to dissipating the head. Consequently, a reasonable solution might be obtained by excluding the sand from the analysis and treating the vertical contact between the two materials as a boundary. The decision as to whether the sand should be included in the analysis must also be made in light of the question, "Does the negative pore-water pressure in the sand contribute to increasing the gradient in the clay?" If it does, the sand must be included in the analysis.

The accuracy with which the hydraulic conductivity needs to be specified depends to some extent on the objective of the analysis. If the primary objective is to compute the distribution of pore-water pressure, then an approximate function may be adequate. On the other hand, if the objective of the analysis is to make reliable time predictions, then it may be necessary to define the storage and hydraulic conductivity with the assistance of laboratory tests.

The level of effort required to define the material functions can be evaluated by performing several analyses with different assumed functions. Performing such a sensitivity analysis can greatly increase the confidence level of the computed results.

In summary, a hydraulic conductivity function must be specified for each material included in an analysis, even if the function is only an approximation.

An approximated curved conductivity relationship in the unsaturated zone results in a much better solution than using a straight, horizontal line.

4.5 Frozen ground hydraulic conductivity

VADOSE/W can be used to model transient seepage behavior in frozen, partially frozen, or actively freezing ground. An example of seepage flow being diverted around an active freezing region is illustrated in Figure 4-6 and Figure 4-7. VADOSE/W uses knowledge of the soil temperature so that it can estimate the reduction in hydraulic conductivity associated with pore-water becoming pore-ice. This estimate is based on knowledge of the soil's unfrozen water content function.

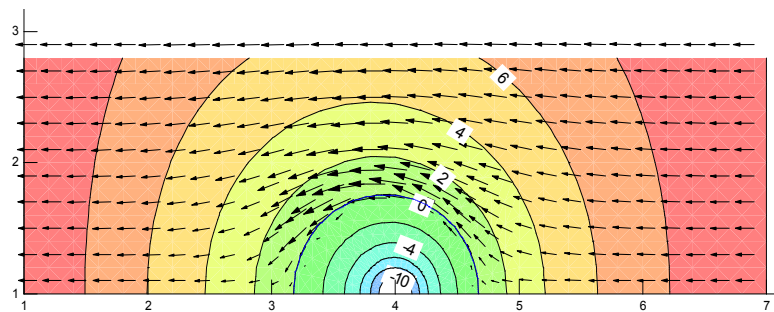


Figure 4-6 Temperature contours and water flow

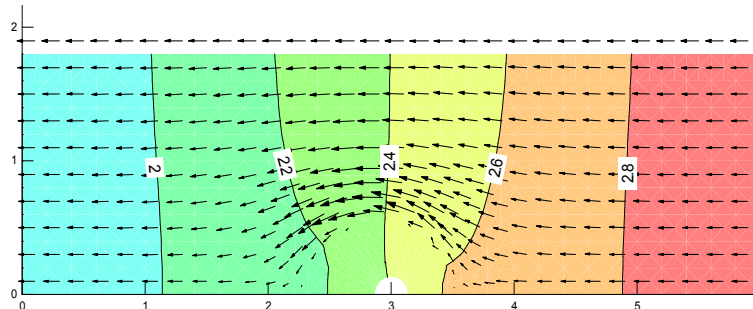


Figure 4-7 Head contours and water flow

The unfrozen water content function relates the amount of unfrozen water to a temperature below freezing and its curve is very similar in appearance to a soil water characteristic curve when plotted on a semi-log scale. The unfrozen water content curve can serve three purposes. It can be used to determine the freezing point depression for pore-water in soils at a given water content below saturation; it can be used to determine the amount of water that remains unfrozen at any given temperature below freezing; and the slope of the curve determines how much latent heat is added to the system by the phase change during the heat and mass transfer analysis.

Ideally, a soil freezing curve should be measured, but this is difficult to do. It is possible to estimate the curve using a measured soil water characteristic (storage) curve and the Clapeyron equation, which relates changes in suction to change in temperature based on equilibrium thermodynamics. Analysis of the Gibbs

free energy for any two phases in equilibrium can be used to derive the Clapeyron equation, which relates how the equilibrium pressure changes with a change in temperature. The reduced form of the Clapeyron equation as applied to the soil freezing scenario is given by Black and Tice (1989) as follows:

$$\text{Equation 4-1} \quad \Delta\Psi = -1110\Delta T$$

where:

$$\begin{aligned} \Delta\Psi &= \text{the soil matric suction (kPa), and} \\ T &= \text{the soil temperature below zero Celsius.} \end{aligned}$$

The constant value equal to 1110 kPa/oC combines the latent heat of fusion value, specific volume, and the conversion between the freezing temperature of water in Kelvin and degrees Celsius.

If the soil temperature below zero Equation 4-1 is used to estimate what the approximate frozen condition suction would be such that this suction is used to determine the hydraulic conductivity at each gauss point with freezing temperatures (Newman, 1996).

Seepage analysis in freezing ground can be very complicated, especially in the direct vicinity of the phase change region. At this location it is possible for certain types of soil to experience “cryogenic suction” which results in very steep pressure gradients that can draw water towards the freezing front where it can accumulate and cause frost heave. In the VADOSE/W model, this phenomenon is not accounted for. While the suctions are estimated based on temperature and used to determine frozen ground hydraulic conductivity, they are not directly coupled with the thermal equation and therefore only change due to the solution of the seepage partial differential equation.

4.6 Conductivity function estimation methods

The difficult task of measuring the unsaturated hydraulic conductivity function directly is often overcome by predicting the unsaturated hydraulic conductivity from either a measured or predicted volumetric water content function, such as the one illustrated in Figure 4-1. Consequently, this is the preferred approach if a suitable predictive model is available. These estimation methods generally predict the shape of the function relative to the saturated conductivity value which is easily obtained.

VADOSE/W has three separate methods built into the model that can be used to predict unsaturated hydraulic conductivity functions using either a measured or estimated volumetric water content function or a saturated hydraulic conductivity function.

Method 1 (Fredlund et al, 1994)

This method consists of developing the unsaturated hydraulic conductivity function by integrating along the entire curve of the volumetric water content function. The governing equation of this method is:

$$k_w = k_s \frac{\sum_{i=j}^N \frac{\Theta(e^y) - \Theta(\Psi)}{e^{y_i}} \Theta'(e^{y_i})}{\sum_{i=1}^N \frac{\Theta(e^y) - \Theta_s}{e^{y_i}} \Theta'(e^{y_i})}$$

where:

$$k_w = \text{the calculated conductivity for a specified water content or negative pore-water pressure (m/s),}$$

- k_s = the measured saturated conductivity (m/s),
 Θ_s = the volumetric water content,
 e = the natural number 2.71828,
 y = a dummy variable of integration representing the logarithm of negative pore-water pressure,
 i = the interval between the range of j to N ,
 j = the least negative pore-water pressure to be described by the final function,
 N = the maximum negative pore-water pressure to be described by the final function,
 Ψ = the suction corresponding to the j^{th} interval, and
 Θ' = the first derivative of the equation ...

$$\Theta = C(\Psi) \frac{\Theta_s}{\left\{ \ln \left[e + \left(\frac{\Psi}{a} \right)^n \right] \right\}^m}$$

where:

- a = approximately the air-entry value of the soil,
 n = a parameter that controls the slope at the inflection point in the volumetric water content function,
 m = a parameter that is related to the residual water content, and
 $C(\Psi)$ = a correcting function defined as

Equation 4-2

$$C(\Psi) = 1 - \frac{\ln \left(1 + \frac{\Psi}{C_r} \right)}{\ln \left(1 + \frac{1,000,000}{C_r} \right)}$$

where:

- C_r = a constant related to the matric suction corresponding to the residual water content.

A typical value is about 1500 kPa. The value 1,000,000 in Equation 4-2 corresponds to the matric suction (in kPa) at which there is zero moisture remaining in the soil in a liquid or vapor phase.

Method 2 (Green and Corey, 1971)

The Green and Corey equation is:

Equation 4-3

$$k(\Theta)_i = \frac{k_s}{k_{sc}} \cdot \frac{30 T^2}{\mu g \eta} \cdot \frac{\xi^p}{n^2} \cdot \sum_{j=i}^m \left[(2j + 1 - 2i) h_i^{-2} \right]$$

where:

- $K(\Theta)_i$ = the calculated conductivity for a specified water content or negative pore-water pressure (cm/min),

$\frac{k_s}{k_{sc}}$	=	the matching factor (measured saturated conductivity / calculated saturated conductivity),
i	=	the last water content class on the wet end (e.g. $i=1$ identifies the pore class corresponding to the lowest water content, and $i = m$ identifies the pore class corresponding to the saturated water content),
h_i	=	the negative pore-water pressure head for a given class of water-filled pores (cm of water),
n	=	the total number of pore classes between i and m ,
Θ	=	volumetric water content (cm ³ /cm ³),
T	=	surface tension of water (Dyn/cm),
ξ	=	the water-saturated porosity,
η	=	the viscosity of water (g/cm •s-1),
g	=	the gravitational constant (cm/s-1),
μ	=	the density of water (g/cm ³), and
p	=	a parameter that accounts for the interaction of pore classes.

The following are some suggested values of p given by various authors: Marshall (1958): 2.0; Millington and Quirk (1961): 1.3; and Kunze, Vehara and Graham (1968): 1.0.

The shape of the conductivity function is controlled by the term:

$$\sum_{j=i}^m \left[(2j + 1 - 2i) h_i^{-2} \right]$$

in Equation 4-3.

The term:

$$\frac{30 T^2}{\mu g \eta} \cdot \frac{\xi^p}{n^2}$$

is a constant for a particular function and can be taken to be 1.0 when determining the shape of the hydraulic conductivity function. This is the assumption made in VADOSE/W.

VADOSE/W first computes the hydraulic conductivity at the zero pressure value using the equation,

$$k_{sc} = \sum_{j=i}^m \left[(2j + 1 - 2i) h_i^{-2} \right]$$

The saturated conductivity k_s is a user-defined value in VADOSE/W. When k_s is specified, the entire conductivity function is moved up or down by a constant ratio of k_s / k_{sc} .

In summary, VADOSE/W uses the Green and Corey equation to estimate the shape of the conductivity function and then moves the curve up or down so that the function passes through the user-specified value of k_s .

Method 3 (Van Genuchten, 1980)

Van Genuchten (1980) proposed the following closed form equation to describe the hydraulic conductivity of a soil as a function of matric suction:

$$k_w = k_s \frac{\left[1 - (a\Psi^{(n-1)}) \left(1 + (a\Psi^n)^{-m}\right)\right]^2}{\left(\left(1 + a\Psi^n\right)^{\frac{m}{2}}\right)}$$

where:

- k_s = saturated hydraulic conductivity,
 a, n, m = curve fitting parameters,
 n = $1/(1-m)$, and
 Ψ = required suction range.

From the above equations, the hydraulic conductivity function of a soil can be estimated once the saturated conductivity and the two curve fitting parameters, a and m are known.

Van Genuchten (1980) showed that the curve fitting parameters can be estimated graphically based on the volumetric water content function of the soil. According to van Genuchten, the best point to evaluate the curve fitting parameters is the halfway point between the residual and saturated water content of the volumetric water content function.

The slope of the function can be calculated as:

$$S_p = \frac{1}{(\Theta_s - \Theta_r)} \left| \frac{d\Theta_p}{d(\log \Psi_p)} \right|$$

where:

- Θ = the saturated and residual volumetric water contents respectively,
 Θ_p = the volumetric water content at the halfway point of the volumetric water content function, and
 Ψ_p = the matric suction at the same point.

Van Genuchten (1980) proposed the following formula to estimate the parameters m and a when S_p is calculated:

$$m = 1 - \exp(-0.8S_p)$$

for S_p between 0 and 1;

$$m = 1 - \frac{0.5755}{S_p} + \frac{0.1}{S_p^2} + \frac{0.025}{S_p^3}$$

for $S_p > 1$; and

$$a = \frac{1}{\Psi} \left(2^{\frac{1}{m}} - 1 \right)^{(1-m)}$$

4.7 Interface model parameters

The interface model allows you to assign a material model to a line and to give that line a thickness. In a seepage application, you may want to use an interface model to simulate a thin liner or a wick drain. When you assign an interface model to a line you must give it hydraulic conductivity values that are both normal and tangent to the direction of the line as shown in Figure 4-8. The thermal conductivity value you specify is independent of direction.

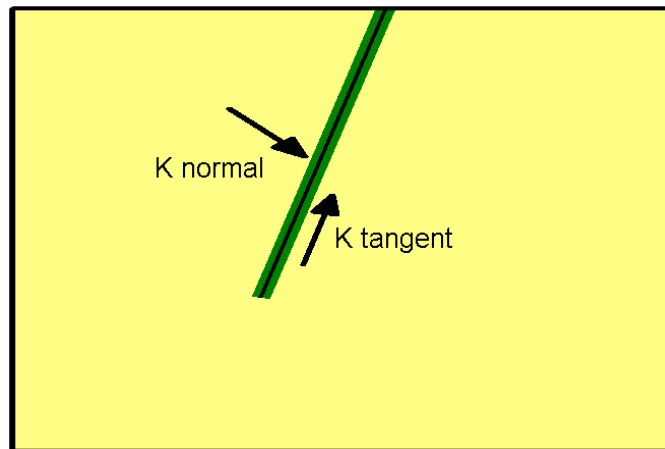


Figure 4-8 Illustration of interface model assigned to a line

4.8 Thermal functions

Unfrozen water content function

Fundamental to the formulation of a general freeze-thaw thermal analysis of soil systems is an understanding of how energy stored in the soil varies as the soil temperature changes. An example of this relationship is shown in Figure 4-9. The function represents the relative energy required for the soil medium to sustain a certain temperature. The steep part of the function in the region of the freeze-thaw front represents the latent heat absorbed or released by a soil due to phase changes of the soil water. The slope of the function away from the freeze-thaw zone represents the volumetric heat capacity of the frozen and unfrozen zones.

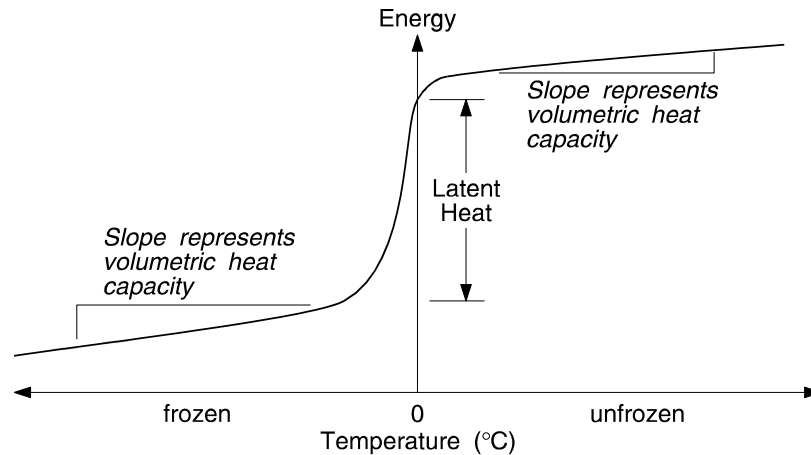


Figure 4-9 Significance of an energy storage function

Unlike the case of a pure water medium, water within a soil changes phase over a temperature range. In other words, not all of the water within the soil experiences a phase change at a single temperature. The percentage of the soil water volume that remains unfrozen at a certain temperature is referred to as the unfrozen water content. Examples of the unfrozen water content function for a variety of soils are illustrated in **Error! Reference source not found.** In general, the unfrozen volumetric water content function is very steep for coarse grained soils and shallower for fine grained soils.

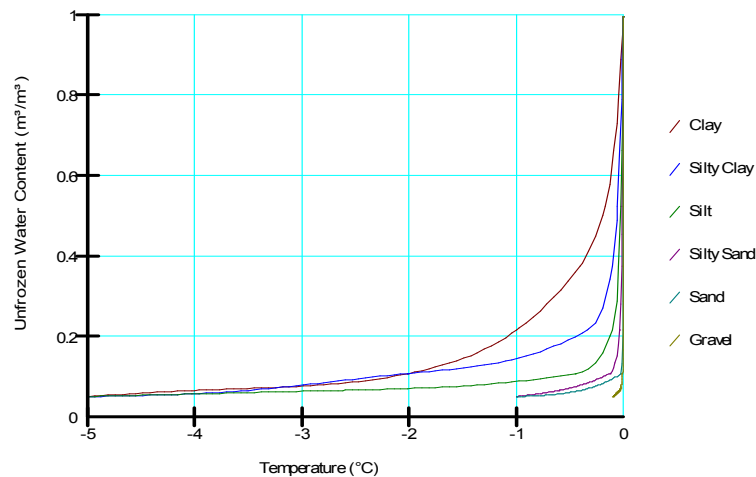


Figure 4-10 Sample unfrozen water content functions

In GeoStudio, the unfrozen water content is normalized to the porosity and therefore varies between 0 and 1.0. Accordingly, a single function could be used for different soils by adjusting the user-input insitu volumetric water content. Both the Full thermal and Coupled convective thermal models require an unfrozen volumetric water content function. The Simplified thermal model does not require an unfrozen volumetric water content function because it assumes that all water in the soil changes phase at a single temperature.

Thermal conductivity

Thermal conductivity k , which characterizes the ability of a soil medium to transmit heat by conduction, is defined as the quantity of heat that will flow through a unit area of a soil of unit thickness in unit time under a unit temperature gradient. Thermal conductivity units are commonly given as J/(sec.m.°C), kJ/(day.m.°C) or Btu/(hr.ft.°F).

At temperatures above zero (0°C), the thermal conductivity tends to increase with increasing water content (see Harlan and Nixon, 1978, pp. 103-163). At temperatures below zero (0°C), the thermal conductivity is usually greater than that of an unfrozen soil, since the thermal conductivity of ice is much higher than water. The thermal conductivity of frozen soil is highly dependent on the unfrozen water content within the soil.

Furthermore, coarse-grained soils are commonly dominated by quartz, which has a relatively large thermal conductivity; fine-grained soils are dominated by clayey minerals, which generally have a substantially lower thermal conductivity.

The Simplified thermal model assumes that the frozen and unfrozen thermal conductivities are constant with temperature. The material model also makes the tacit assumption that the water content is constant throughout the duration of the analysis. The Full thermal model also assumes constant water content, but the thermal conductivity is a function of temperature (Figure 4-11).

In a coupled convective analysis, the volumetric water content is known from the water transfer analysis; so the user must specify a thermal conductivity versus volumetric water content function for the unfrozen soil. The thermal conductivity of frozen soil is computed internally by the solver as a function of ice, water, air and soil mineral content.

If the ice content is greater than zero, the soil particle thermal conductivity is back-calculated. The frozen soil thermal conductivity at the given water content is calculated assuming all water is frozen according to:

$$K_f = (K_{ice})^{wc} (K_{soil})^{1-wc}$$

This relationship is based on that proposed by Johansen (1975) and described in the following section.

Once the fully frozen conductivity is known, the partially frozen thermal conductivity of the ground is assumed to be linearly partitioned between the unfrozen and frozen states by the ratio of ice content to water content.

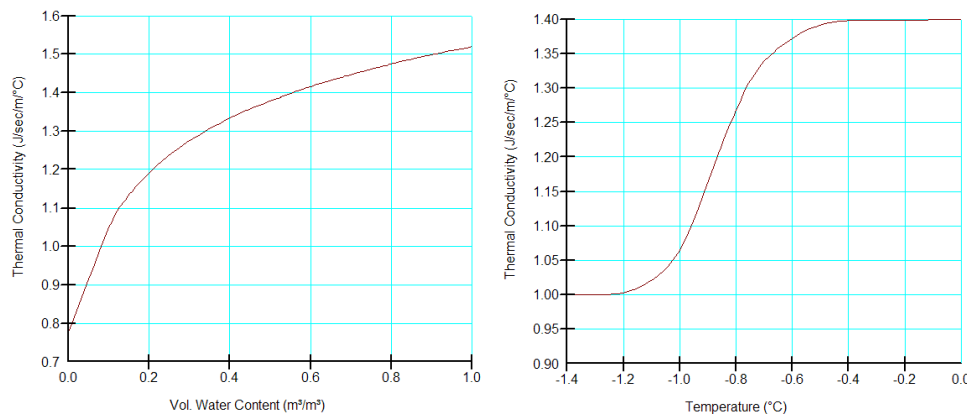


Figure 4-11 Two types of thermal conductivity functions

Estimating thermal conductivity for soils

Various empirical or semi-empirical methods have been developed for estimating the thermal conductivity of soils. These methods have been evaluated in detail by Farouki, (1981), who concluded that different types of soils may require different estimation methods. The method developed by Johansen (1975), however, appears to be the most general method. Since it is beyond the scope of this chapter to present the various estimation methods, only Johansen's method is presented in this section.

For dry, natural soils, the thermal conductivity k_{dry} can be estimated based on its dry density using the following equation:

$$K_{dry} = \frac{0.135\gamma_d + 64.7}{2700 - 0.947\gamma_d} \pm 20\%$$

where the dry density γ_d is in kg/m³ and the unit weight of soil particles is taken as 2700 kg/m³.

For dry crushed rock materials, the thermal conductivity k_{dry} can be estimated based on its porosity n using the following equation:

$$K_{dry} = 0.039n^{-2.2} \pm 25\%$$

For a saturated unfrozen soil, the thermal conductivity k_{sat} is estimated based on the thermal conductivities of its components and their respective volume fractions.

$$K_{sat} = (K_s)^{1-n} (K_w)^n$$

where, k_s is the thermal conductivity of the soil particles, and k_w is the thermal conductivity of the pore water.

For a saturated frozen soil containing some unfrozen water content, w_u , the thermal conductivity k_{sat} becomes:

$$K_{sat} = (K_s)^{1-n} (K_i)^{n-w_u} (K_w)^{w_u}$$

where k_i is the thermal conductivity of ice.

For an unsaturated soil, the thermal conductivity k_{unsat} is estimated based on its saturated conductivity, dry conductivity and degree of saturation S using the following equation:

$$K_{unsat} = (K_{sat} - K_{dry})K_e + K_{dry}$$

where:

$$\begin{aligned} K_e &= 0.7 \text{ Log}S + 1.0 \text{ for unfrozen coarse grained soil,} \\ K_e &= \text{Log}S + 1.0 \text{ for unfrozen fine grained soil, and} \\ K_e &= S \text{ for frozen soil.} \end{aligned}$$

The above equations may be used for an approximate estimation of the thermal conductivity of a soil. It is the user's responsibility to ensure the applicability of the above equations to the respective soils.

Typical values of thermal conductivity

Error! Reference source not found. provides typical values of thermal conductivity for various materials (extracted from Johnston, Ladanyi, Morgenstern, and Penner, 1981). When using this data in the function estimation routine in GeoStudio, make sure the engineering units of the data you select match the units set you have chosen for the model and make sure you have set your time units prior to estimating these functions.

Figure 4-12 and Figure 4-13 show typical thermal conductivity functions for both the full thermal and coupled convective thermal models. These functions were based on sample functions available directly in the function estimation routine. If you use the estimated functions, you are required to enter some guiding parameters which are available in the table below.

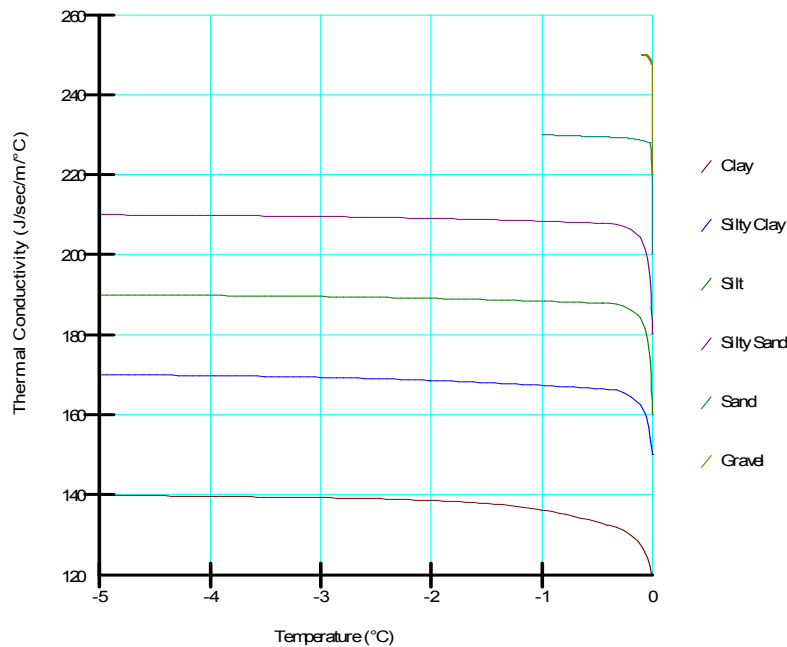


Figure 4-12 Sample K vs temperature functions

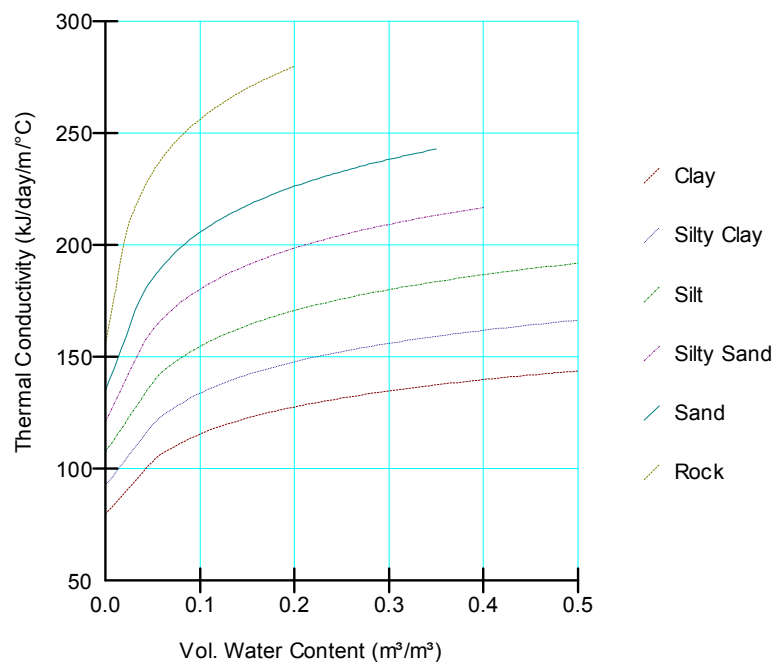


Figure 4-13 Sample K vs water content functions

Volumetric heat capacity

The heat capacity of a material is defined as the quantity of heat required to raise the temperature of the material by a unit degree. When expressed on a per unit weight basis, this quantity of heat is referred to as the specific heat capacity; when expressed on a unit volume basis, the quantity is known as the volumetric heat capacity. The units for specific heat capacity are J/(kg.°C) or kJ/(kg.°C) and Btu/(lb.°F), and the units for volumetric heat capacity are J/(m³.°C) or kJ/(m³.°C) and Btu/(ft³.°F).

TEMP/W users need only specify the function for the unfrozen zone and, based on this, the volumetric specific heat in the frozen zone will be computed internally by the solver as a function of ice, water, air and soil mineral content using the relationships described in the following section.

Table 4-1 Unit weight and thermal conductivity of various materials

Material	Unit Weight	Conductivity		
	lb/(ft ³)	Btu/(hr-ft-°F)	J/(sec-m-°C)	kJ/(day-m-°C)
Water	62.4	0.35	0.605	52.27
Ice	57	1.29	2.23	192.7
Air (dry, still)	0	0.014	0.024	2.07
Snow				
loose, new	–	0.05	0.086	7.43
on ground	–	0.07	0.121	10.45
dense, compacted	–	0.20	0.340	29.37
Soil and rock minerals				
shale	–	0.9	1.5	129.6
evaporites	–	3.1	5.4	466.6
limestone	168	0.75-2.9	1.3-5.0	112-432
dolomite	178	2.9	5.0	432
sandstone	–	1.1-2.4	1.8-4.2	155-86.4
schist	–	0.90	1.6	138.24
gneiss	–	1.4	2.5	216
greenstone	–	1.9	3.3	285.12
slate	–	2.2	3.8	328.3
argillite	–	1.9	3.3	285.12
quartzite	–	2.6-4.1	4.5-7.1	388.8-613
granite	–	1.0-2.3	1.7-4.0	146.9-345.6
diabase	–	1.2	2.1	181.4
gabbro	–	1.4	2.5	216
grandiorite	–	1.5	2.6	224.6

Estimating volumetric heat capacity

TEMP/W uses the volumetric heat capacity in its formulation. The volumetric heat capacity of a soil can be approximated by the dry density of the soil and the sum of the specific heat capacities of its different constituents (namely, soil particles, water, ice, and air). The air component is very small and generally is neglected. A general equation for estimating unfrozen and frozen volumetric heat capacity is: (see Johnston, Ladanyi, Morgenstern and Penner, 1981, pp. 73-147).

$$C = c\gamma = \gamma_d [c_s + c_w w_u + c_i w_f]$$

where:

- C = volumetric heat capacity of the soil,
 c = specific heat capacity of the soil,
 γ = bulk density of the soil,
 γ_d = dry density of the soil,
 c_s = specific heat capacity of soil particle,

c_w	=	specific heat capacity of water,
c_i	=	specific heat capacity of ice,
w_u	=	unfrozen water content expressed in % of dry weight of the soil, and
w_f	=	frozen water content expressed in % of dry weight of the soil.

Examples

The following examples illustrate how to estimate the volumetric heat capacity for various soils.

Example 1

For a dry mineral soil with dry density of 120 lb/ft³ or 1923 kg/m³, the volumetric heat capacity of the soil can be estimated as:

$$\begin{aligned} C &= 120 \text{ lb/ft}^3 * 0.17 \text{ Btu/(lb} \cdot ^\circ\text{F)} \\ &= 20.4 \text{ Btu/(ft}^3 \cdot ^\circ\text{F)} \end{aligned}$$

or in SI units as:

$$\begin{aligned} C &= 1923 \text{ kg/m}^3 * 0.71 \text{ kJ/(kg} \cdot ^\circ\text{C)} \\ &= 1365 \text{ kJ/(m}^3 \cdot ^\circ\text{C)} \end{aligned}$$

Example 2

For an unfrozen mineral soil with dry density of 120 lb/ft³ or 1923 kg/m³, and unfrozen water content of 0.25, the volumetric heat capacity of the soil can be estimated as:

$$\begin{aligned} C &= 120 \text{ lb/ft}^3 * [0.17 \text{ Btu/(lb} \cdot ^\circ\text{F)} + 1.0 \text{ Btu/(lb} \cdot ^\circ\text{F)} * 0.25] \\ &= 50.4 \text{ Btu/(ft}^3 \cdot ^\circ\text{F)} \end{aligned}$$

or in SI units as:

$$\begin{aligned} C &= 1923 \text{ kg/m}^3 * [0.71 \text{ kJ/(kg} \cdot ^\circ\text{C)} + 4.187 \text{ kJ/(kg} \cdot ^\circ\text{C)} * 0.25] \\ &= 3378 \text{ kJ/(m}^3 \cdot ^\circ\text{C)} \end{aligned}$$

Typical values of volumetric heat capacity

Table 4-2 below provides typical values for the specific and volumetric heat capacity of various materials, (extracted from Johnston, Ladanyi, Morgenstern and Penner, 1981 and Harlan and Nixon, 1978). Sample functions based on water contents in the coupled convective model are given in Figure 4-14.

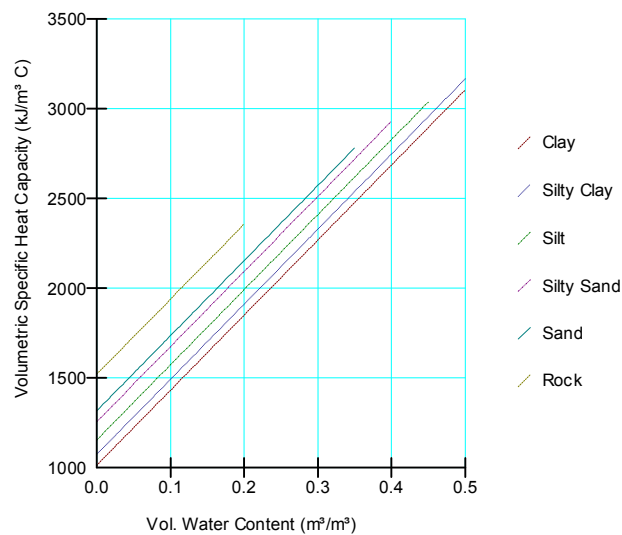


Figure 4-14 Sample heat storage capacity functions

Table 4-2 Specific and Volumetric Heat Capacities of Various Materials

Material	Mass Specific Heat Capacity		Volumetric Heat Capacity	
	Btu/(lb·°F)	kJ/(kg·°C)	Btu/(ft ³ ·°F)	kJ/(m ³ ·°C)
Water	1.00	4.187	62.4	4187
Ice	0.50	2.094	28.1	1880
Air	0.24	1.0	0.0187	1.25
Soil minerals	0.17	0.71	28.0	1875
Organic soil minerals	0.40	1.674	37.5	2520
Extruded polystyrene insulation	0.24	1.0	0.65	43.5
Concrete	0.21	0.895	30.0	2010
Asphalt	0.40	1.674	37.5	2520
Snow, fresh	—	—	3.11	209
Snow, drifted and compacted	—	—	7.80	523.5
Granite	—	—	37.1	2490
Limestone	0.29	1.2	48.9	3285
Dolomite	0.21	0.88	37.4	2510
Sandstone	—	—	37.4	2510
Shale	—	—	27.4	1840
Glass	—	—	26.2	1760
Steel	0.11	0.46	56.0	3890
Wood	0.19	0.8	7.79	523

4.9 Sensitivity of hydraulic results to material properties

How sensitive is a model to changes to the air-entry value, the slope of the function, the residual volumetric water content and the saturated hydraulic conductivity? The effect of altering each of the four material property functions is highlighted below, through a series of steady-state and transient analyses where only one parameter is changed at a time to clearly evaluate the influence of each parameter. Figure 4-15 shows a cross-section of a system where both saturated and unsaturated conditions exist. This cross-section represents a two-dimensional view of a flow system in which water from a canal passes through an unconfined, homogeneous, fine sand aquifer and is collected in a series of collection wells located along the right edge of the cross-section.

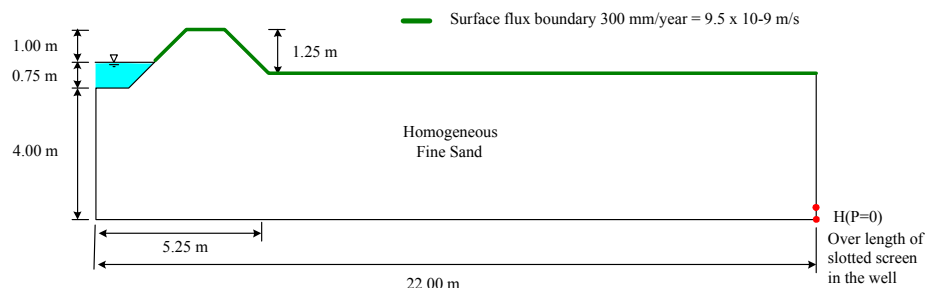


Figure 4-15 Diagram of system used in sensitivity analysis

Changes to the air-entry value (AEV)

To show how sensitive the model is to changes in air-entry value, a steady-state simulation was conducted where the AEV of a function was increased from 3 to 10 kPa. A volumetric water content function is not required for a steady-state analysis, however it is good practice to always make changes to the volumetric water content function when conducting a sensitivity analysis, and then let the changes be reflected in the hydraulic conductivity function by recalculating the function from the value of the saturated hydraulic conductivity and the newly specified volumetric water content function. Figure 4-16 shows the adjusted volumetric water content function and the predicted hydraulic conductivity functions used in the simulations. It is important to note that if the K-function was presented on a log-log plot (hydraulic conductivity functions are usually presented in the literature on a log-log scale), the effect of increasing the air-entry value and adjusting the rest of the curve accordingly would appear to also steepen the slope of the function. In VADOSE/W however, the functions are always presented on a log-arithmetic scale and the AEV can be increased while the slope of both functions remain similar in shape. Figure 4-17 and Figure 4-18 show the VADOSE/W modeling results for both the 3 kPa and 10 kPa AEV simulations respectively.

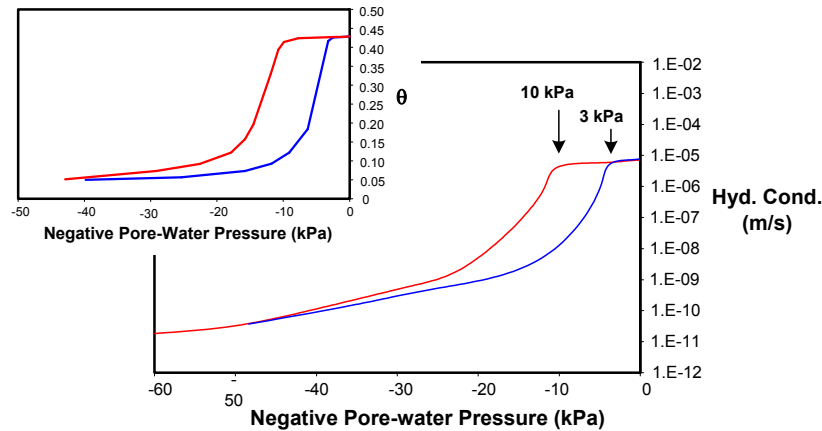


Figure 4-16 Material property functions used in the AEV sensitivity analyses

To compare the results in Figure 4-17 and Figure 4-18, it is probably easiest to consider the height of the capillary fringe that is emphasized in the magnified sections. A dimension arrow has been superimposed to show the extent of capillary rise that develops for both simulations. The capillary rise is the height above the water table where negative pore-water pressures exist, but the soil remains saturated due to capillary tension. The air-entry value, when converted from pressure (kPa) to a pressure head (m), is approximately equal to the height of the capillary fringe. In the capillary fringe, water is transported through the soil at a rate equal to the saturated hydraulic conductivity, so more water can be transported in a larger capillary fringe than in a smaller one. As an interesting aside, note how the structure of the model (i.e., the downstream side of the berm) controls the shape of the unsaturated flow system. Even though saturated flow occurs in the berm, the water table is still at depth and negative pore-water pressures exist on the downstream face so a seepage face never develops.

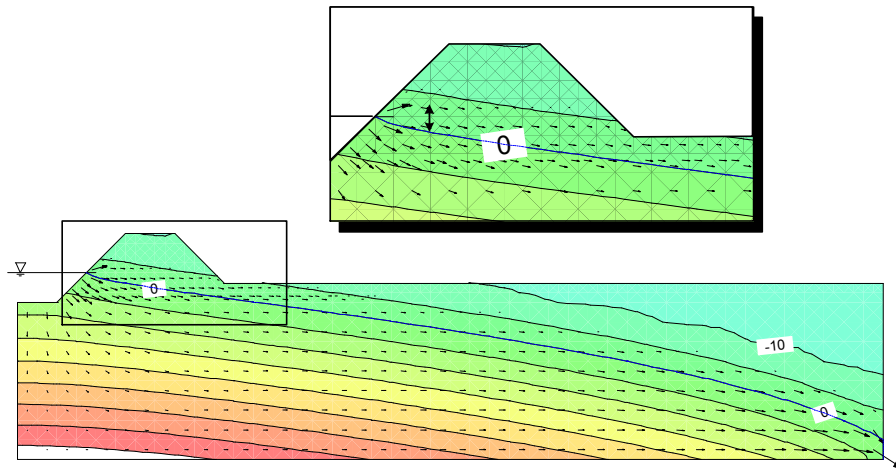


Figure 4-17 Pressure contours and flow vectors for a 3 kPa AEV material

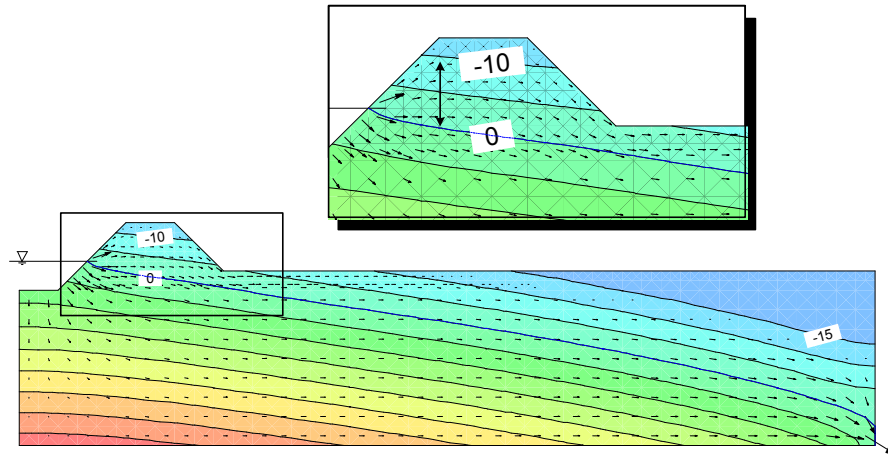


Figure 4-18 Pressure contours and flow vectors for a 10 kPa AEV material

Changes to the saturated hydraulic conductivity

Six steady state simulations were conducted to evaluate the effect of changing the saturated hydraulic conductivity (Table 4-3). Basically, the first three simulations compared the effect of both increasing and decreasing the saturated hydraulic conductivity and the last three showed the effect of conducting a saturated hydraulic conductivity sensitivity analysis with the added influence of an applied surface flux boundary condition.

Table 4-3 Summary of simulations for Ksat sensitivity analyses

Simulation	Ksat (m/s)	Surface Flux (m/s)
1	7.5×10^{-4}	none
2	7.5×10^{-6}	none
3	7.5×10^{-8}	none
4	7.5×10^{-4}	9.5×10^{-9}
5	7.5×10^{-6}	9.5×10^{-9}
6	7.5×10^{-8}	9.5×10^{-9}

The three hydraulic conductivity functions that were used in the simulations are presented in Figure 4-19. The general shape of the function remained unchanged while the saturated hydraulic conductivity was adjusted.

Figure 4-20 to Figure 4-22 show the results obtained from simulations 1 to 3 (see Table 4-3). A surface flux was not applied and the Ksat was varied by two orders of magnitude between each simulation. The resulting total head contours and total flux values that were determined near the well screen are included in the figures. One of the most significant comparisons to make is with respect to the total head contours. Altering the saturated hydraulic conductivity does not alter the shape of the flow net, so the total head contours should be and are the same. The only obvious difference between the results can be found in the value associated with the flux section near the well. The flux varies along the same order of magnitude that the Ksat was varied, so increasing the saturated hydraulic conductivity results in a greater flow rate to the well and decreasing it reduces the amount of flow to the well.

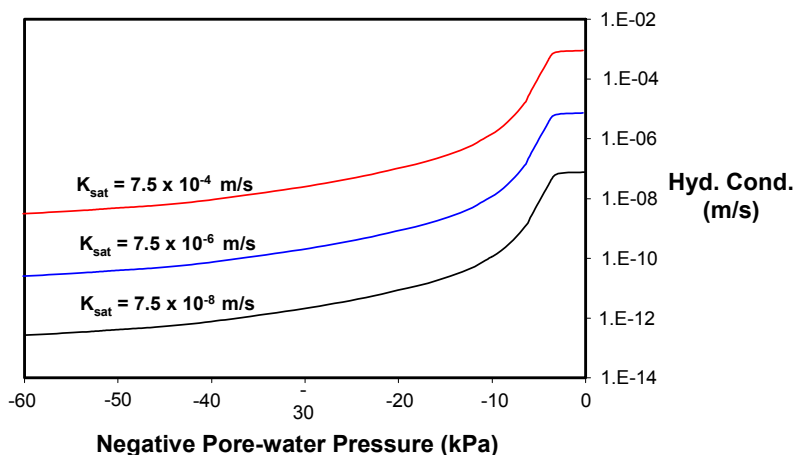


Figure 4-19 Hydraulic conductivity functions used for Ksat sensitivity analyses

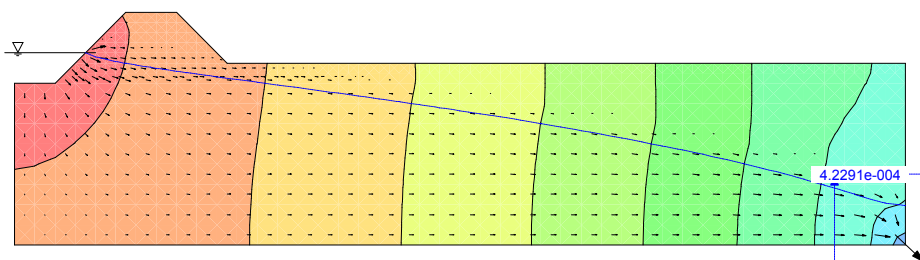


Figure 4-20 Simulation #1 total head contours (Ksat 7.5×10^{-4} m/s)

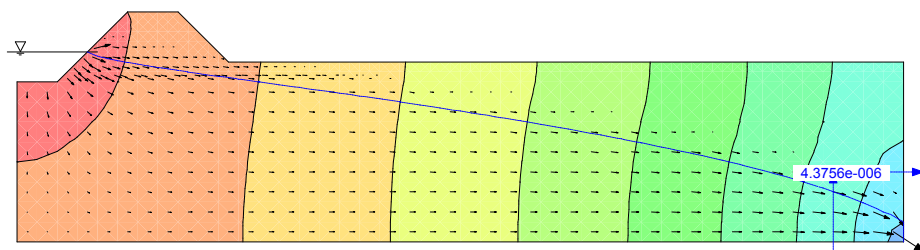


Figure 4-21 Simulation #2 total head contours (Ksat = 7.5×10^{-6} m/s)

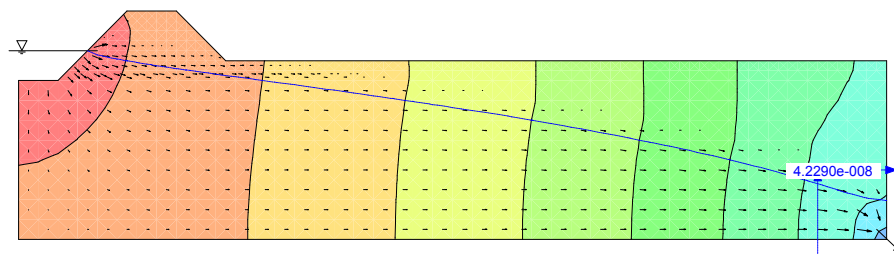


Figure 4-22 Simulation #3 total head contours (Ksat = 7.5×10^{-8} m/s)

The results presented in the above figures did not include a surface flux boundary condition. Results obtained from sensitivity analyses (regarding Ksat) where surface fluxes are applied, are not nearly as easy to compare. The next three figures show the results from simulations 4 to 6 from Table 4-3. In these cases, a surface flux boundary condition of 9.5×10^{-9} m/s (equivalent to 300 mm/year net infiltration)

was applied over the surface and the K_{sat} was once again varied by two orders of magnitude between simulations.

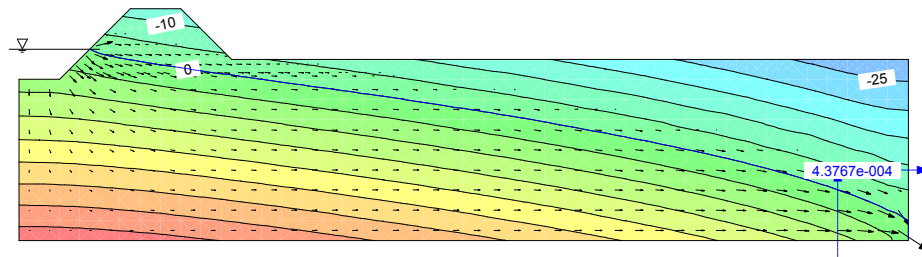


Figure 4-23 Simulation #4 pressure head contours ($K_{sat} = 7.5 \times 10^{-4}$ m/s)

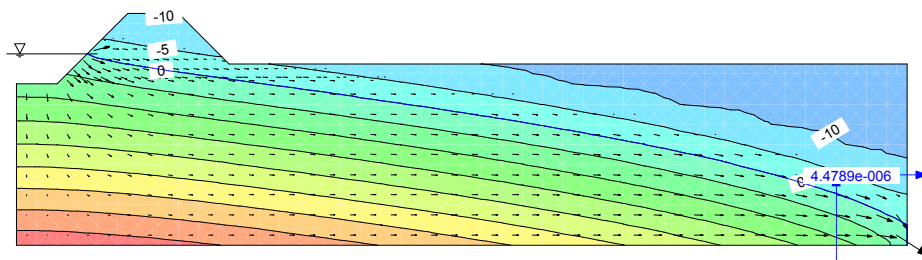


Figure 4-24 Simulation #5 pressure head contours ($K_{sat} = 7.5 \times 10^{-6}$ m/s)

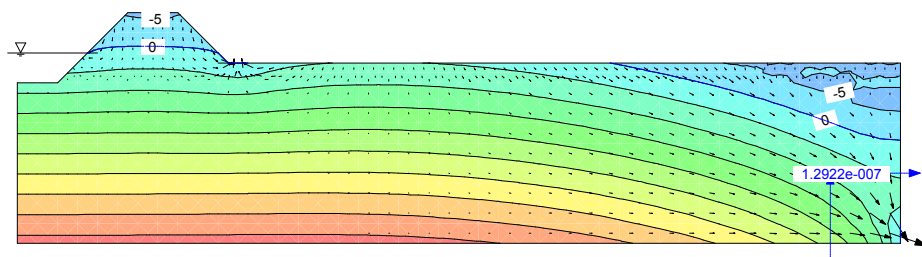


Figure 4-25 Simulation #6 pressure head contours ($K_{sat} = 7.5 \times 10^{-8}$ m/s)

The pressure head contours (and consequently the total head contours) are very different between the three simulations where a surface flux was applied. This time the system has two water sources to contribute to the total flow; the upstream ponded water and the applied surface flux. The effect on the flow system is minimal in Figure 4-23 because the K_{sat} is much greater than the applied surface flux (10^{-4} compared to 10^{-9} m/s). As the difference between the K_{sat} and the applied flux gets smaller, the effect on the pressure profiles becomes more significant. In Figure 4-25, the system is close to becoming fully saturated and a seepage face develops on the downstream side of the berm. The rate at which the water can leave the system (i.e., the well), is still controlled by the saturated hydraulic conductivity, but in the case of analysis with a surface flux applied, the total flux value leaving the profile is greater.

Changes to the slope of the VWC function

In a steady-state analysis, the amount of flow into the system corresponds to the flow rate out of the system. However, in a transient seepage analysis the flow into the system may differ from the flow out of the system because the system stores or releases water. It therefore becomes necessary to account for the change of water stored within a soil profile with time. The amount of water stored or retained is a function of the pore-water pressures and the characteristics of the soil structure and is described by the volumetric water content function. A transient analysis can be used to evaluate the effect of altering the slope of the

volumetric water content function (mw). In any transient analysis there are two main considerations; how fast the water is flowing (a function of the hydraulic conductivity) and how much water is flowing (a function of the change in storage and the amount of water in the system). As a result, both material property functions must be defined. Storage is the amount of water that remains in the pores of a soil under negative pore-water pressures. If the slope of the VWC function is flat, the change in volumetric water content for increasingly negative pore-water pressures would be less than for a soil with a steeper slope function. Figure 4-26 shows the volumetric water content and hydraulic conductivity functions used for the sensitivity analysis regarding the slope of the VWC function. Creating a function with a flatter slope represents a soil which is non-uniform and has a larger distribution of pore sizes. The air-entry value (a function of the largest pore size) has not been changed, nor has the residual water content (a function of the smallest pore size). The modifications were made to the VWC function and the changes were then reflected in the hydraulic conductivity function through the use of predictive methods.

In order to obtain initial head conditions, steady-state analyses were conducted using both the modified and unmodified material property functions. A pond depth of 0.75m was included for the steady-state analyses and was then removed for the start of the transient analyses, allowing the system to drain into the well for 40 days. The results from both transient analyses are presented in Figure 4-27.

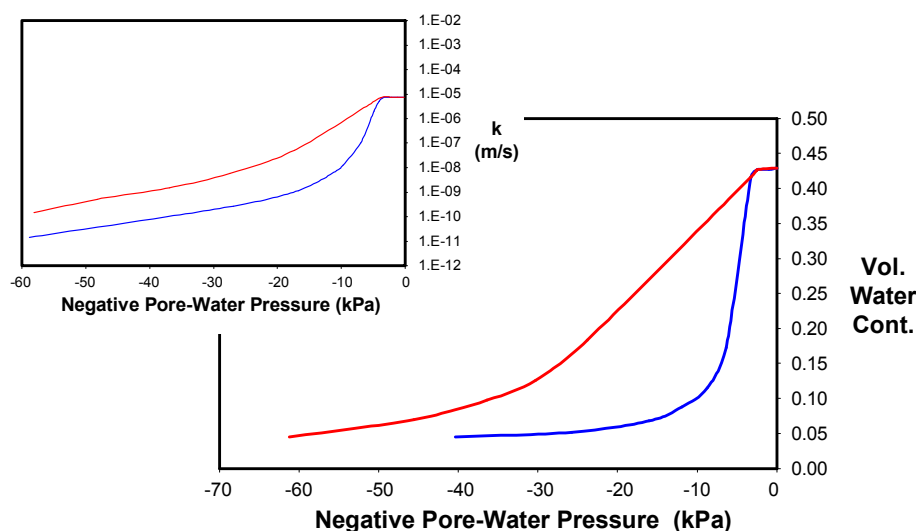


Figure 4-26 Material property functions used in the sensitivity analyses for changes to the slope of the storage function

One way to evaluate the effect of altering the slope of the VWC function is to compare how long it takes each simulation to lower the water table to the same elevation. As can be seen in Figure 4-27, it only took 22 days of drainage, using the modified function, to lower the $P=0$ contour (water table) to the same elevation as that of the unmodified function after 40 days of drainage. The time difference can be explained in part by comparing water content profiles taken at the same location. Figure 4-27 shows the initial water content for both simulations as a vertical, solid black line. The red line indicates the water content profile after 22 days of drainage using the modified function and the blue line indicates the water content profile after 40 days of drainage using the unmodified function (the one with the steeper slope). The amount of water removed from the system for each soil type can be estimated as the area between the black line and the red or blue line respectively. The water content profile of the modified soil (red) shows that the soil is wetter, having stored more water in the unsaturated zone than the unmodified soil (blue). As a result, the amount of water released from the system is less than that of the unmodified VWC

function. The majority of the water removed for both soils was through the saturated flow system, and since the K_{sat} remained unaltered between the simulations, it took less time to drain less water.

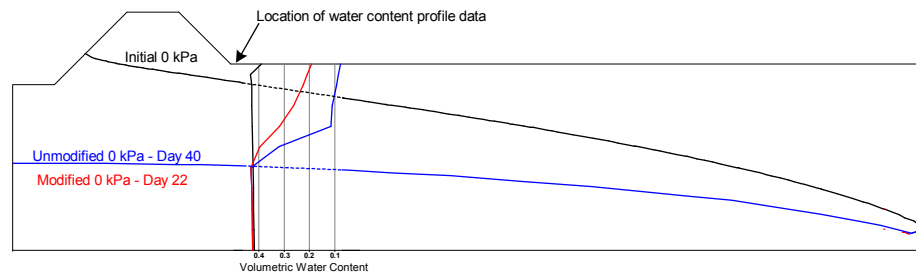


Figure 4-27 Location of $P=0$ kPa contour and water content profiles for the modified function (day 22) and unmodified function (day 40)

Changes to the residual volumetric water content

The last feature of the volumetric water content function to evaluate in the sensitivity analysis is the residual water content. The effect of changing the residual volumetric water content does not alter the hydraulic conductivity function, so only the VWC function was adjusted such that the residual water content for the modified function was much greater than the unmodified function as shown in Figure 4-28.

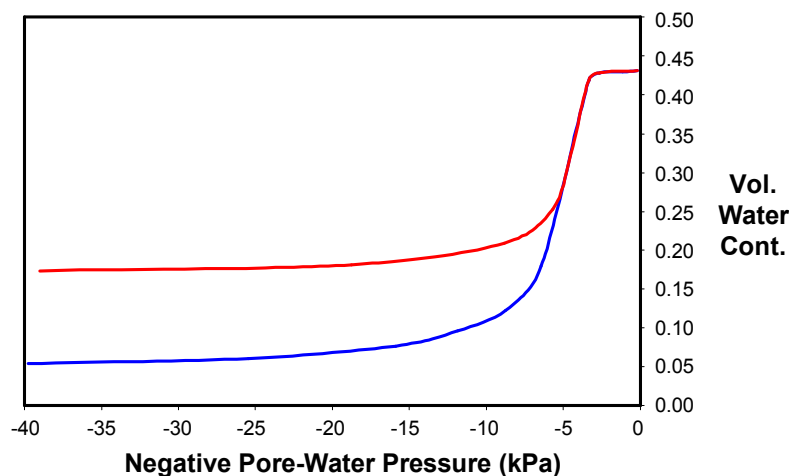


Figure 4-28 Modified and unmodified residual water contents used in analyses

Both steady state and transient analyses were conducted in a manner similar those described in the last section in terms of having the pond in place for the steady-state simulation and then letting the system drain over a 40 day period. Intuitively, altering the volumetric water content to have higher volumetric water content at residual should result in a wetter unsaturated profile. To confirm this thinking, the length of time that it took to lower the $P=0$ pressure contour (water table) to the same level as in Figure 4-27 was determined. The results are presented in Figure 4-29.

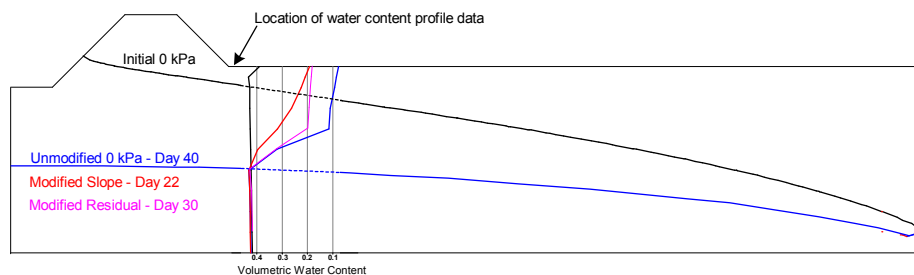


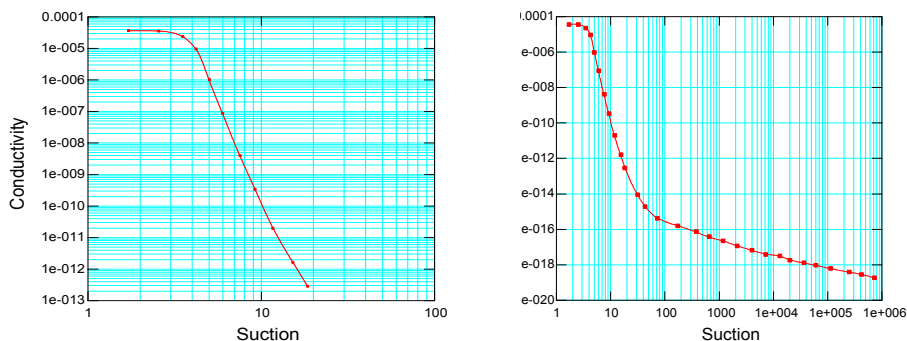
Figure 4-29 Location of $P=0$ kPa contours and water content profiles for the modified slope function (day 22), the modified residual (day 30) and the unmodified function (day 40)

With the completely unmodified function, it took 40 days to lower the $P=0$ contour (water table) to the location represented in Figure 4-29. It took the function with the shallower slope 22 days to have the $P=0$ contour lower to the same elevation. Increasing the residual water content of the unmodified function resulted in the $P=0$ contour reaching the same elevation after 30 days.

Therefore, increasing the residual water content of the volumetric water content function resulted in a wetter profile above the $P=0$ contour (as shown by the pink water content profile) than that of the unmodified function (as shown by the blue water content profile). Less water was released from the system and so it took less time to release the water. The greatest amount of water storage results in the least amount of water being released from the system. This occurred using the volumetric water content function with the shallow slope.

Fully defined conductivity function in evaporation analyses

When carrying out evaporation analyses it is important to define the conductivity function over a reasonable range of suctions. Consider the case illustrated below in which VADOSE/W was used to model actual evaporation from a column of uniform sand in an environmentally controlled laboratory. The function on the left in Figure 4-30 is defined to a suction of 20 kPa while the one on the right is defined to a suction of 1 million kPa. The exact shape of the function is not critical at higher suctions but it is critical that the conductivity is shown to decrease several orders of magnitude over the higher



pressure range.

Figure 4-30 Partially and fully defined conductivity function for sand

In this experiment, the column of sand was initially saturated and the climate conditions in the chamber were established such that the approximate Potential Evaporation rate was equal to about 8 mm/day.

Based on this evaporative demand, after about 3 or days surface of the sand began to desaturate such that the ability of the sand to release water at the potential evaporation rate was reduced.

Figure 4-31 shows the modeled performance of the column of sand using both the partially and fully defined conductivity function. In the left of this figure, the liquid flow to the surface is shown to decrease slightly on the second day but then flatten out at a fairly high unit flux rate. The vapor flow is shown to increase dramatically at about the same time the liquid flux rate is reducing. It is important to remember that the total flow in the vertical direction is therefore the sum of the liquid and vapor flow and both are stabilizing at relatively high flux rates. The figure on the right shows the liquid flow shutting down dramatically early in the experiment and the vapor flow increasing dramatically at the same time. This is the correct mechanism. When the correct liquid and vapor flows are summed, they produced a modeled response that matches the observed actual evaporative loss from the columns as shown in Figure 4-26.

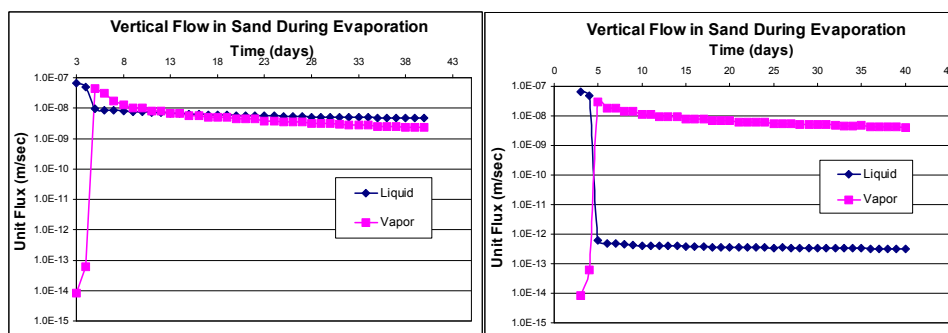


Figure 4-31 Incorrect and correct partitioning of flows

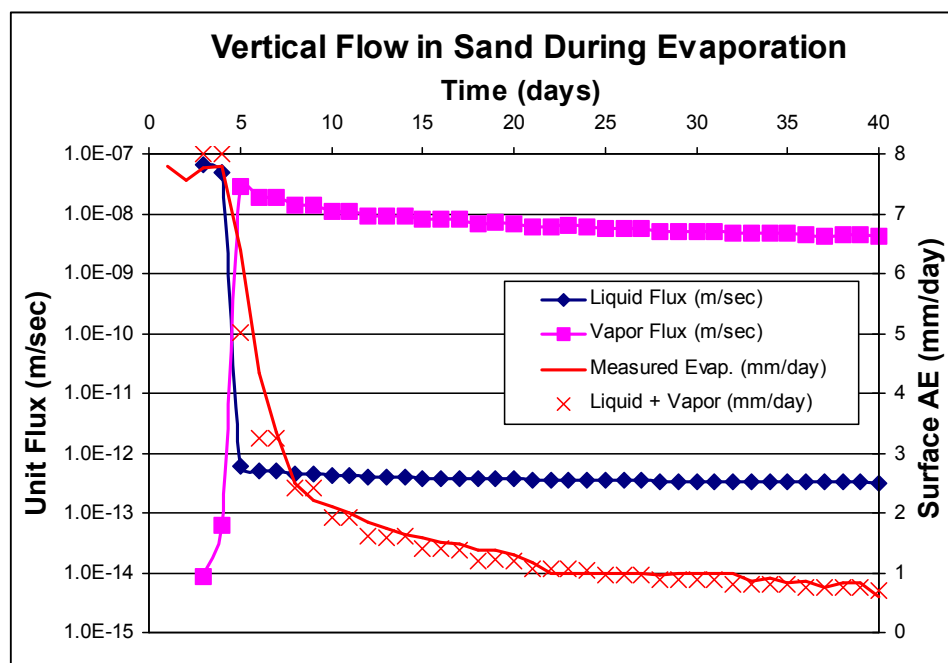


Figure 4-32 Actual computed and measured surface loss from column of sand

In summary, in modeling unsaturated systems, appropriate definition of the volumetric water content and conductivity functions are critical to achieving a representative solution. It is important to know how the results can be affected by varying the main features of the function and how to conduct a sensitivity analysis if you are unsure of your material property functions. Conducting a sensitivity analysis will help

you gain confidence in the results and to increase your understanding of how the system being modeled will respond to changes in the material properties.

4.10 Sensitivity of thermal results to material properties and water content in soil

In seepage analyses where the hydraulic conductivity values can change many orders of magnitude a sensitivity study usually considers multiplying or dividing values by a factor of 10 in order to see a change in output data. With thermal properties, the change in values (be they thermal conductivity or heat storage) generally occur within a 1/3 order of magnitude. In addition, if freezing is taking place, the amount of unfrozen water that freezes and releases latent heat can be a significant factor.

In this discussion, the attempt to calibrate a thermal model to real site data is used for illustrative purposes. The geometry of the model was established and default material properties were used in the initial simulations based on previous modeling for the site. An iterative approach was then used to adjust material properties until a reasonable agreement between computed and actual observed temperatures was obtained. The calibrated model was needed for future site planning.

There are three primary material properties that can be adjusted. These are listed below with an explanation of the affect they have on the computed temperature trends. The comparison between actual measured and best fit calibrated data is provided in Figure 4-33.

Thermal Conductivity: Increasing this value increases the rate at which the temperature drops to the freezing point and then after the phase change has occurred. It is evident in the slope of the curves in the figure at temperatures above freezing and at temperatures below about -4°C when most of the pore-water is frozen.

Volumetric Water Content: Adjusting the water content affects the length of time the temperature profile “hovers” around the freezing point before it starts to drop off rapidly again. This length of time is directly related to the latent heat that is released so the more water there is, the more latent heat, and the longer it takes to be removed.

Slope of Unfrozen Water Content Function: This parameter controls the rate at which the water is frozen at temperatures just below freezing. If the function is steep, all the water freezes just below 0°C and the temperature decay curve drops off quickly at a rate almost equal to the rate before the freezing point was reached. If the function is shallow and unfrozen water is still present at temperatures around -2 to -4°C , then the temperature decay curve shows a slower drop in the temperature range just below 0°C . Steep functions are typical of very coarse-grained material and shallow functions are typical of fine-grained materials.

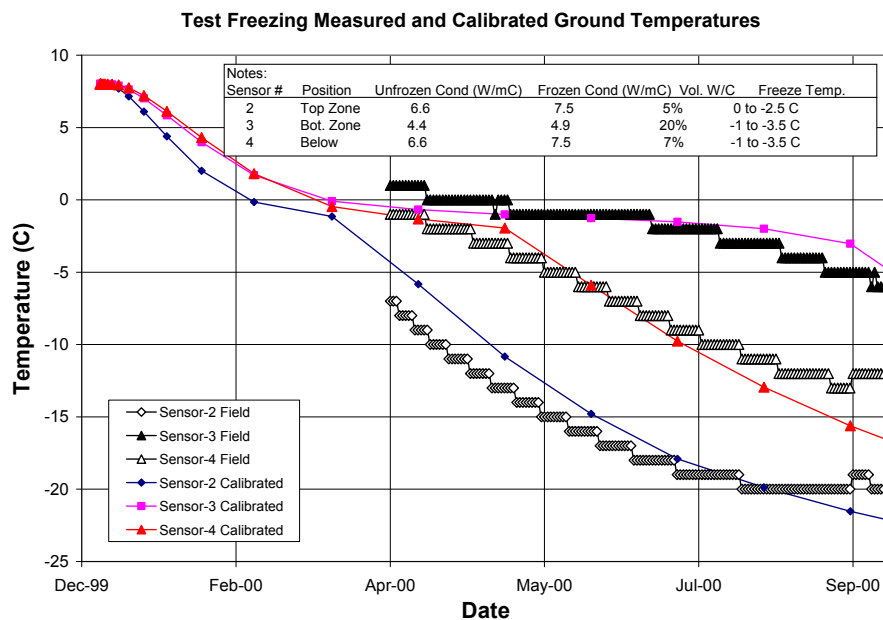


Figure 4-33 Comparison between actual and calibrated ground temperatures

When the model was initially run using assumed material properties the predicted freezing times were much longer than those observed. In fact, the temperatures were just starting to pass through the 0 C point by the end of the test freezing period. The slopes of the decay curves from the initial temperature of +8 C to the 0 C point indicated that the material thermal conductivity was too low. Sensors 2 and 3 were assumed to be in a clay/ore type ground with very low thermal conductivity and sensor 4 was assumed to be in a broken sandy type ground. The model was re-run a few times with slight increases to the thermal conductivity on each subsequent iteration. When the drop in temperature from +8 C to 0 C agreed somewhat with the measured data the thermal conductivity was held constant.

Once the thermal conductivity was adjusted it was necessary to adjust the volumetric water contents in order to match the time the temperature profile “hovered” near the freezing point. The final calibrated water contents are likely lower than one may expect, but even a slight increase in the calibrated values resulted in several more weeks of freezing delay near the freezing point. The final calibrated values are within the ranges originally reported by the project owner.

Finally, the shape of the unfrozen water content function was adjusted in order to approximate the rate of decay of the temperatures after they have passed through the freeze point. No extreme changes were made to the material properties (compared to earlier modeling), but they were adjusted somewhat to approximate a more fine-grained, than coarse-grained material.

In carrying out all of the above changes it was important to ensure that the final combination of material properties for any given soil made sense for that soil. In other words, care was taken to not have water contents typical of clay, combined with a thermal conductivity obtained from a solid rock core sample, applied to a soil with an unfrozen water content function found in beach sand.

4.11 Gas diffusion parameters

Gas diffusion, decay and dissolution plays an important role in many physical geotechnical problems. Gas analysis in VADOSE/W is separate from vapor phase mass transfer. Gas transfer refers to chemical

transport in response to concentration gradients in the air phase. Vapor transfer is already included in the VADOSE/W formulation.

One example of gas diffusion in unsaturated soil is in the modeling of oxygen gas diffusion through engineered covers over waste rock at mining operations, where the transport of oxygen into the waste rock results in the oxidation of sulfide bearing minerals. The oxidation process results in low pH effluent containing high concentrations of metals. The supply of oxygen to these reactive materials occurs primarily by diffusion, and must be modeled using complex boundary conditions, material properties, and soil profiles.

In municipal landfill operations, there must be a balance between the amount of oxygen entering the system and the amount of oxygen required to decompose organic matter in addition to any other oxygen consuming reactions. If the amount of oxygen is not sufficient, clogging mats can form at infiltration interfaces which lead to undesirable moisture redistribution mechanisms. In nuclear hazardous waste containment facilities, the amount of radon gas being released to the atmosphere must be controlled.

VADOSE/W is formulated to rigorously analyze the influences of the climate on the heat, mass and vapor transfer phenomenon in all types of natural and man-made soil systems exposed to the atmosphere. The addition of gas diffusion, and decay analysis is another key component to consider in many of these designs and as such, it has been built into the VADOSE/W solver.

The user does not need to directly specify any soil property functions to use the gas diffusion option as these parameters are computed internally based on the degree of saturation of the soil. The only exception is the decay constant property if used. The decay constant is really the half life value and it is entered with units of years, not in the inverse (1/years) as in some circumstances. More discussion of this is provided in the Theory chapter.

5 Boundary Conditions

5.1 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.

While SEEP/W is formulated for application of hydraulic boundary conditions only, VADOSE/W is formulated for simultaneous application of hydraulic, thermal and gas transfer boundary conditions. Much of the discussion that follows is focused on hydraulic boundary conditions because they are the most extreme types of conditions applied in this model from a physical perspective (wetting / drying) and from a numerical perspective (extremely non-linear soil property functions). Special consideration is given to climate boundary conditions and mention is made of available types of thermal and gas boundary conditions.

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, in essence, the driving force. What causes seepage flow? It is the hydraulic total head difference between two points or some specified rate of flow 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 conditions that exist along the bottom of a reservoir. It is simply the elevation head at the top of the reservoir. 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 along a seepage face. The size of the seepage face is not known and needs to be determined from the solution. Furthermore, the conditions on the boundaries may change with time during a transient analysis, which can also add to the complexity.

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 the user with this aspect of an analysis, VADOSE/W has tools that 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.

5.2 Fundamentals

All finite element equations just prior to solving for the unknowns ultimately 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 seepage analysis the equation is:

$$\text{Equation 5-1} \quad [K]\{H\} = \{Q\}$$

where:

$\{H\}$ = a vector of the total hydraulic heads at the nodes, and
 $\{Q\}$ = a vector of the flow quantities at the node.

The prime objective is to solve for the primary unknowns, which in a seepage analysis are the total hydraulic head at each node. The unknowns will be computed relative to the H values specified at some nodes and/or the specified Q values at some other nodes. Without specifying either H 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 H condition. The specified H 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 H or the Q at a node. It is very useful to keep this in mind when specifying boundary conditions. You should always ask yourself the question: “What do I know? Is it the head H or the flow, 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, flow across a boundary can also be specified as a gradient or a rate per unit area. Such specified flow boundary conditions are actually converted into nodal Q values. So, even when we specify a gradient, the ultimate boundary condition options still are either H or Q.

There are cases where we may know either H or Q. A seepage face is a boundary condition where this is the case. We actually know that the pore-water pressure is zero (H equals elevation), but we do not know the size of the seepage face. In such a situation, it is necessary to use an iterative procedure to try either H or Q boundary conditions until the correct solution is obtained. A complete section is devoted to this special case later in this Chapter. The point here is that in the end we can still only specify H or Q - which one is to be specified, needs to be guided by the solution itself.

Remember! When specifying seepage boundary conditions, you only have one of two fundamental options – you can specify H 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 H, the solution to the finite element Equation 5-1 will provide Q. Alternatively, when you specify Q, the solution will provide H. The equation always needs to be in balance. So when an H is specified at a node, the computed Q is the Q that is required to maintain the specified H, you cannot control the Q as it is computed. When Q is specified, the computed H is the H that is required to maintain the specified flow Q.

Recognizing the relationship between a specified nodal value and the corresponding computed value is useful when interpreting results. Let's say you know the specified flow across a surface boundary. Later when you check the corresponding computed head at that node, you may find that a significant depth of water impoundment is required to provide the computed head. Then you can judge whether that is reasonable or not.

VADOSE/W always provides the corresponding alternative when conditions are specified at a node. When H is specified, Q is provided, and when Q is specified, H is provided. The computed Q values at nodes where a head is specified are referred to as Boundary Flux values with units of volume per time. 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 H nor Q is specified at a node, then the computed Q is zero. Physically, what it means is that the flow coming towards a node is the same as the flow leaving the node. Another way to look at this is that no flow is entering or leaving the system at these nodes. Water leaves or enters the system only at nodes where H 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 drains.

The heads in a seepage analysis are the primary unknowns or field variables. A boundary condition that specifies the field variable (H) at a node is sometimes referred to as a Type One or a Dirichlet boundary condition. Flow 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 seepage modeling simply refers to boundary conditions as head (H) or flux (Q) boundary conditions. Later we will differentiate between nodal flux Q and specified gradients (rates of flow per unit area) across an element edge.

5.3 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 5-2 and Figure 5-3 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.

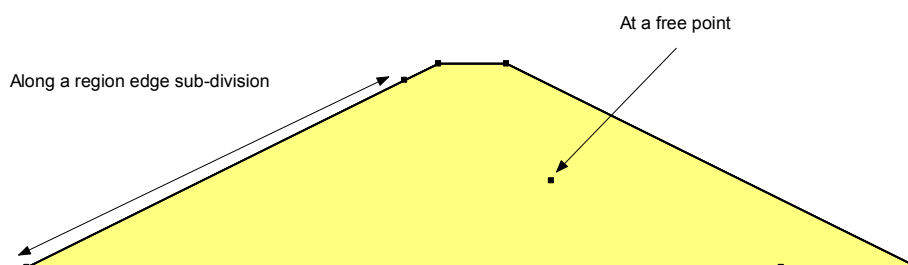


Figure 5-1 Desired BC locations

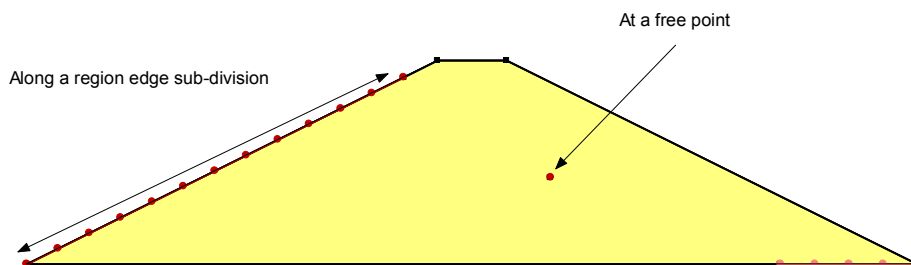


Figure 5-2 BC's attached to geometry

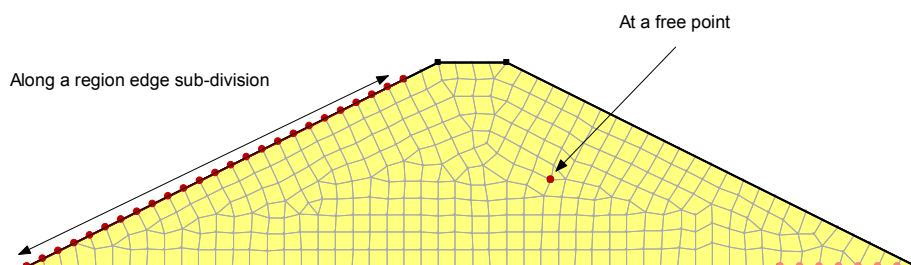


Figure 5-3 BC's with underlying mesh visible

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.

5.4 Head boundary conditions

Definition of total head

In VADOSE/W the primary unknown or field variable solved in the equation is pressure because soil water pressure can be coupled with temperature. In reality, water flows in response to changes in total head, not changes in pressure but the conversion between these two parameters is quite simple. Total head is made up of pressure head and elevation head, where the elevation head represents the gravitational component. In equation form the total head is defined as:

$$H = \frac{u}{\gamma_w} + y$$

where:

- | | | |
|------------|---|--|
| H | = | the total head (meters or feet, for example), |
| u | = | the pore-water pressure (kPa or psf), |
| γ_w | = | the unit weight of water (kN/m ³ or pcf), and |
| y | = | the elevation (meters or feet). |

The term u / γ_w is referred to as the pressure head – represented in units of length.

When specifying head boundary conditions, it is necessary to always think of both the pressure and elevation components. The significance of these components is illustrated with the following series of examples of flow through a pipe filled with sand.

Figure 5-4 shows a situation where the pipe is horizontal. The elevation is the same at both ends, but the pressure head is higher on the left than on the right. The total head on the left is 20 while on the right the total head is 10. There is a total head difference, and consequently, there will be flow from the left to the right. In equation form, the total difference is:

$$\Delta H = (20 + 5) - (10 + 5) = 10$$

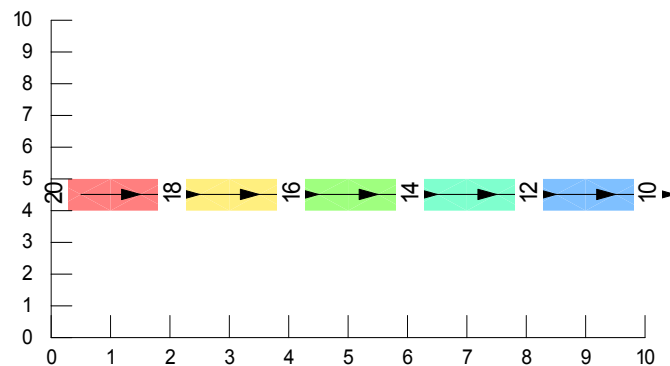


Figure 5-4 Flow in horizontal pipe due to head gradient only

Now consider the case where the left end of the pipe is higher than the right end as in Figure 5-5. In this case, the pressure head is the same at both ends. There is, however, a total head difference between the two ends due to the elevation difference and, consequently, once again there will flow from the left to the right. Now the total head difference is:

$$\Delta H = (0 + 10) - (0 + 0) = 10$$

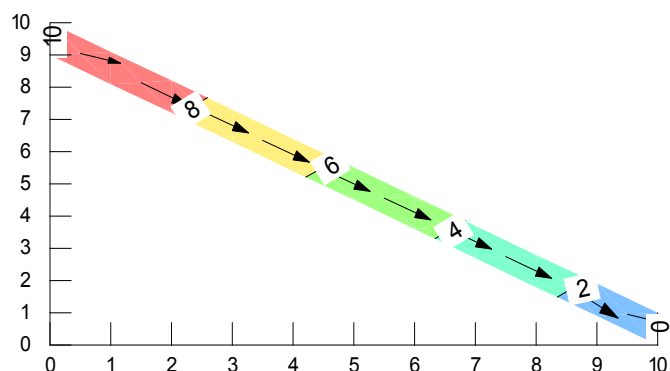


Figure 5-5 Flow in inclined pipe due to elevation head gradient only

In Figure 5-6 the pipe is again inclined as was the previous case, but the water pressures are different at each end. The total head difference now is zero and, consequently, there is no flow.

$$\Delta H = (5 + 10) - (15 + 0) = 0$$

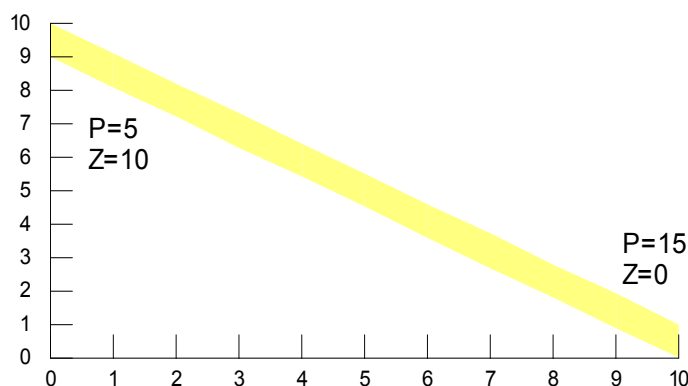


Figure 5-6 No flow in inclined pipe if zero total head change

Now consider the case where the total head is higher on the right than on the left, as in Figure 5-7, even though the pipe slopes from left to right. The total head difference is:

$$\Delta H = (5 + 10) - (20 + 0) = -5$$

The negative value indicates the flow is from right to left.

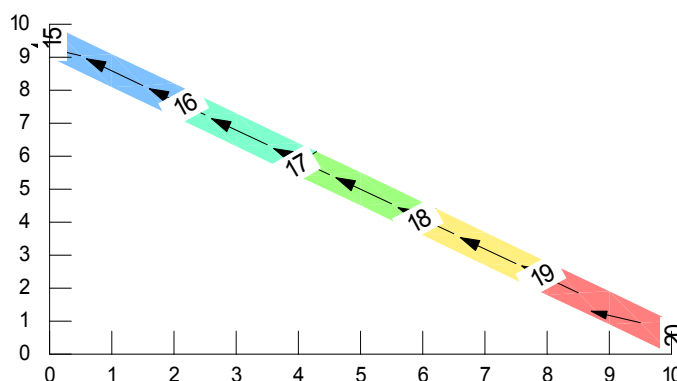


Figure 5-7 Upward flow due to pressure head and lower elevation head gradient

These simple examples all illustrate that the flow is in response to a total head difference between two points and, when defining head boundary conditions, it is necessary to always consider the pressures head together with the elevation.

At least one node in a steady-state analysis needs to have a head-type and a temperature type boundary condition in order to obtain a solution in VADOSE/W.

Head boundary conditions on a dam

Now let us specify the head boundary condition for a seepage analysis through the dam shown in Figure 5-8. The full supply level of the reservoir is 20 m. The ground elevation at the bottom of the reservoir is 10 m. Downstream of the dam the water table is at the ground surface and at the downstream end there is an under-drain. The granular material in the under-drain is highly permeable, making it reasonable to assume that the water level in the drain is the same as the water table downstream of the dam. This

implies that the permeability is high enough that there is no head loss in the drain relative to the small amount of seepage that will come through the low permeability embankment and foundation material.

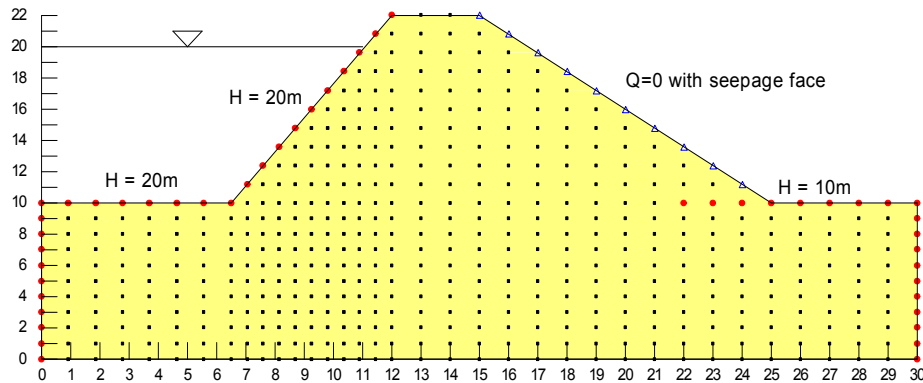


Figure 5-8 Head and seepage face boundary for flow through a dam

On the upstream side, where the reservoir contacts the embankment dam and the original ground surface, the total head is equal to the full supply level. On the upstream face of the dam at the reservoir level, the water pressure is zero, but the elevation is 20 m. The total head at this point then is 20 m. At the bottom of the reservoir, the pressure head is 10 m of water and the elevation is 10 m, making the total head also 20 m. The upstream boundary condition is therefore a constant total head equal to 20 m. This shows the convenience of using total head as a boundary condition. Even though the water pressures are different at every node on the upstream sloping face under the reservoir, the total head is nonetheless a constant. Without using total head as a boundary condition a different pressure would have to be specified at each node on the upstream dam face. Specifying this condition as a constant total head is more convenient.

Downstream of the dam toe, the water table is at the ground surface; that is, the water pressure is zero at the ground surface. The total head, therefore, is the elevation of the ground surface, which in Figure 5-8 is 10 m.

The water level in the drain is the same as the water table beyond the downstream toe as reasoned earlier. Therefore, the conditions around the perimeter of the the drain are known. The total head around drain perimeter in this case is 10 m.

The total head difference between the upstream and downstream conditions then is 10 m, resulting in the flow shown in Figure 5-9.

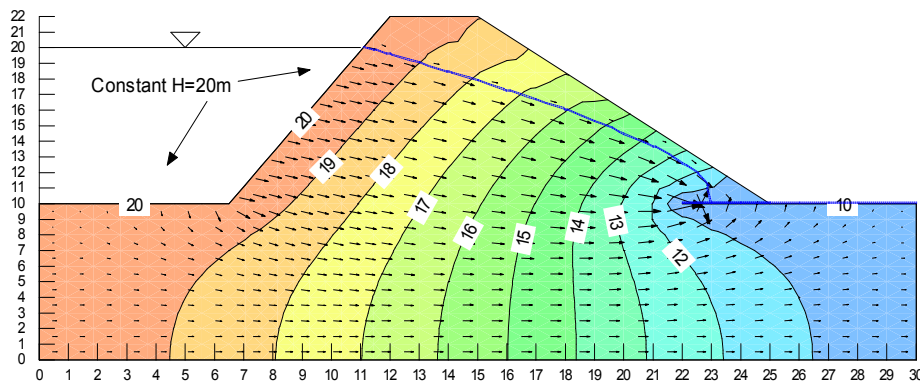


Figure 5-9 through reservoir dam with toe under-drain

Constant pressure conditions

Sometimes it is the pressure head that is constant on sloping ground and the total head varies at every node. Figure 5-10 illustrates a case like this. The natural ground surface beyond the embankment toe slopes away from the embankment. The water table is considered to be at the ground surface. From a seepage analysis point of view, the water pressure is zero at the ground surface. The elevation of each node in this area is different and therefore the total head is different at each node.

VADOSE/W has a special feature to handle this condition. You can specify the head with a special condition that makes the pressure zero. When you select this option, VADOSE/W finds the y-coordinate of each node and sets the total head equal to the y-coordinate. You will notice that the boundary condition is specified as a head-type with the action equal to the y-coordinate of the node.

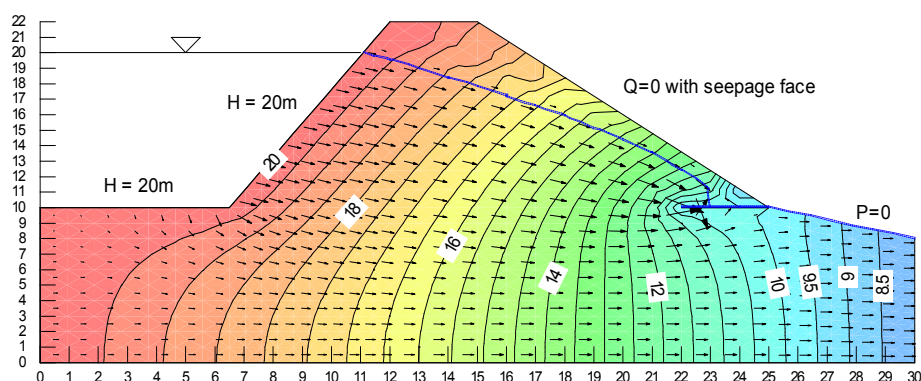


Figure 5-10 Sloping down stream face with $P=0$ boundary (non constant heads)

Far field head conditions

There are many situations where it is necessary to specify the boundary conditions at the far extents of a problem. Figure 5-11 shows an example where the main interest is the seepage into an excavation. The excavation is below the initial water table. In a case like this it is necessary to specify the condition on the vertical boundary some distance away from the excavation. This is often referred to as the far field boundary.

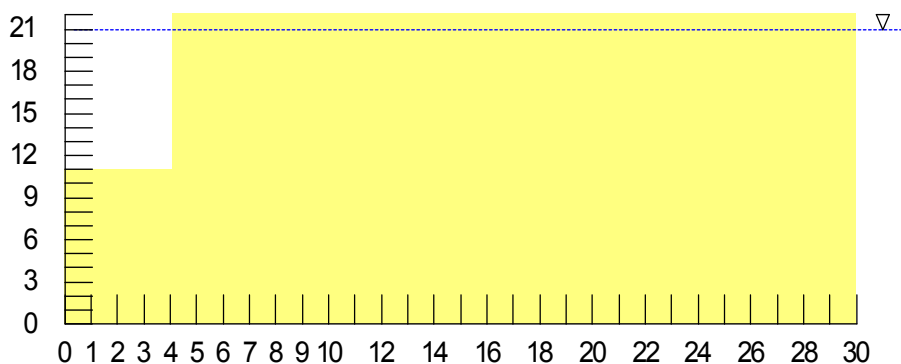


Figure 5-11 Excavation region with initial water table shown

In reality, the boundary conditions at the far field are unknown. It is common, however, to approximate the boundary condition by specifying a head condition reflective of the initial water table. In other words,

the boundary condition is specified as a total head equal to the elevation of the water table. This is a reasonable thing to do, but it is important to understand the physical significance of this type of a boundary condition.

Specifying a constant total head as a far field boundary condition implies that sufficient water is somehow going to come to that location so that the head remains a constant. Physically this is the same as if there was a water reservoir up against the far field end of the problem, as illustrated in Figure 5-12, and that the reservoir remains at a constant level. This is not reality, but specifying the constant head has the same physical significance.

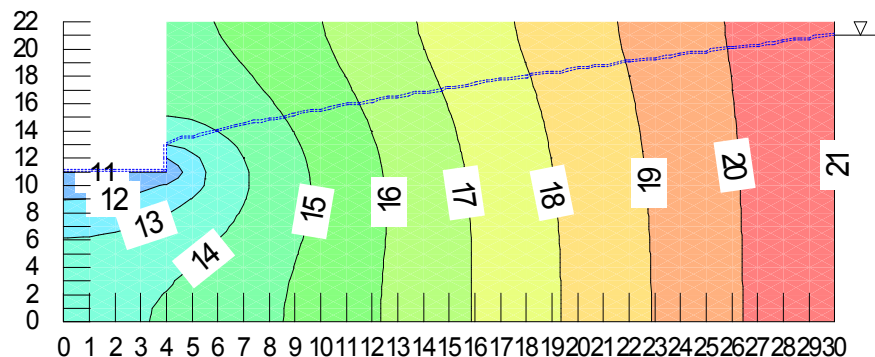


Figure 5-12 Far field boundary with head equal to water table elevation

Specifying a constant head far field boundary condition is legitimate in a transient analysis until the point in time when the water table would naturally start to drop at the far field. For further time steps, it is only an approximation of reality the same as it would be if used in a steady-state analysis. A steady-state analysis is physically a transient analysis run to infinity, and during this long time water somehow arrives at the far field to maintain the constant head.

The objective in a finite element analysis is to extend the far field boundary far enough away from the point of engineering interest that the head approximation does not significantly influence the engineering results. Extending the far field boundary can sometimes be conveniently accomplished with infinite elements, which are discussed in greater detail later in this chapter, the Meshing chapter, and Appendix A.

Once again as discussed in Section 5.2, it is important to remember that when you specify a head, the software will always compute a flux Q into or out of the flow system at that node.

5.5 Specified boundary flows

The second of two options for specifying boundary conditions is to specify a rate of flow across the edge of an element. An example may be the rate of infiltration or application of precipitation. This is often referred to as a flux boundary.

Thinking back to the discussion on fundamentals in Section 5.2, when it comes to solving the unknowns in the finite element equations, it is necessary to specify or compute the flow at the nodes. Consequently, when specifying a unit rate of flow across the edge of an element, it is necessary to integrate along the edge of the element and convert the unit rate of flow (q) into nodal flows (Q). Even though VADOSE/W automatically does the integration, it is nonetheless useful to have an understanding of how the integration is done. Understanding the relationship between unit rates of flow across an element edge and nodal flows can be useful in understanding and verifying results. Sometimes in unusual situations, it can also be

useful to know how to manually compute the nodal Q flows from unit rates of flow (q) and then specify Q at the node instead of q on the edge of the element.

First of all, VADOSE/W only handles uniform rates of flow across the edge of an element. The uniform rate of flow can be set to vary with time, but not with distance across an edge of any individual element. Formulations for non-uniform rates of flow across an edge are available, but these have not been implemented in VADOSE/W.

Since the flow across the edge of an element is uniform, the total flow across the edge is simply the flow rate (q) times the length of the element edge. The manner in which the total flow across the edge gets distributed to the nodes depends on the number of nodes on the edge. In VADOSE/W the edge can have either 2 or 3 nodes.

When the edge of an element has only two nodes, the total specified flow across the edge is evenly divided between the end nodes. Half goes to one end node, the other half goes to the other end node. This is graphically illustrated in Figure 5-13. When two or more edges have a common node, the contributions from each edge accumulate at the common node as illustrated in Figure 5-13.

Higher-order elements with three nodes along the edge of an element are usually not required in a seepage analysis. Sometimes, however, it is desirable to do a SIGMA/W or QUAKE/W analysis on the same mesh, and for these types of analyses, higher order elements are required. Consequently, sometimes higher order elements are used in a seepage analysis not because they improve the seepage analysis results, but because mesh consistency is required when integrating with other types of analyses.

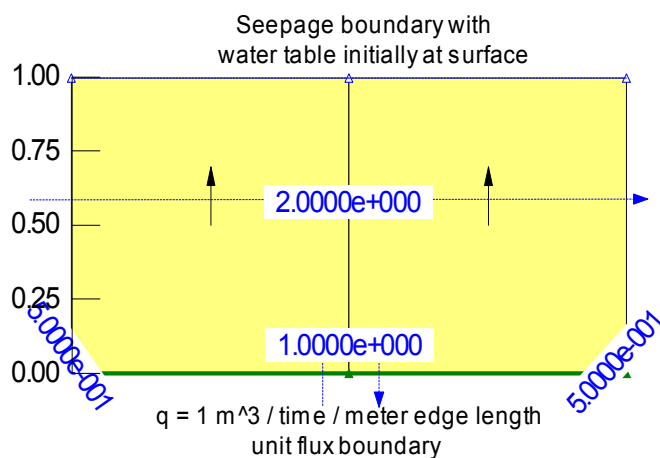


Figure 5-13 Unit and total nodal flux boundary condition relationships

When there are three nodes along the edge of an element, the total flow across the edge is distributed as 1/6 to each corner node and 4/6 to the middle node. This is graphically illustrated in Figure 5-14. Once again, when one node is common to more than one edge the 1/6 end contribution from each edge is accumulated at the common node. The distributions of the nodal fluxes come directly from the numerical integration of a variable, such as a gradient along the edge of an element. Further details on this are presented later in the Theory Chapter and the Visualization of Results Chapter.

For an axisymmetric case the Q boundary flux values are a function of the radial distance from the vertical symmetric axis. For elements with nodes located only at the corners as shown in Figure 5-15, the nodal boundary flux, Q, is the contributing area from each element multiplied by the radial distance from the symmetric axis times the element thickness which is expressed in terms of radians. The nodes further away from the axis of symmetry have more contributing area so their flux values are greater. In the case

of the middle node, it has a total flux value of 1.0, but this is comprised of two flux quantities of 0.5, each contributed by the element edges on either side of it. The node on the right has a total flux of 0.833333, but only half the contributing area as the middle node. Consequently, as the distance from the axis of symmetry increases so does the flux quantity.

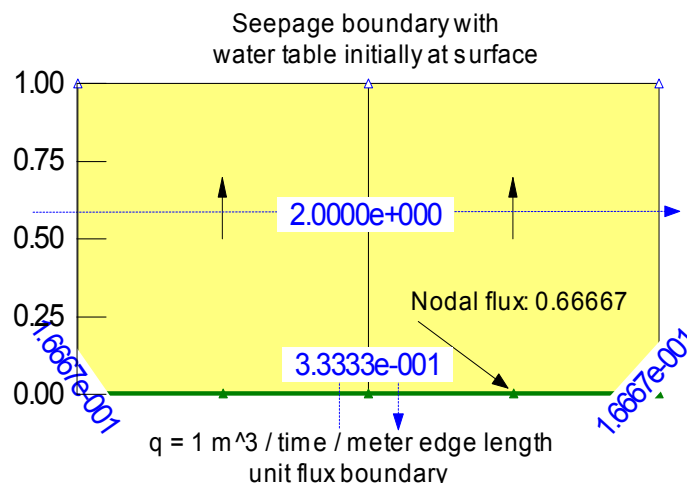


Figure 5-14 Distribution of unit flux in element with secondary nodes

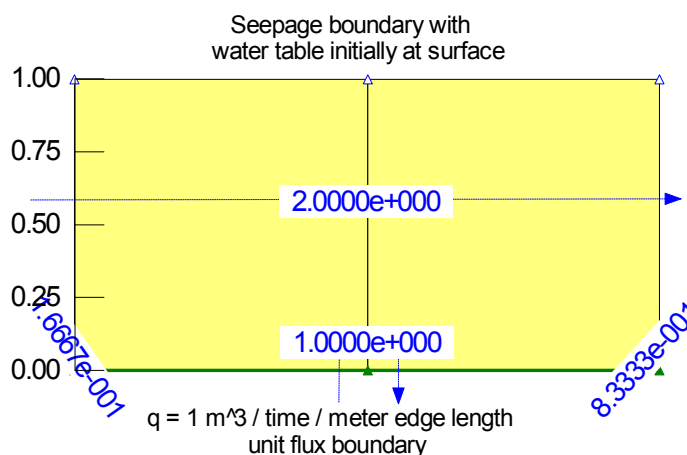


Figure 5-15 Distribution of unit flux in axisymmetric analysis without secondary nodes

The situation is not quite as straightforward for higher order elements where three nodes exist along the element edge, as illustrated in Figure 5-16. The detailed formulas for these cases are provided in the Theory Chapter. The case described in Figure 5-15 is fairly straightforward and easy to remember for quick spot-checking the computed nodal boundary flux values.

Conversion of specified flow rates (gradients) across element edges is dependent on the specified element thickness. For a two-dimensional vertical section the thickness, by default, is one unit, although the thickness can be some other specified value. For axisymmetric cases, the thickness is in terms of radians. The default is 1 radian. Sometimes it is useful and convenient to specify the thickness as 2π radian so that the computed nodal boundary flux values are for the entire circumferential area. Specifying the thickness is simply a user preference. It is important to remember the element thickness when interpreting the computed Q values.

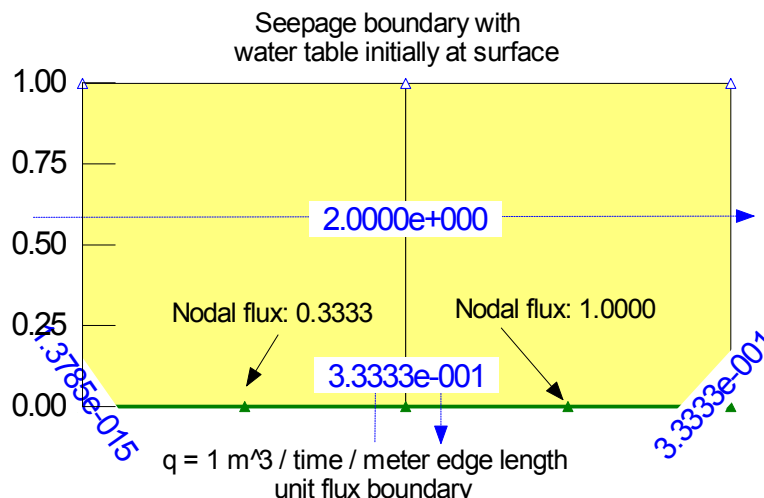


Figure 5-16 Distribution of unit flux in axisymmetric analysis with secondary nodes

In VADOSE/W, the specified in-flow or out-flow rates (gradients) are always deemed to be normal to the element edges.

In VADOSE/W, flow into the system is positive. Flow out of the system is negative.

Another important concept to keep in mind when specifying and interpreting flow quantities is that nodal boundary flux values Q are scalar values. Nodal Q values have no specified or computed direction. The direction of flow can only be inferred from the computed gradients or unit flow vectors inside the elements. VADOSE/W can display velocity vectors in each element, which are a graphical representation of flow rates and direction.

5.6 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. A source could be an injection well. The important concept about sinks and sources is that they represent flow into or out of the system.

Consider the situation in Figure 5-17, which simulates the effect of an under-drain on the downstream face of a dam. The simplest way of including the effect of a drain at that location is to specify a “sink” type boundary condition at those nodes. We assume that the drain will be capable of removing all the seepage that arrives at the drain. In other words, the drain will not be under positive pressures at any time; the water pressure in the drain will be zero. We can specify this boundary condition by specifying a head (H) at the desired drain nodes equal to the elevation (y -coordinate) of those nodes. This is equivalent to specifying the pressure to be zero at those nodes ($P=0$). By specifying the H condition, VADOSE/W will compute the boundary flux (Q) that must exist to ensure the pressure is always 0 at each node.

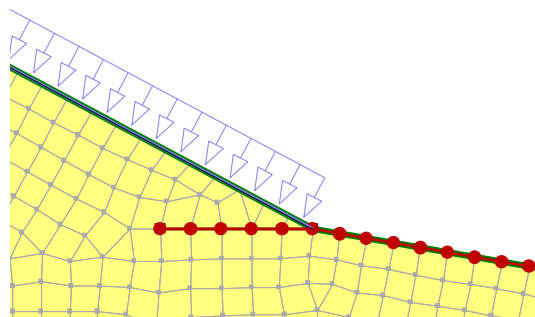


Figure 5-17 Under-drain nodes beneath toe of down stream dam face

In this example the specified H is a sink, since water leaves or disappears from the flow system as a result.

From a behavioral point of view, any specified H or Q on the perimeter of a problem has the same action as a specified H or Q inside the mesh. The difference is only in terminology. Along the problem perimeter the specified H and Q are usually referred to as boundary conditions. Inside the mesh, a specified nodal H or Q is often referred to as a sink or source type of boundary condition.

It is often tempting to specify piezometric measurements at certain nodes inside a mesh. This leads to erroneous results. The physical consequence of including piezometric measurements in a seepage analysis is that water needs to enter or escape from the flow system in order to achieve the specified water pressure at the point where the piezometer is located. Remember that when we specify H (piezometric measurement), VADOSE/W will compute Q . Piezometers are not a sink or a source and therefore it is not appropriate to specify the field measurements as a boundary condition. A useful way of thinking about this situation is that the flow regime was created before the piezometer was installed and the installation of the piezometer does not change the flow regime. Specifying the piezometric measurements may alter the flow regime since the specified conditions may act like a sink or a source, which is not the intention.

5.7 Seepage faces

It has been noted several times earlier that in seepage analyses only the head (H) or flow (Q or q) can be specified as a boundary condition. There are, however, situations where neither H nor Q are known. A typical situation is the development of a downstream seepage face such as illustrated in Figure 5-18. Another common situation is the seepage face that develops on the upstream face after rapid drawdown of a reservoir. Other examples may include the drain/soil interface inside a lysimeter where water accumulates until pressures build sufficiently to form a drip surface. For this type of situation, there are periods of time where there is no flow across the drain boundary.

The pore pressure on a seepage face is zero, but this cannot be specified for all times because a $P=0$ situation also reflects the location of the phreatic surface and it may inadvertently become a source for water. Another problem with seepage faces is that the size of the seepage face may not be known and consequently needs to be determined as part of the solution through an iterative process.

In VADOSE/W, all climate boundary nodes are, by default, seepage faces. It is also possible to apply a manual potential seepage face by flagging nodes as a special boundary condition type. At the end of each iteration the conditions along the specified potential seepage face are “reviewed” to see if they meet the correct criteria. This is why it is called a potential seepage face review.

Consider the simplest case where the boundary flux is zero along a seepage face. In this situation, the boundary conditions along the entire potential seepage face are set to $Q = 0$ (flux-type), indicating that no

additional flux is going to be added or removed at these nodes, and with the specification that the conditions will be reviewed and adjusted as necessary. At the end of the first iteration after the heads are computed for all nodes along the potential seepage face, VADOSE/W checks to see if any of the nodes have a positive pressure (H greater than elevation). Nodes with computed pressures greater than zero are not allowed, as positive pressure on the surface indicates ponding, which cannot happen along the sloping boundary. The water would run off, not pond. The specified boundary condition of Q equal to zero is therefore not correct. Physically, it means water wants to exit the system, but the Q equal zero condition does not allow the water to exit. To allow water to leave, VADOSE/W converts the boundary condition to a head-type with H equal to the y -coordinate (zero water pressure) at each node with a computed positive pressure, and a new solution is computed.

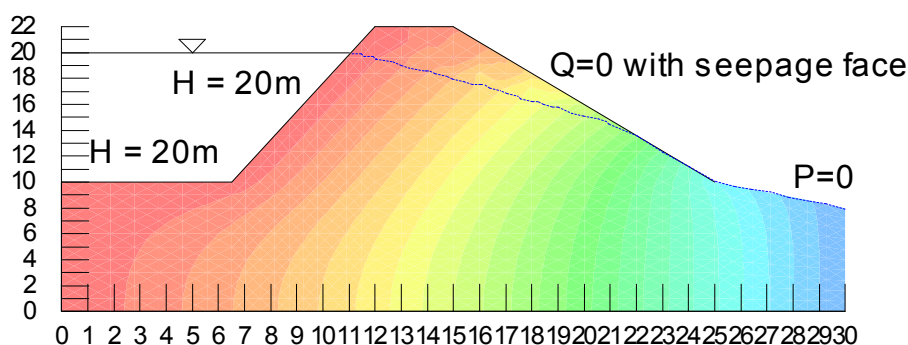


Figure 5-18 Seepage on down slope dam face (no toe under drain in this case)

At the end of the repeated solution step, water can now leave or enter the system at the nodes that were converted from a Q -type to an H -type. Now the program checks to see whether the computed Q is negative (out of the system) or positive (into the system). Computed flow out (negative) of the system is acceptable – a computed flow into (positive) the system is not acceptable. At nodes along the potential seepage face with a positive flux, VADOSE/W then converts the H -type boundary back to the original specified Q -type and then repeats the analysis. The process is repeated until all nodes on the potential seepage face have either a computed zero water pressure ($H = y$) or a nodal Q equal to zero, the original specified boundary condition. In a steady state analysis, once the seepage face is determined, the solution solves to completion. In a transient analysis, the seepage face is determined for every transient time step as necessary.

The initially specified flux on a potential seepage face does not have to be zero. The initially-specified flux can be some other positive or negative value. A positive value could represent infiltration and a negative value could represent evaporation. Nodes that are not converted to an H -type along a potential seepage face in the end must have the specified flux.

During a transient analysis, potential seepage face review nodes are set to a flux-type boundary condition at the start of each time step. This includes all nodes that were converted to a head type boundary condition during the previous time step. The applied flux is set to the initial action specified at the review nodes. If the review nodes follow a flux-type boundary function, the flux at the review nodes is computed from the function for the start of each time step. The size of the required seepage face must be determined separately for each time step in a transient analysis.

Review nodes can be located anywhere along a boundary. For example, the nodes may be located on the downstream seepage face and on the upstream drawdown face at the same time. All review boundary nodes are considered in each review procedure. Consequently, depending on the solution, the modification of boundary conditions may jump from one area to another with each successive iteration.

Sometimes conditions may follow a head-type boundary function; such as the upstream face of an embankment dam experiencing drawdown. The head changes as the reservoir is lowered. Above the changing surface of the reservoir, there is potential for a seepage face to develop as the pore-water pressures within the embankment redistribute. In this case, a function that describes the changing head boundary with time can be developed and a secondary condition that will change the head boundary to a flux boundary if the total head becomes less than the elevation head at any node. When the head boundary is assigned to the reservoir nodes, the boundary review option can then be flagged. The boundary review procedure is then followed to determine the required seepage for that particular time step. This is required to ensure that all nodes with a y-coordinate greater than the boundary function head (pool elevation) have a condition of flux equal to zero at the start of each time step.

It is important to remember that the node along a potential seepage face must have a flux type boundary at the start of the time step. Nodes with a specified constant head boundary condition cannot be reviewed.

Care must taken to not specify potential seepage boundary conditions that are unrealistic or unnecessarily too large. The computing time and associated potential convergence difficulties increase significantly as the number of nodes along all potential seepage faces increases. A little preliminary planning and guessing as to where seepage face may develop and specifying the boundary conditions accordingly helps to mitigate these issues.

5.8 Free drainage (unit gradient)

A free drainage boundary condition can be useful in certain circumstances, but it can also be easily misused. Consider the pressure profile of the Kisch problem for steady state infiltration through a clay barrier over a coarse sandy soil as illustrated in Figure 5-19. In this figure, both the surface and base boundary conditions are specified as head boundaries. There is in effect a pressure equal to zero at the surface and a water table at the base. Consider now what the bottom boundary condition would be if the water table was not 2.5 meters below the surface, but was 30 meters below the surface. While technically it would be possible to construct a mesh to represent this situation, it would likely not be practical.

We know from the illustrated Kisch pressure profiles that at some point beneath the clay (near surface) layer, the water contents and pressures in the sand become constant with depth. When this is the case, the total head gradient within the sand is equal to unity and the downward flux is equal to the hydraulic conductivity at that point. Closer inspection of the pressures in Figure 5-19 indicate that the unit gradient condition could exist under the clay soil until a specific depth, which is dependent on the infiltration rate and the hydraulic properties of the underlying soil, when the pressures have to transition towards $P=0$ near the water table. If we do not want to model the entire profile and we are certain that for our real field conditions there is a fairly constant water content and pressure with depth, we can use the free drainage or unit gradient boundary condition option for the base of our geometry and apply it at some fixed distance AWAY from our prime area of interest in the model. Figure 5-20 shows the correct pressure profile for the Kisch problem with a free drainage base boundary condition applied one meter beneath the clay cover.

Use of the free drainage boundary condition should ideally be applied in transient analysis and only specified on bottom mesh boundaries that are relatively far away from your main area of focus. They will work for a steady state analysis, but the solution can be hard to obtain from a convergence perspective, as you are in effect applying an unknown Q boundary with unknown conductivity values at the base of the problem and the solution can tend to oscillate if not carefully controlled.

In a transient analysis, however, the unit gradient boundary condition is obtained by setting the Q flux boundary to be equal to the actual hydraulic conductivity value present at the nearest gauss point from the previous iteration multiplied by the contributing edge boundary length. Therefore, the solution of the

correct Q to apply is closely controlled by the initial or previous time step and actual pressure and conductivity conditions in the finite element at the point of application. In a transient analysis the solved Q drainage is free to increase or decrease with time, depending on the small changes in pressures in the elements above the free drainage boundary. In turn, the water content at the bottom can, with time, slowly increase or decrease in response to the free drainage or infiltration from above.

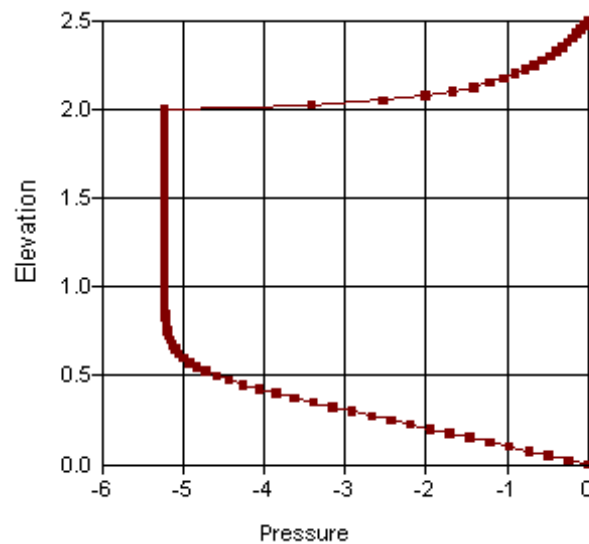


Figure 5-19 Kisch pressure profile with head top and head base boundary condition

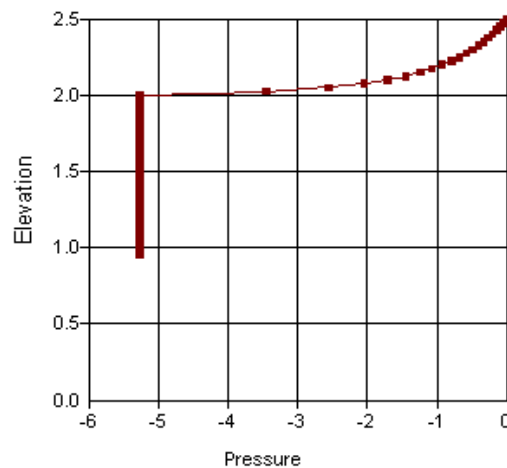


Figure 5-20 Kisch pressure profile with head top and free drainage base boundary condition

5.9 Far field boundary conditions

In many cases the boundary conditions far away from the main point of interest are undefined, such as the boundary conditions far away from a pumping well or from an excavation. These are referred to as “far field” boundary conditions.

One approach to dealing with far field boundary conditions is simply to extend the problem boundaries; that is, make the mesh bigger and longer away from the point of main interest. The disadvantage of this

approach is that it requires more elements and therefore more computing time, and sometimes a very big, long mesh can make it awkward to draw and define the problem and to interpret and present the results.

An alternative to extending the mesh is to use what are called infinite elements. These are very convenient and powerful elements, but they need to be used with care and only under certain circumstances. The interpolating shape functions and detailed element characteristic are presented in the Theory Chapter. The discussion here concentrates on the behavior of infinite elements and on guidelines for using infinite elements.

The fundamental concept of the infinite element formulation is that the far field edge of the problem is extended away from the problem on the basis of an exponential decay function or hyperbolic function. A minimum of three points are required to describe such a function. The VADOSE/W formulation uses the interior corner nodes, the intermediate nodes and a pole point to make up the three points, as illustrated in Figure 5-21. The nodes on the right perimeter are deemed to be at infinity. For computation purposes the intermediate nodes are displaced in the direction of infinity by an amount equal to the distance between the pole point and the interior corner nodes. The pole point, interior corner node and the extended position of the intermediate node are then used to form the exponential decay function, which in turn is used to develop the element shape functions.

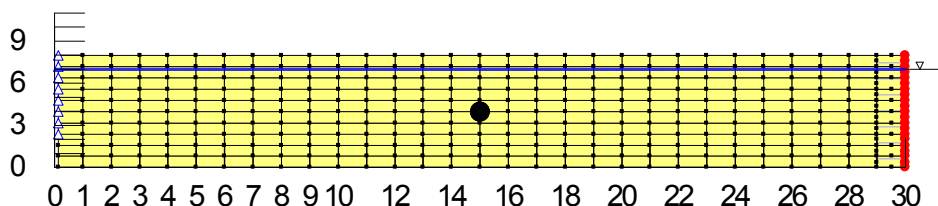


Figure 5-21 Axisymmetric pumping well with far field elements

The infinite elements are very useful and function well when heads (H) are specified at the far field. More specifically, they function very well when the primary unknown variable, which in VADOSE/W is the total head, is specified at the far field. The infinite elements do not always function well when flow rates are specified at the far field. The results can be acceptable if the boundary condition is a Q -type and the action is zero. Non-zero specified flux conditions can be troublesome and using infinite elements is not recommended when it is necessary to specify a non-zero flux boundary condition, particularly when specifying gradients or unit rates of flow.

Boundary conditions should not be applied on infinite elements perpendicular to the direction of infinity. Specifying for example surface infiltration at the ground surface on an element that extends horizontally to infinity can lead to unrealistic results. If it is deemed absolutely necessary to specify such a surface flux, then the mesh should be extended using ordinary elements instead of using infinite elements.

Interpreting or viewing results with infinite elements can be somewhat tricky. For this reason the results can be viewed with or without the infinite elements. The problem is that the infinite elements are displayed at the positions where they are drawn, but they are extended for computational purposes. When interpreting the results, it is necessary to mentally think of the boundary actually being a far distance beyond the edge of the mesh. Whether the infinite elements are or are not displayed when viewing results is a matter of personal preference. Once again, remember that the far field has been extended towards infinity, but is not displayed at infinity.

The pole position can have some effect on the solution. Earlier it was explained that three points are required to form the exponential decay function, and the distance between these points affects the decay function. The larger the distance between the pole point and the interior corner nodes of the infinite

elements, the further the outside edge will be projected to infinity. So to extend the outer edge as far as possible the distance between the pole and the interior corner nodes should be as large as conveniently possible. Fortunately, the results are usually not very sensitive to the pole position, provided the pole position is a reasonable distance from the interior corner nodes.

Sometimes results can appear unreasonable when using infinite elements, particularly for a steady-state analysis. Consider the case of axisymmetric flow to a pumping well. For this situation, the vertical dimension is small relative to the horizontal, as illustrated in Figure 5-21. When infinite elements are added at the far left side of the mesh, away from the well, the results may indicate that there is very little drawdown within the ordinary element portion of the mesh. The interface between the ordinary elements and the finite elements contains a sharp curve in the phreatic line. For this situation, if the infinite edge could be displayed at its actual horizontal position, the solution would appear reasonable, but it is not practical or even possible to draw the edge at infinity and consequently the majority of drawdown that occurs inside the infinite elements appears unreasonable as illustrated in Figure 5-22. Numerically, the flux values and pressure contours in the ordinary elements are correct, but the solution looks suspect, as it is not usually an anticipated solution.

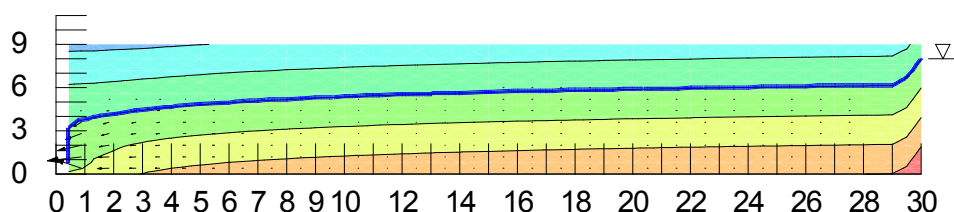


Figure 5-22 Draw down cone phreatic line using far field elements

It is always good practice at the start of the analysis to NOT use infinite elements. It is highly recommended that you obtain a reasonable result using ordinary elements before proceeding with infinite elements. Once you are satisfied with the results, you can then add the infinite elements and evaluate whether they provide any advantage for your particular analysis.

In summary, the infinite elements can be convenient and powerful, but they need to be used with caution and care.

5.10 Hydraulic boundary functions

VADOSE/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 heads (or pressure) or fixed flux values. In a transient analysis however, the boundary conditions can also be functions of time or in response to flow amounts exiting or entering the flow regime. VADOSE/W accommodates a series of different boundary functions. Each one is discussed in this section.

General

A non-fixed boundary condition must be entered as a user-defined function. In VADOSE/W all functions are defined using a combination of manually entered or cut and paste data points, and all functions can be customized to suite your exact needs. In certain cases, it may be desirable to have a stepped function. The additional functionality of automatically fitting the data with a step function has been added to the program. There is also an option to have a cyclic function repeat itself over time, which saves you the task of defining it repeatedly.

In general, all functions are comprised of a series of x and y data points that are fit by a spline curve. A spline curve is a mathematical trick to fit a curved shape between a series of points. The simplest way to fit a series of data points is to draw a straight line between the points. This is often a very poor way to represent a non-linear function. The advantage of the spline is that it joins all data points with a continuous smooth curve.

During the solution process, the solver uses the “y” value along the spline curve for any required “x” value. It is therefore important to make sure the spline fit, not your original data, portrays how you want the boundary condition applied.

Head versus time

A very useful boundary function is user-specified Head versus Time. Consider the example in Figure 5-24 where the drawdown in the reservoir is to be applied as a boundary condition so that the dissipation or pore-water pressures in the dam can be modeled. A Head versus Time function (Figure 5-23) with the $Q=0$ if $H < \text{elevation}$ option has been specified on the reservoir side of the dam.

The advantage of using a Head versus Time function on the reservoir side of the dam is that it avoids a “shock” unloading of the water pressure on the dam if the water level in the reservoir were instantly drawn down to the 11 meter elevation. Whenever possible, it is a good idea to apply changing boundary conditions as realistically as possible, to avoid shocking the system.

In the drawdown example, the boundary function has an added criteria imposed on it that requires the boundary flux on the head nodes to be zero if the head at the node becomes less than the elevation of the node. This means that seepage cannot flow out of the upstream face of the dam above the water table. This may not be desired in some cases, such as if there were a higher water table on the right side of the dam that caused reverse flow through the dam, or if there were some surface infiltration that could cause water to flow back into the reservoir through the upstream face.

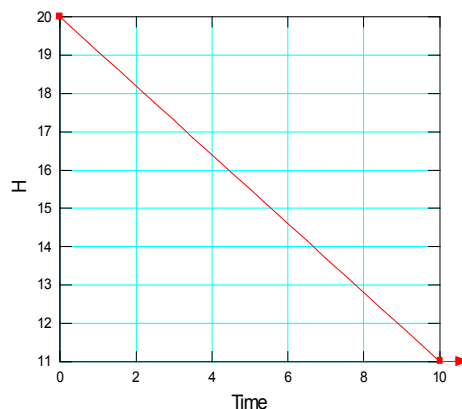


Figure 5-23 Head versus time function for reservoir draw down

There are occasions where the boundary function may cycle, or repeat itself over time. This may be the case if the reservoir water level rises and drops on an approximately constant cycle. Instead of defining the cyclic nature of the function from start to finish, you have the option to define it over the first “period” of time and then have it repeat itself for as long as you defined time steps to solve. An example of a cyclic function is given in Figure 5-25 where the data represents the water level in the reservoir fluctuating between 20 and 16 meters over a 100 day period.

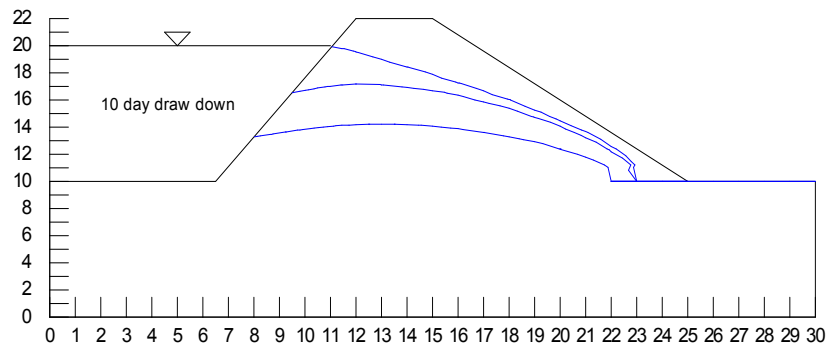


Figure 5-24 Phreatic surface in dam over time after reservoir draw down

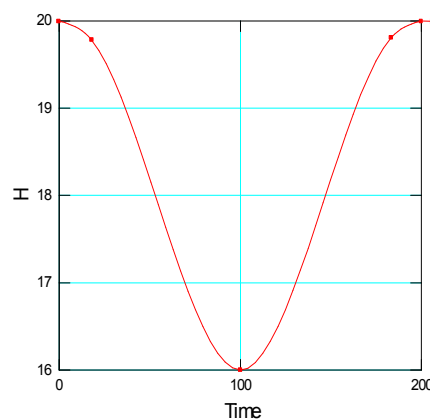


Figure 5-25 Cyclic head versus time function

In any “time” function, make sure the units of time you specify in the function match those used to define the conductivity function (e.g. seconds, hours, days etc.) For long transient solutions, it is often useful to define the conductivity in terms of m/day so that all time steps and functions can be set up with “day” units. This avoids having to input time values of 864000 seconds to represent 10 days.

Head versus volume

In certain circumstances you may want to determine the amount of seepage that exists and how deep a pond may be as a result of the outflow. Consider that you have a rising river level and you need to determine the depth of ponded water that develops in a depression adjacent to the river.

VADOSE/W is formulated to automatically track and accumulate the volume of water from a user-specified area, such that the volume of water can be compared with a user input function to determine the actual head value at that point. Consider the simple illustration in Figure 5-26. In this example, a river level is rising according to a user input Head versus Time function. The objective is to determine how deep the seepage pond will get when the river reaches its peak.

To carry out this analysis, you must create a Head versus Volume function for the area being filled by seepage water. A schematic of this function is given in the figure below. As the analysis solves, the total

outflow from each Head versus Volume boundary node is obtained and summed. The total summation of these nodal volumes is equal to the total volume of ponded water. Prior to the next time step, the program will consider the total volume of ponded water and use the Head versus Volume function to determine the head boundary to apply at each node.

It is important to consider the ponded water head in this case, because the total outflow into the pond is a result of the difference in the driving head from below AND from above.

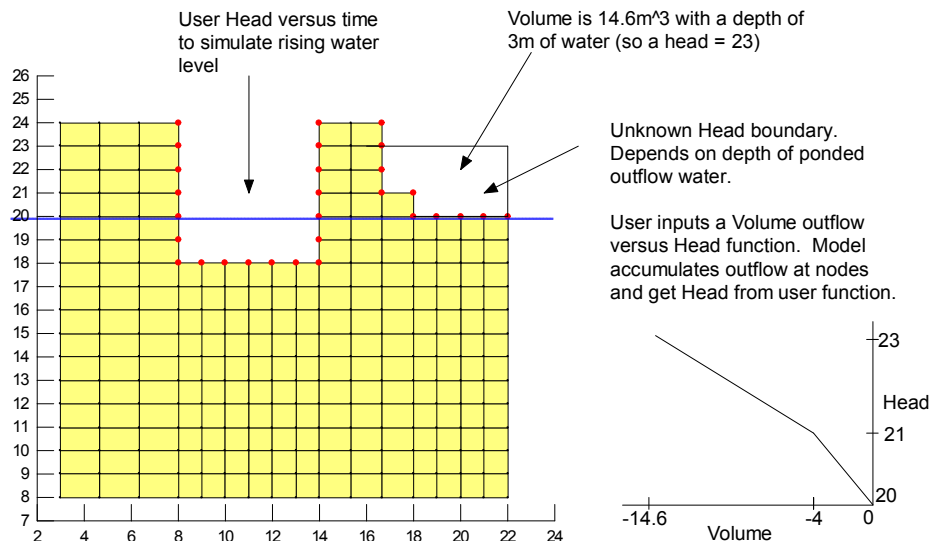


Figure 5-26 Simple illustration of head versus volume boundary function

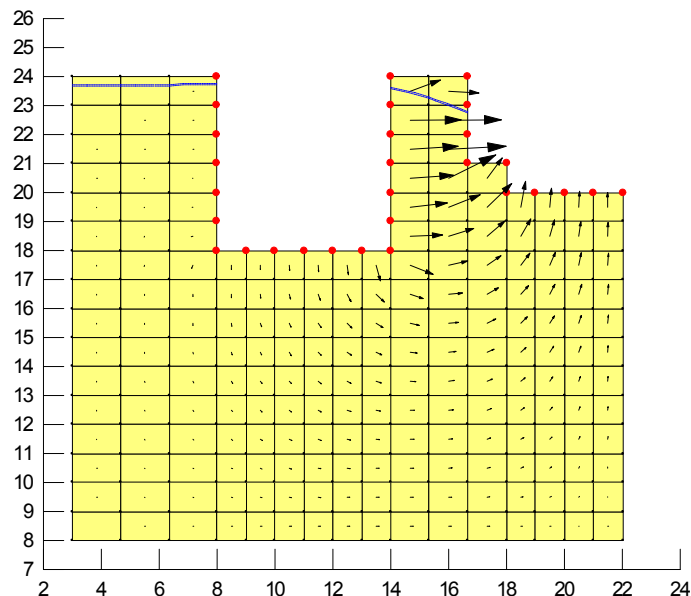


Figure 5-27 Seepage into ponded volume

The illustration in Figure 5-27 shows the position of the phreatic line at the end of the analysis when the river level is at its peak. You can see that the flow vectors indicate there is still some seepage out of the

soil and into the pond at this stage. Had the analysis been carried out for slightly longer with the river level remaining at its peak, then the ponded depth would rise to match that of the river. However, in a real life application, it is likely that the river level would peak and then subside. This analysis method could be used to determine the full transient nature of the rise and decline of the ponded water in response to the river's rise and drop.

Nodal flux Q versus time

As discussed previously, there are only two fundamental types of boundary conditions: either a head or flux boundary. Head boundaries can be applied as total head, pressure head, or a time/volume function of head. Likewise, flux boundaries can be applied as fixed values of total or unit flux or a time dependent function of either.

In many cases it is useful to apply a total nodal flux (Q) boundary that is a function of time such as the function illustrated in Figure 5-28. In this case, a total nodal flux is being applied at one or more nodes such that the flux represents a decaying source of water at those nodes. If the function “y” value is positive, this indicates a water source at the node and if the “y” value is negative, this would indicate a nodal sink flux. When you apply a total nodal flux at a node, you are not taking into account any mesh geometry in the flux quantity. You are simply stating that you are introducing a set volume of water at a single point in the mesh, and the amount that you are introducing changes with time.

During the solver process, the solver will take the elapsed time of the solution and look up from the defined function what the total flux rate of water should be at that time. It will then multiply the function value by the current time step duration to obtain a total volume of water to add at that time step. Be careful when using functions like this. It is very important to make sure the time steps you set up in the solver are small enough to follow the desired shape of the function. For example, for the function shown in the figure below, if the elapsed time was 3 days and the time step being solved was 3 days, then a water volume of $0.05 \text{ m}^3/\text{day} * 3 \text{ days} = 0.15 \text{ m}^3$ would be applied between day 3 and day 6. The specified function amounts over these three days would be $0.05 \text{ m}^3/\text{day}$ between day 3 and day 4, 0.04 m^3 between day 4 and day 5, and 0.025 m^3 between day 5 and day 6. Therefore, the correct total for these three days would be $0.05 + 0.04 + 0.025 = 0.115 \text{ m}^3$. Using too large a time step in this case would in effect introduce more water than indicated by the function for the same time period. As a rule, make the time steps small enough to follow the shape of the function.

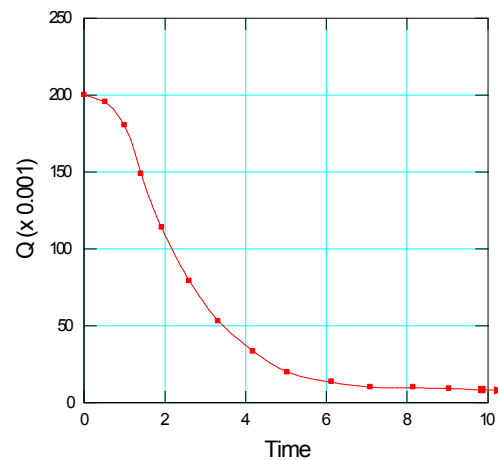


Figure 5-28 Nodal flux (Q) versus time function

Unit flow rate versus time

The previous section discussed application of a total nodal flux boundary function. In this section, a unit flux boundary function is discussed. A unit flux is a flux value applied along a mesh edge such that the length of the mesh edge determines how much flux is applied at the nodes adjacent to the edge. While a unit flux can be applied as a fixed action value, it is very useful to be able to apply it as a function.

A very simple example of a unit flux boundary function applied to an element edge is that of a ground surface daily rainfall minus potential evaporation rate that is known per square meter of surface area. This approach is not recommended for use in VADOSE/W where the real physical mechanisms of evaporation and infiltration are accounted for, but it has been used in SEEP/W which is a seepage only model.

Consider one such function as illustrated in Figure 5-29. In this function, the daily rainfall minus potential evaporation is entered as a step function. If the solver time steps are set up to be less than or equal to a day, they will follow the shape of the function and include data from each step. The data for this type of function can easily be set up in a spreadsheet program and cut and pasted into the function edit box.

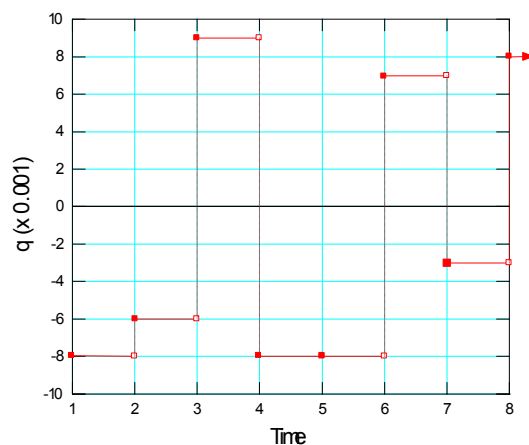


Figure 5-29 Unit flux function showing net rainfall minus evaporation

Modifier function

The previous two types of functions allow you to apply a set total or unit flux at element edges or mesh nodes. They are functions that will let the solver apply the appropriate action value for the stated elapsed time.

A modifier function is a powerful way of having the applied flux be dependent on the pore-water pressures in the soil. Consider the process of evaporation from a soil surface. As the soil dries out at the surface, the amount of actual water that is evaporated is reduced from the potential amount. Wilson (1990) showed that the rate of actual evaporation to potential evaporation is a function of the soil surface temperature and relative humidity. Ideally, the relationship is a result of coupled heat and mass flow processes in the soil (e.g. VADOSE/W); however, the process can be represented in simplified terms by having knowledge of the soil water pressure. It is possible to use SEEP/W to compute an approximate evaporation rate from the soil surface by combining a unit flux boundary condition (such as that specified above) with a modifier function such as the one illustrated in Figure 5-30. Again, this is not the recommended approach in VADOSE/W, because it is formulated for the rigorous method. This is simply an example of how a modifier function may be used.

In this figure, the ratio of actual to potential evaporation is shown as a function of the negative pore-water pressure. As the soil dries out (the pressure becomes more negative), the percentage of the daily potential evaporation as specified by the unit flux versus time function is reduced. At each time step, the solve will look up the appropriate potential evaporation rate and then multiply that value by the percentage value obtained from the modifier function for any given soil pressure state.

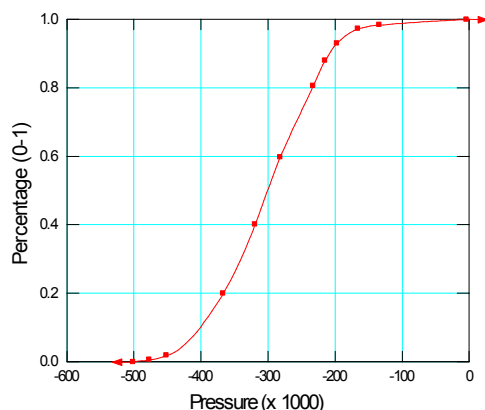


Figure 5-30 Modifier function showing possible ratio of actual to potential evaporation

5.11 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 VADOSE/W.

5.12 Climate – soil boundary conditions

VADOSE/W is specifically formulated to allow for the rigorous coupling of climatic conditions to the ground surface. While the actual boundary conditions are computed based on a complex set of conditions, the boundary conditions applied in the model are one of three basic types; a unit flux water flow rate at the surface which is converted to a total nodal flux based on nodal spacing, a ground surface nodal temperature, or a ground surface gas (radon or oxygen) concentration. The full details of how these values are computed are given in the Theory chapter. It is strongly recommended that you read the section titled Atmospheric Coupling in the Theory chapter in addition to the discussion below.

The climate boundary condition, by default, can only be applied on the edge of a mesh created as part of a special surface mesh region. Surface meshing is discussed in more detail in the chapter on meshes. Once a surface mesh is established, it is possible to use the Draw Boundary condition command to simultaneously set the thermal, hydraulic and gas flux boundary condition on all or part of the surface. In addition, if the analysis is set to include transpiration from plants, this condition is specified as part of the climate boundary condition.

If a climate boundary condition is chosen with the gas transfer analysis option enabled, then the concentration type boundary condition at the ground surface will depend, by default, on what type of gas is used in the analysis. If the gas is oxygen, then the default concentration of oxygen at the ground surface

climate nodes is set to the equivalent of 280 g/m³ which is a typical concentration of oxygen in air. If radon is the gas type used in the analysis, then the radon concentration at the ground surface is set to zero Becquerels/m³, as it is assumed the radon source is within the soil and it is removed by the atmosphere as soon as it reaches the ground surface. For both the radon and oxygen gas transfer processes, it is up to the user to specify a known boundary condition (fixed concentration or source/sink flow rate) at some other point in the geometry.

VADOSE/W will allow different climate data sets to be applied to different parts of the surface mesh. This is a useful feature when it is known that parts of the ground surface are oriented differently to the sun or prevailing winds, or where precipitation or snow accumulation varies across a modeled region. If vegetation is applied in the analysis, any combination of a leaf area index, plant root depth and moisture limiting function can be used at any external element edge with either a single or multiple climate data set.

As with SEEP/W, the surface mesh in VADOSE/W tells the solver to make special considerations when it comes to dealing with water from a seepage face or precipitation runoff (or snowmelt runoff etc.) The solver attempts to determine the high and low points across a surface mesh such that water that does not infiltrate or that leaves the ground as seepage face water is not lost from the analysis but is stored at low points in the profile. The volume of the low points is computed and the amount of water that flows to the low points is used to determine the level of ponding. The level of ponding determines what the total head boundary condition should be on subsequent time steps. Even if rain is falling on a ponded section of the mesh, the program tracks the existing pond depth, the amount of rainfall and the amount of evaporative loss prior to applying the appropriate heat or flux boundary condition on the next time step.

5.13 Thermal and gas boundary conditions

VADOSE/W allows the thermal and gas boundary conditions to be applied throughout the mesh, independent of climate boundary conditions as required by the problem definition. The following types of boundary conditions can be applied at either the nodes or element edges:

- Fixed or time varying nodal concentration or temperature,
- Fixed or time varying nodal total heat flux or gas flux rate, and
- Fixed or time varying element edge unit heat flux or gas flux rate.

Finally, for both gas and thermal analyses, a modifier function can be used to automatically update a head or concentration boundary condition function based on current ground temperatures or concentrations. Use of a modifier function is described earlier in this chapter.

6 Analysis Types

There are two fundamental types of finite element seepage analyses, steady-state and transient. Numerous additional constraints and conditions can be applied within each fundamental type. A description of each type and the implications associated with each type are discussed in this chapter.

6.1 Steady state

Think about the meaning of the words “steady state.” They describe a situation where the state of the model is steady and not changing. In a seepage analysis for example, the “state” means the water pressures and water flow rates. If they have reached a steady value, it means that they will be in that state forever. In many cases where the geotechnical problem is exposed to nature with its cyclical conditions, it is possible that a steady state will never be reached. Flow beneath a cutoff wall may come close to steady state if the upstream conditions are held fairly constant over time. Net surface infiltration and evaporation will never reach a steady long term constant value. When simulating a constantly changing boundary condition such as surface infiltration and evaporation, the model does not know what the steady-state reality might be, it only knows how the initial input parameters change in response to the boundary conditions applied over the length of time being modeled. If you make the assumption that the boundary conditions are constant over time, then the model can compute the long term ground conditions in response to your assumption.

This type of analysis does not consider how long it takes to achieve a steady condition and that is something you need must understand. The model will reach a solved set of pressure and flow conditions for the given set of unique boundary conditions applied to it and that is the extent of the analysis.

It's very important to understand that when you are doing a steady state analysis you are not making any estimation of how long it takes the final condition to develop, nor how long it will last. You are only predicting what the ground will look like for a given set of boundary values, and it is implied that you are pretending the boundary values have been in place forever and will be in place forever.

Because steady state analyses are taking out the “time” component of the problem it greatly simplifies the equations being solved. However, at the same time it can make convergence harder to achieve – depending on the degree of non-linearity of your soil property functions. The steady state seepage equation leaves out the actual “time” variable and omits the entire volumetric water content function. They are not needed in the solution. However, VADOSE/W requires that you still input a function as it is used in the determination of water contents – which are required for the vapor flow coupling diffusion coefficients.

The volumetric water content is used for telling how much water is gained or lost in the soil if there is a change in pressure. In a steady state analysis, there is no starting pressure, and so there is no change in pressure to worry about. Remember, it is only looking to find out what the pressures will be throughout the problem geometry, given the fact you know what they are at only a few known locations and for all points in time.

Unfortunately, simplifying the equations does not mean that there is a reduced set of numerical issues associated with solving them. Recall that the soil hydraulic conductivity can and usually does change several orders of magnitude between the wet and dry states of the soil. Because the solution is not starting from a known water content or pressure state at all points in the finite element mesh, it does not have the numerical luxury of letting the solution march forward in time from a start condition to its end condition. Since there is no start condition, the solver also has no idea what the soil hydraulic conductivity value is at all points in the soil. The objective, therefore, is to be able to get the pressures and hydraulic conductivities to match throughout the mesh domain by only giving the solver a “known” condition at a

very small part of the domain when the solve process begins. The way the solver gets the final answers is by iterating – that is, trying different things and moving slowly towards the singular answer. The answer is singular because for the fixed set of boundary conditions (whether pressures or fluxes) there is only ONE unique perfectly converged solution. The objective is to get as close to the unique solution as possible – without driving yourself crazy!

Boundary condition types in steady state

In a steady state analysis there are two choices of boundary conditions: a constant pressure (or head) and a constant flux rate. There is no climate data boundary condition. For convenience the flux rate can be specified as a total nodal flux or a unit flux applied to an element edge, but the end result applied to the equations is identical. It is either a known pressure at this point, or there is a continuous inflow or outflow of water.

A few other boundary condition features have been added to the analysis to help model different real life scenarios such as seepage faces, but these are just different ways of telling the model how to come up with an H or Q boundary value to put into the equation solver. A more detailed discussion of boundary condition options is given in the dedicated chapter dedicated to Boundary Conditions.

6.2 Transient

A transient analysis by definition means one that is always changing. It is changing because it considers how long the soil takes to respond to the user boundary conditions. Examples of transient analyses include predicting the time it takes the core of a dam to “wet up” when the reservoir is filled quickly; or predicting where the seepage will exit the face of a dam if a heavy rainfall event is applied over the ground surface. When choosing a climate controlled analysis it is necessary to have a transient solution in order to capture the transient nature of climate data throughout any given day and also over changing seasons and years.

In order to move forward in time during a transient analysis, you must tell the solver what the soil pressure conditions are at the start of the time period in question. In other words, you must provide initial conditions as well as current or future boundary conditions.

Initial conditions

For a transient analysis it is essential to define the initial (or starting) total head, temperature and gas concentration at all nodes. If you do not specify a gas concentration or temperature, a value of zero is assumed for each node which is likely a very incorrect assumption. You can not leave out the hydraulic initial condition state.

VADOSE/W allows you to specify the initial hydraulic conditions by either reading the data from an initial conditions file created in a separate analysis, or by drawing the initial water table position or by specifying the value as a material property.

It is important to recognize that the initial conditions for a transient analysis can have a significant effect on the solution. Unrealistic initial conditions will lead to unrealistic solutions which may be difficult to interpret, especially in the early stage of the transient analysis.

As stated, you can specify initial conditions by instructing the solver to use data from a previously completed analysis. The initial conditions file must be identical in geometry to the current file and can be from one of the following sources:

A VADOSE/W file created by a steady-state analysis,

A VADOSE/W file created by a transient analysis at a specific time step,

A VADOSE/W file created by the current analysis at a previously saved time step to that which the current analysis is starting,

Establishing the initial hydraulic conditions are often more difficult than thermal or gas conditions as hydraulic conditions are strongly influenced by gravity and are often related to the very non-linear soil properties present in the soil. For this reason, the discussion that follows is focused towards hydraulic issues. In most cases, the initial conditions are established by running a steady-state analysis. Figure 6-1 illustrates two examples of steady-state flow problems that can be used to define the initial conditions for a transient analysis. The initial conditions for seepage from a pond (part “a” in figure) might be the steady-state regional groundwater flow defined by the water table elevation underneath the pond. The initial conditions for seepage through a dam (part “b” in figure) might be the steady-state flow condition of the dam due to the small water impoundment upstream from the dam.

In a steady-state analysis, the pore-water pressure in the unsaturated zone above the water table will vary in a linear manner when the surface flux is specified as zero, as shown in Figure 6-2 part “a”. This means that the negative pore-water pressure near the surface may become too high. A more realistic estimate of the initial negative pore-water pressure can be established by specifying a small infiltration along the ground surface. The small surface flux has the effect of changing the pore-water pressure profile as illustrated in Figure 6-2 part “b”.

The magnitude of the maximum negative pore-water pressure is dependent on the shape of the hydraulic conductivity function and, to a lesser extent, on the rate of infiltration. The infiltration rate must be less than the saturated conductivity. In general, applying a small non-zero surface flux tends to give a more realistic initial pore-water pressure estimate than a zero surface flux.

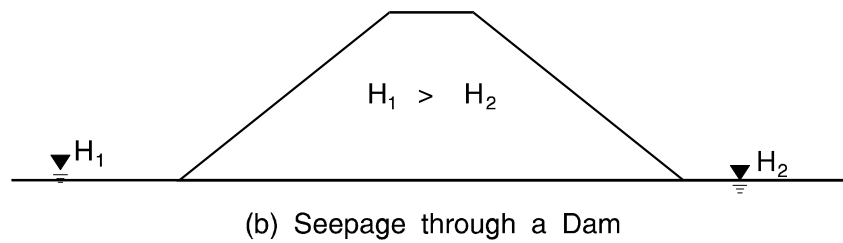
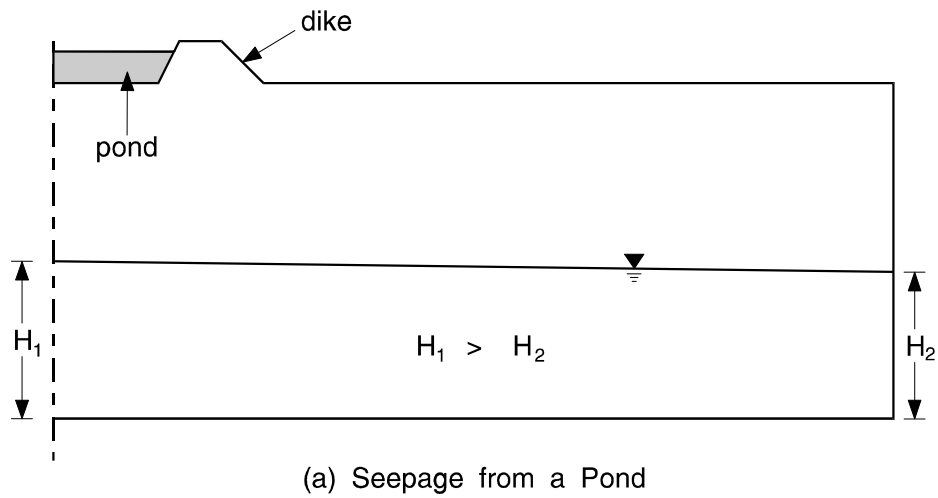
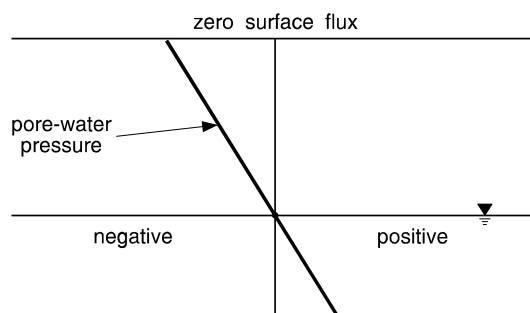
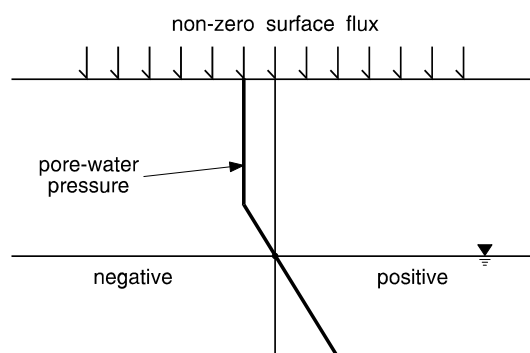


Figure 6-1 Establishing initial conditions



(a) Pore-Water Pressure with Zero Surface Flux



(a) Pore-Water Pressure with Non-Zero Surface Flux

Figure 6-2 Effect of surface flux on negative pore-water pressures under steady state conditions

Drawing the initial water table

With this option, you specify initial conditions directly by using the Draw Initial Water Table command in VADOSE/W. This is particularly useful when the location of the initial water table is known in advance. When you define an initial water table, the initial total head at each node is computed proportionally to the vertical distance between the node and the defined water table. The effect is that the pore-water pressure varies hydrostatically with distance above and below the water table. Above the water table, the negative pore-water pressure can be set to a limit to produce a pressure distribution such as shown in Figure 6-2 part “b”. Below the water table, the pressures increase hydrostatically with depth.

The definition of an initial water table gives an accurate pore-water pressure distribution when the water table is perfectly horizontal. If the water table is curved, this option gives an approximation of the actual initial conditions. Whether this approximation is or is not acceptable will depend on the nature of the problem. If this approximation is not considered adequate, then you will have to perform a VADOSE/W analysis to establish the initial conditions.

Activation values

If you have a new soil region becoming active and you know it has a certain initial pressure, temperature or concentration, you can use the material property activation value to initialize the parameter 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 value 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 values conditions will be by applying a spatial function. You can define a spatial function for pressure, temperature or concentrations and have the solver point to this function result. An example of a spatial function is shown below.

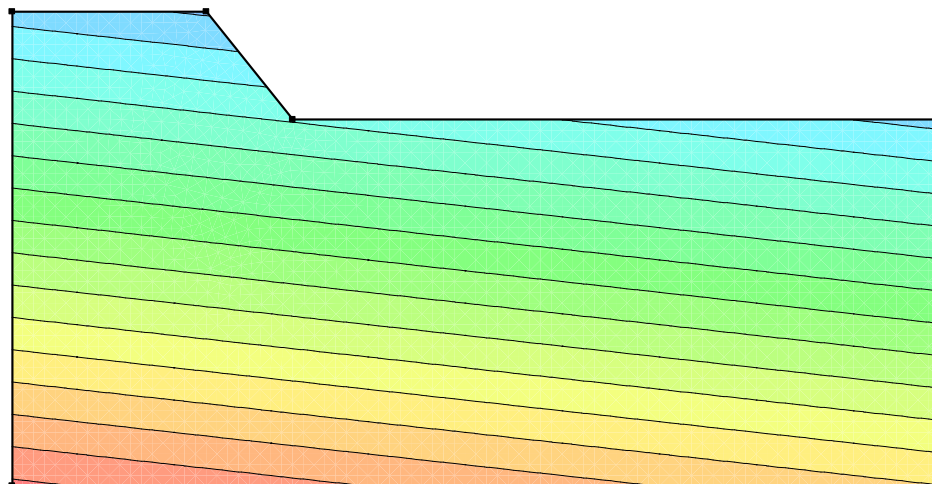


Figure 6-3 Spatial function assigned for initial pressures

No initial condition

In the event initial hydraulic conditions are not specified, VADOSE/W will not proceed with the transient analysis. The solver will bring up an error message informing you that no initial data is available and no water table has been defined.

In summary, a reasonable initial condition must be specified in a transient analysis.

6.3 Time stepping - temporal integration

An incremental time sequence is required for all transient analyses and the appropriate time sequence is problem-dependent. In most cases it will likely be necessary to try a reasonable sequence and then adjust the sequence as necessary in response to the computed results. For example, if the migration of the wetting front is too rapid, the time steps need to be decreased; if the migration is too slow, the time steps need to be increased.

The accuracy of the computed results depends to some extent on the size of the time step. Over the period of one time increment, the process is considered to be linear. Each time step analysis is equivalent to a mini steady-state analysis. The incremental stepping forward in time is, in reality, an approximation of the nonlinear process. For the same rate of change, large time steps lead to more of an approximation than small time steps. It follows that when the rate of change is high, the time steps should be small, and when the rate of change is low, the time steps should be large.

When a climate controlled analysis is done, it is important to have time steps that are one day or less in duration. This is necessary in order to capture the day to day change in thermal and moisture conditions. If you attempt to have time steps that are too large, the VADOSE/W solver will report an error. There is a more detailed discussion of climate modeling and time steps in the following chapter.

Finite element temporal integration formulation

The following discussion is presented here and again in more detail in the Theory chapter, where the full development of the equations is given. At this point, it is important now to simply show the equation to highlight a key point that will enhance your understanding of the transient finite element method.

The finite element solution for a transient analysis is a function of time as indicated by the $\{P\}_t$ term in the finite element equation. The time integration can be performed by a finite difference approximation scheme.

Writing the finite element mass transfer equation (leaving vapor flow out for the moment) in terms of finite differences leads to the following equation (Segerlind, 1984):

$$\left(\omega \Delta t \left[\frac{K}{\rho g} \right] + \left[\frac{M}{\rho g} \right] \right) \{P_1\} = \Delta t \left((1 - \omega) \{Q_0\} + \omega \{Q_1\} \right) + \left(\left[\frac{M}{\rho g} \right] - (1 - \omega) \Delta t \left[\frac{K}{\rho g} \right] \right) \{P_0\} - [K] \{Y\} \Delta t$$

where:

- Δt = time increment,
- ω = a ratio between 0 and 1,
- $\{P_1\}$ = pressure at end of time increment,
- $\{P_0\}$ = pressure at start of time increment,
- $\{Q_1\}$ = nodal flux at end of time increment,
- $\{Q_0\}$ = nodal flux at start of time increment, and
- $[K]$ = element characteristic

Look at this equation carefully for a moment. You can ignore the braces and brackets, as they just indicate a grouping of node and element information with some geometry tied in. The thing to focus on is that in order to solve for the new heads at the end of the time increment, it is necessary to know the pressure at the start of the increment, along with the average material properties calculated at the average of the new and old pressures. If you do not have reasonable values for starting pressure, then you make the equation difficult to solve because you use these starting pressure directly in the equation AND also in the calculation of the average material properties.

Problems with time step sizes

The detailed discussion of how to compute optimum time steps is very advanced and is left to those with advanced understanding of finite element mathematics (see Segerlind, 1984, pp 190-199). For our purposes, let us just point out some key issues and make some safe conclusions.

As discussed directly above, the shape and size of an element is tied into the assembly of the $[K]$ and $[M]$ matrices. It is also plain to see that changing the time step magnitude can change the solution of the computed pressures. Small time steps can cause overshoot in the calculation of the new pressures and time steps that are too large can result in poor averaging of material properties at the mid point of the time step. Elements that are too large can also result in poor material property averaging, while elements that are too small can lead to overshoot problems as well.

The mathematical formulations for time step sizes generally take into account the soil's water storage capability, its hydraulic conductivity, and the size of the element. In a homogeneous, fully-saturated soil sample, the optimum time step can be readily estimated. However, the problem in a 2D analysis with multiple soil types quickly becomes apparent. What may be an optimum time step for one region of the problem can also be a very poor choice of time step for another region; and, unfortunately, the entire problem must be solved with the same time step.

Some programs have attempted to use adaptive meshing and adaptive time stepping to deal with these issues, but the bottom line is that they cannot be applicable to all points in a mesh at all times. So, you are going to have to try some different things and use some common sense.

General rules for setting time steps

So, now that we have made the issue of time steps somewhat unclear, what do we recommend are some methods to deal with it? Some of the following points have a strong theoretical basis and some are just common sense based on years of experience.

The finite element shape is important. Triangular elements should not have any interior angles greater than 90° . Square elements can have double the time step size as triangular elements.

Since the element size is directly proportional to time step size, doubling the element size means you can double the time step. The corollary of this is that decreasing the element size and not decreasing the time steps accordingly will not improve the calculated results.

If you have a "instantaneous loading" of the system, such as instantaneous pore pressure increases due to external loading, you should set the initial time step size to be approximately equal in order of magnitude to the Mv value divided by the saturated conductivity value of the soil that is instantaneously loaded.

If you are modeling a rapid filling of a reservoir, you can "instantaneous load" the model by having it be filled instantaneously, or you can use a Head versus Time boundary function to more accurately simulate the filling of the reservoir over a short, finite time period.

If you are using a detailed surface boundary flux versus time function with many different values (such as simulating the on / off nature of rainfall) make sure your time steps are small enough to allow the solver to follow the shape of the function. For example, 2 week long time steps don't work if rain falls on day 3, 8 and 17. The program would make its first flux value be that at day 14 (2 weeks), but you have no value on day 14 in your function. Also, note that if the rainfall on day 8 is 5 mm/day, and if you have solver time steps of 4 days, your function will get a value from the function on day 8, but the actual applied flux in the model would be 5 mm/day applied over 4 days for a total of 20mm of rainfall. Make sure you use 1 day time steps in this case.

If you are solving a climate boundary condition, you should use one day time steps with adaptive time stepping activated.

Adaptive time stepping

VADOSE/W will permit you to activate an adaptive time stepping routine that will insert extra time steps between your specified time steps in the event the solution is not meeting your specified time stepping or convergence criteria. Full details of the adaptive time stepping options are discussed in the Numerical Issues chapter.

6.4 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 6-4 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.

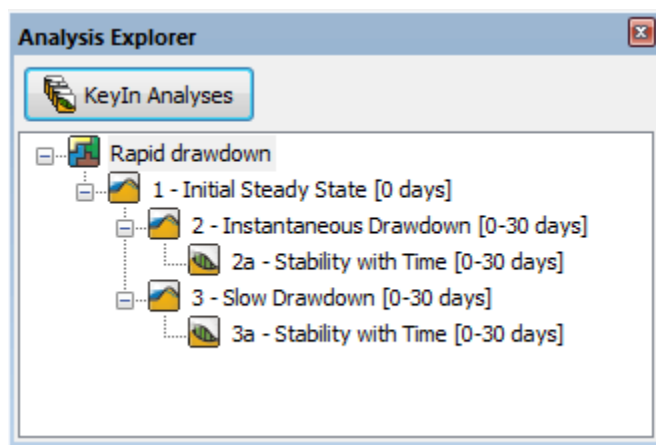


Figure 6-4 Example of an Analysis Tree in GeoStudio

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.

6.5 Axisymmetric

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. A typical example of an axisymmetric analysis is the flow into a single pumping well or flow out of a single recharge well into a uniform aquifer.

In VADOSE/W the vertical symmetric axis of rotation is always at x-coordinate equal to zero. The x-coordinates in an axisymmetric finite element mesh must, therefore, all be greater or equal to zero. A typical case for an axisymmetric analysis is the drawdown cone formed by a single pumping well, as illustrated in Figure 6-5. In this figure, the pressure head contours are plotted for a steady state condition of continual pumping from the well at a rate of 0.22 cubic meters per day per radian about the x-axis.

For an axisymmetric analysis, the computed 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., 2π radians) before you do the analysis, or simply multiply the above value by 2π after the solution is finished. You can change the element thickness for the entire mesh with the Draw Element Properties command.

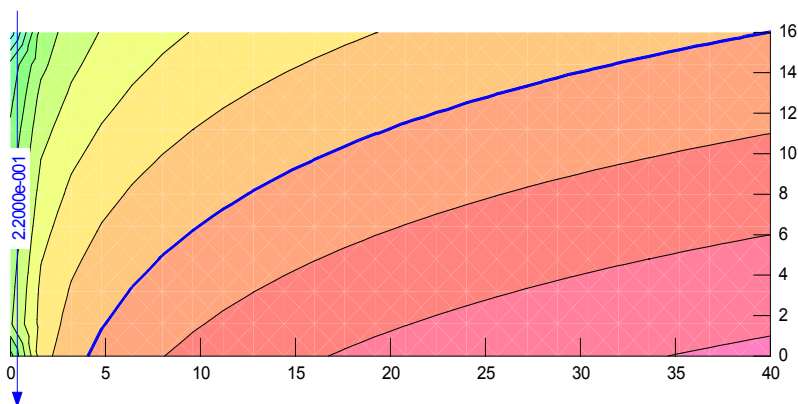


Figure 6-5 Well drawdown for an axisymmetric case (note zero x- coordinate axis)

Infinite elements may be used for the outside far field edge of the axisymmetric mesh (right side away from the axis of symmetry). However, the application of non-zero q (unit flux) boundary conditions along the infinite element edges is not allowed. This is because the nodal contributing area is dependent on the distance of the node from the rotation axis, and since the far nodes of the infinite elements are at infinity, the nodal contributing area becomes undefined. Even though VADOSE/W may still compute a solution to the problem in some simple cases, the solution becomes suspect and the use of q -type boundary conditions in this case is therefore not recommended.

It is also not relevant to apply a small “ q ” unit flux boundary to the left edge of the mesh if it is at an “ x ” coordinate of zero because then there is no area (no radius) to compute an area over which the flux should be applied. You can, however, apply a big “ Q ” flux, because when you do this you are including the area of flow inside the Q value you specify.

6.6 Plan view

VADOSE/W does not support a plan view analysis as it is not applicable to modeling climate – ground interaction.

6.7 Vegetation, ground freezing, runoff and gas transfer

In the VADOSE/W model there are options to enable vegetation, ground freezing, runoff ponding, gas transfer or any combination of the above. A brief description of how these analysis types are used is provided in the section below.

Vegetation can be turned on / off so that the effects of its inclusion versus exclusion can be established. If the vegetation routine is enabled, then the appropriate vegetation boundary condition functions must be applied when specifying climate boundary conditions. If no vegetation data is applied, but the check box for vegetation is enabled, then the program will inform the user of an error. The vegetation check box can be set to disable vegetation even if vegetation data is applied as a boundary condition. This makes it possible to test the results with and without vegetation, while not forcing the user to change the overall defined boundary conditions of the problem.

The ground freezing option should be enabled if you want to include the effects of latent heat in the solution of the thermal partial differential equation. If the check box is disabled, the solver will still solve for temperatures below the phase change point, it will still accumulate and melt snow etc. The solver will simply omit the latent heat component of the solution. This may or may not be a significant issue. Enabling the latent heat option can sometimes increase the time required to solve the simulation, as it is necessary to iterate on a converged solution in order to find the correct position of the freeze front at each time step.

There is an optional check box to turn off the ability to pond seepage face and runoff water at low points you defined geometry. If the box is disabled, then water that leaves the ground surface (or that does not infiltrate) is assumed lost from the solution for the remainder of the analysis. This may be a desired feature such as the case when ponded water is pumped away from the site for treatment. In this case, it does not sit idle and remain available for infiltration and evaporation. Ponding water automatically is not valid for an axisymmetric analysis.

The gas transfer check box simply tells the solver to solve the gas transfer differential equation or not. If the equation is not solved, then there will be no output data of relevance for gas concentrations or fluxes. If it is solved, the process will take a little longer due to the necessity to set up and solve another equation after the primary coupled heat and mass equations are solved at each time step. If gas transfer is applied, then the surface gas concentration boundary condition is assumed to be that of oxygen in air (280 g/m³) or zero grams of radon; depending on whether the analysis is for oxygen or radon transfer.

6.8 Using VADOSE/W Basic edition for 1D modeling

This section is about how to use VADOSE/W for one dimensional analysis. There are features and settings in the full feature software that should not be applied in a 1D case. There are also some settings that work better in a 1D case that will hinder the efficiency of a two dimensional model. The VADOSE Basic edition license will limit the extents of the geometry modeled such that the x-coordinates of all nodes are either zero, or 1.0. It is up to the user to ensure all other solution parameters are appropriately defined.

1D versus 2D Models

In reality it is not that common for a field site to display true one dimensionality. Aside from laboratory studies using physical columns, the only “field” case where one dimensionality is valid is a centrally located position on a large, flat plateau. However, with some careful thought about the objectives of the modeling and the various site factors that may control these predicted results, it is possible to use 1D modeling to better understand the physical process in effect.

Consider the two dimensional cross section of a pinch out soil cover placed over a mine waste rock dump shown in Figure 6-6. The superimposed data on the section is the computed actual evaporation from the ground surface along the slope and crest of the cover system. The water table is shown as a dashed, blue line and the red dots at the base of the soil indicate an estimated total head boundary condition that may

exist at that point in the profile. The numbers on the left axis are cumulative mm/m² of actual evaporation over a five year period.

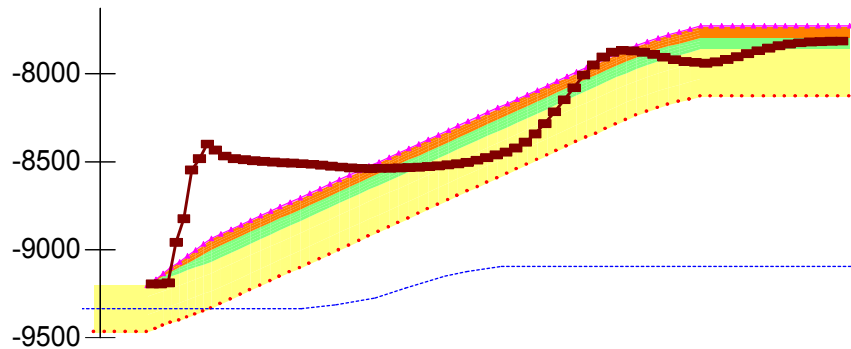


Figure 6-6 Actual evaporation (mm) superimposed on mine waste cover cross section

While there is an obvious two-dimensionality to the problem, careful observation suggests that there are three distinct evaporation trends: at the toe of the cover, along the lower slope section, and along the upper slope and crest. Is it possible to capture the key mechanisms controlling the overall performance of this system in a series of 1D models?

Consider the three 1D sections superimposed on the mine waste cross section in Figure 6-7. Is it possible that data from these three 1D models will provide a sufficient understanding of actual evaporation conditions along the 2D slope? In asking this question, we must understand what the differences between the three 1D sections are. There is a difference in cover layer thickness for the section at the toe of the slope. There is a difference in the depth to the water table at all three locations. The 1D sections are flat at the top and base (there is no advantage in a 1D model to slope the ground surface). And, most importantly, there is no lateral flow from one section to the other.

One of the objectives of the series of 1D models should be to determine the sensitivity of surface conditions to the possibility of lateral flow at the interface between cover layers. This lateral flow may either introduce or remove water from the system. While it will not be possible to know how much water this may be unless you carry out a 2D analysis, it should be possible to use a trial and error approach to see how much water it would take to change the performance of the system.

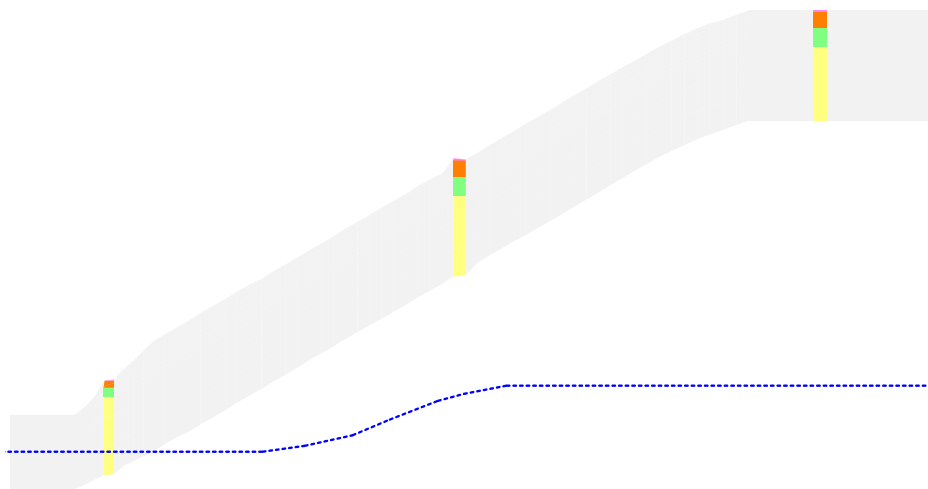


Figure 6-7 Conceptual series of 1D models to represent a 2D domain

The main boundary condition locations that could be applied in a one dimensional model are identified In Figure 6-8. In this case, the one unknown that can not be determined by the 1D model is the interflow. The climate and vegetation parameters will control the surface and near surface boundary conditions and the net percolation at the base will be determined by the type of hydraulic boundary condition applied there (e.g., pressure, unit gradient, flux rate). At first it would not be a good idea to include any interflow values but after several results are generated for the cases where it is excluded, the user may observe some wetting trends at the interface between the green and yellow soils that may not actually exist there if the profile was located on a slope. Once this is observed, it may be possible to try to add some interflow or at least prevent any positive head build up by specifying a seepage face boundary condition at that location.

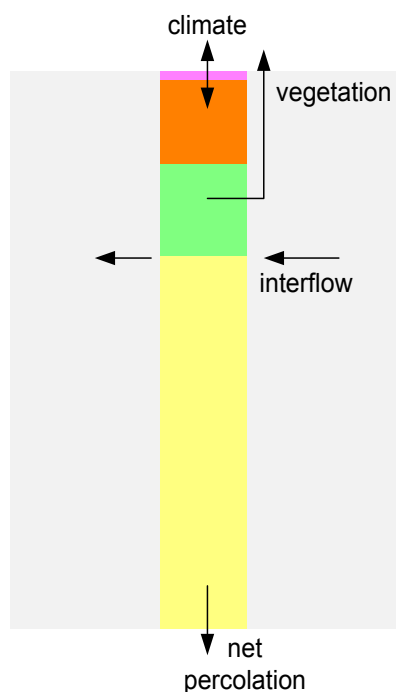


Figure 6-8 One dimensional representation of main boundary condition locations

Boundary conditions

While initial conditions are a snap shot of what the soil profile looks like just prior to the start of the main, transient analysis, it is boundary conditions that control how any analysis proceeds. Boundary conditions are pressures, temperatures or flow rates that are applied to the soil model to control how the model changes with time during the analysis. In VADOSE/W Basic edition the main objective is to determine the soil's response to climatic conditions. If appropriate climate data sets are defined in the model, they can be applied to the ground surface nodes and used by the model to predict ground surface temperatures and water flux rates across the soil-atmosphere boundary. Water flux rates may be evaporation, rainfall, pond infiltration, snow melt, or plant transpiration. The model will determine the portioning of these parameters based on the current climate conditions and soil state.

The bottom boundary condition in a 1D model is a little harder to determine. Some options for the bottom boundary are illustrated in Figure 6-9. The left of the image shows a pressure head BC of 3m. This corresponds with the initial condition pressure of 3m at that location. The middle image shows a pressure head of zero at the location of the water table. The right side of the image shows a unit gradient

condition located at an elevation of 8m where we know the pressure profile is vertical with elevation above that point. Be careful with the unit gradient condition... if it is used at this location, the water table must still be drawn as shown in the figure such that the starting pressure in the main analysis is an actual unit gradient condition at this location. If a water table is not used, then you should make sure the initial condition file has solved to a unit gradient condition prior to using it as the starting condition in a transient model.

Other types of boundary conditions that may need to be specified include: water flux rates, temperatures, heat flux rates, gas concentrations or gas flux rates.

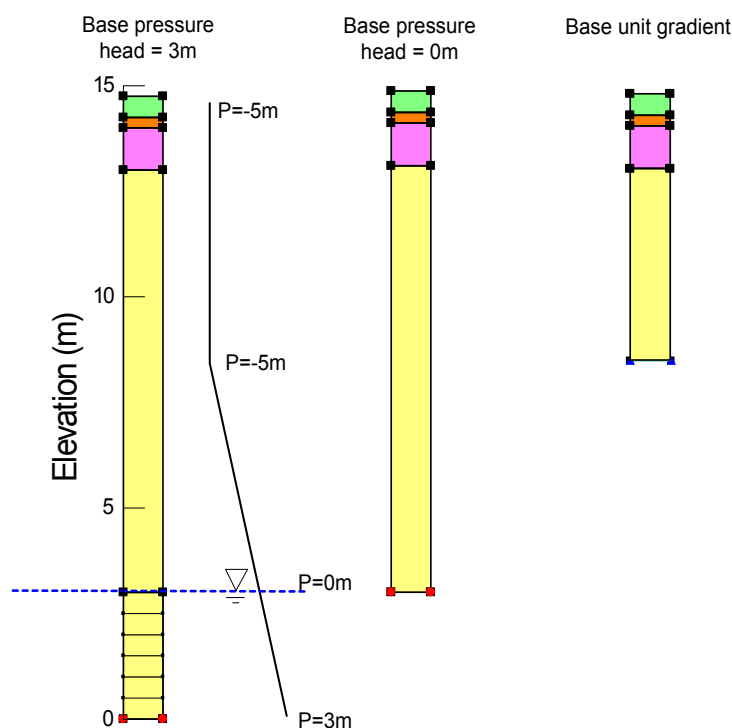


Figure 6-9 Base boundary condition options

Analysis settings

There are some analysis settings that should be specified within VADOSE/W Basic edition to optimize the solution speed and numerical stability. In particular, it is necessary to think about convergence and time stepping.

In general, the default convergence parameters will work for a 2D or 1D model. However, due to the faster solution speed of a 1D model, it is sometimes useful to reduce the maximum number of iterations the solver will attempt before moving on or reducing the adaptive time steps. While the default number of iterations is set to 50, you may want to try 20 along with smaller minimum adaptive time steps as discussed next.

The choice of parameters for the main time step control sequence depends on the units of time you specified in the Set Scale command. In this example, there are 365, one day time steps. The advantage to using “day” time steps is that the step number corresponds with the actual time value, unlike the case if you use seconds such that at the end of step 1, or one day, there is an elapsed time of 86400 seconds. If climate data is used in the analysis, the time steps must be less than or equal to 1 day. If they are set at 1

day, the adaptive time stepping scheme can be used to subdivide them into even smaller units for better convergence and accuracy.

When saving computed data to file, it is a good idea to save it every 10th or 30th day in order to keep the output file size manageable. If necessary, it is possible to manually set any other day as a save step.

The important settings for a 1D model in this case are the adaptive time step control parameters. In a 1D model it is very important to let the adaptive time stepping scheme base its time step size adjustment on the individual nodal head values and not the vector norm of the nodal heads. In a 1D model, sharp wetting or drying fronts within the soil are always moving past a pair of nodes so it is the pair of nodes that is undergoing the greatest change in hydraulic head at any one time. Therefore, if the time steps need to be reduced to accommodate an accurate solution of the flow equations at these nodes, then these nodes should control the time step adjustment. In a VADOSE/W two dimensional model, there are likely many pairs of nodes at a wetting or drying front so it is possible for the vector norm value to capture extreme changes in pressures at these locations and so it is not always necessary to base the time step control on individual nodes.

Other settings

In general, a VADOSE/W Basic edition model is intended to represent a 2-dimensional cross section of a soil profile where the section is 1 distance unit across and 1 distance unit depth into the page. Therefore, the top surface area that the climate is applied to is 1 square meter or 1 square foot. If an axisymmetric analysis view is chosen and the x-coordinates of the model are at zero and 1.0, then the top surface area of the model is equal to the area of a circle with radii of 1, or 1.57 m² or ft². There is no real advantage in VADOSE/W Basic to choose an axisymmetric view and it should not be used in this case.

Optional solution parameters include ground freezing, vegetation, gas diffusion or surface water runoff. If the ground freezing option is selected, then the latent heat of freezing will be included in the heat transfer solution when ground temperatures fall below the phase change temperature. In addition, ice will build up in the pores and will reduce the ability of water to infiltrate through frozen soil. If this option is left off, the ground temperatures will still solve to below freezing but no latent heat will be included and no ice will block pores. When ground freezing is enabled, the Gauss regions / iteration value should be set to 2 in a 1D model. In both cases, snow pack will develop and melt on the ground surface if the climate data includes sub-zero air temperatures and precipitation.

Vegetation is an option that can be applied to the model if the appropriate related functions have been defined (e.g. Leaf area index, root depth, moisture limiting function) and a vegetation boundary condition has been applied to the climate data when it was set at the top nodes.

Gas diffusion is optional. If appropriate gas diffusion initial and boundary conditions are specified, the finite element diffusion equation will be solved in addition to the heat / mass transfer equations.

The final “allow ponding...” option is important to understand. Even though the model is a 1D column, if this check box is selected, the model will accumulate on the surface, any water that is applied as precipitation that can not infiltrate. As the water accumulates, it builds up a pressure head. Water that sits on the surface is available to evaporate or infiltrate at later time steps. If this option is disabled, then water that can not infiltrate will be assumed to flow down slope and will not be available for evaporation or subsequent infiltration.

7 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 compiled 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.

7.1 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.

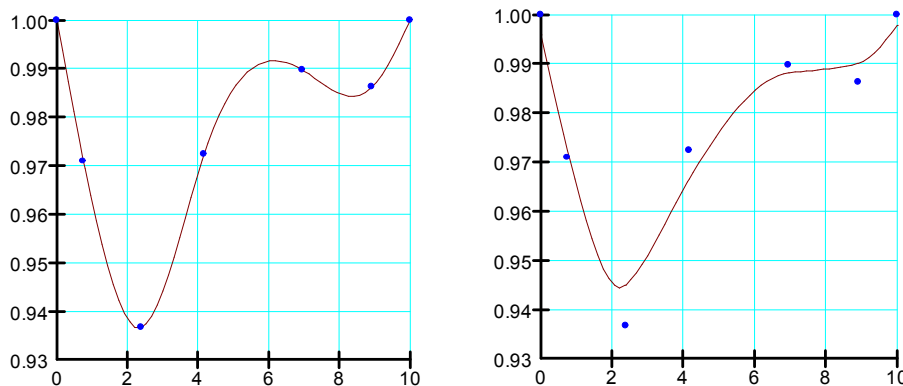


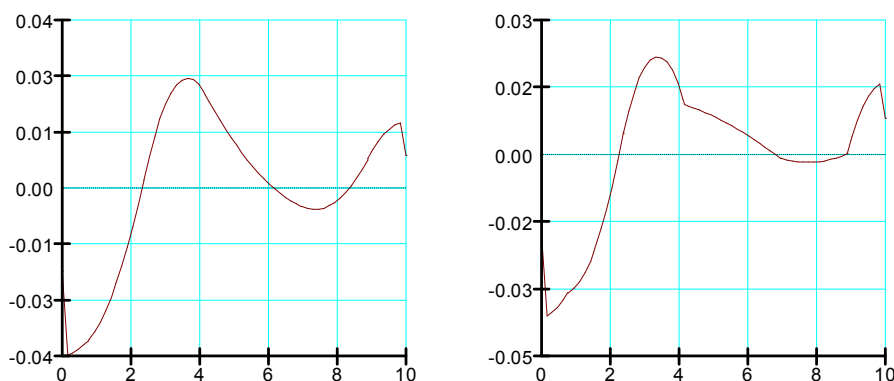
Figure 7-1 Spline functions with different settings

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 7-2 Slope of spline functions**

7.2 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.

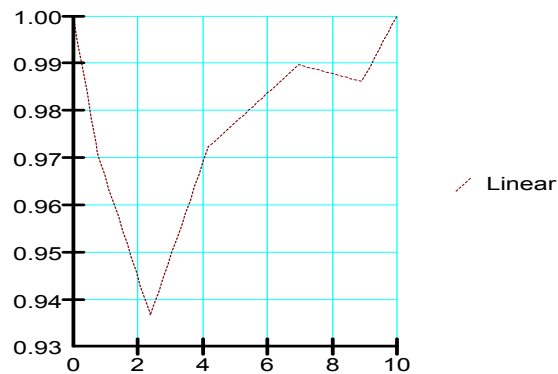


Figure 7-3 Linear fit spline

7.3 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.

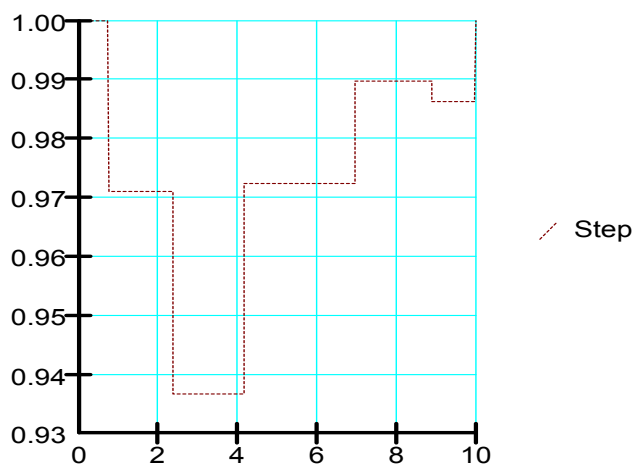


Figure 7-4 Step function

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.

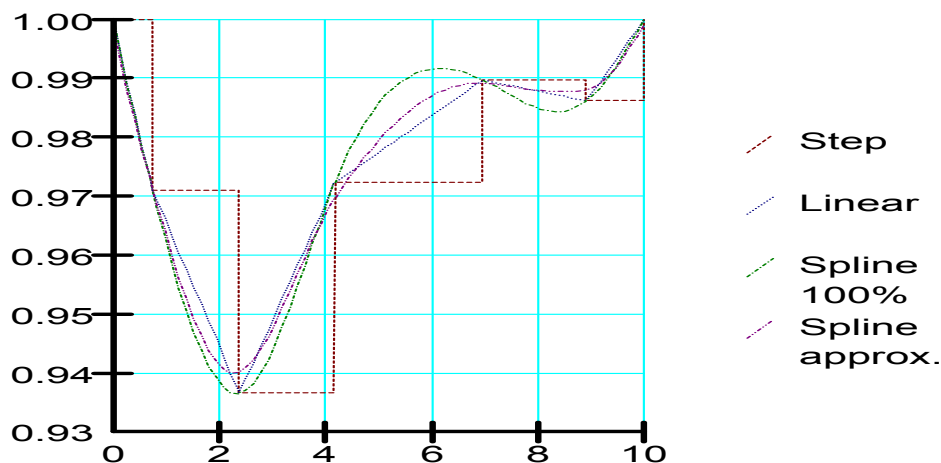


Figure 7-5 Comparison of all data point functions

7.4 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.

7.5 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.

7.6 Spatial functions

A spatial function in VADOSE/W can be used to establish starting pressure, temperature or gas 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.

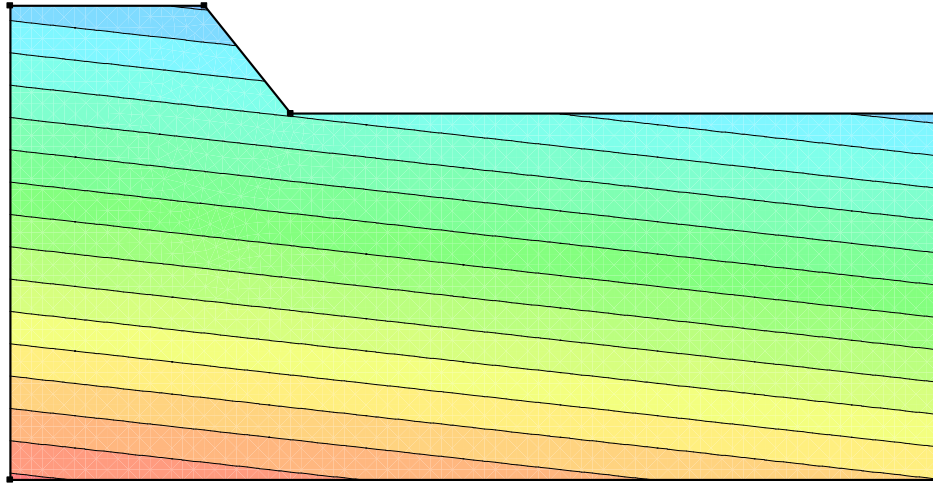


Figure 7-6 Example of spatial function assigned to model

8 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 cannot 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 extreme non-linearity of soil properties; some issues relate to the fact the physical equations being solved do not apply to all cases (for example, flow through unsaturated coarse gravel is not likely Darcian flow); 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 do not 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. 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.

Fortunately, 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 VADOSE/W.

8.1 Convergence

The finite element equation generally takes the form:

$$[K]\{h\} = \{Q\}$$

where $[K]$ is the global property matrix, $\{h\}$ is the vector of nodal primary values, and $\{Q\}$ the right side forcing vector. The global assemblage of finite element matrices contains material properties that could be a function of the solution. A commonly used numerical procedure for coping with material non-linearity involves repeatedly solving the finite element equations and updating the material properties based the solution at the previous iteration. Convergence is obtained if successive solutions are equal within a specified tolerance or the maximum number of iterations is reached. The GeoStudio products determined convergence based on two parameters:

- Significant figures
- Minimum difference

Significant figures

Significant figures of a number are those digits that carry meaning as to the precision of the number. Leading and trailing zeros simply provide a reference as to the scale of the number. Consider a number like 5123.789. If we say that the number is precise to two significant figures its precision is 5.1×10^3 ; if it is three significant figures then its precision is 5.12×10^3 , and if it is four significant figures then its precision is 5.124×10^3 .

In GeoStudio, the user is allowed to specify the desired significant figures or digits for comparison of the primary variable(s) from the finite element solution. Specifying two significant digits means that when the primary variable(s) from two successive iterations are the same to a precision of two significant figures, they are deemed to be the same or they are said to have converged.

Minimum difference

Computer computations inherently produce numerical noise; that is, digits that have no significance. So when comparing floating point numbers it is necessary to filter out the insignificant digits.

GeoStudio does this with a user specified minimum-difference value. If the difference between two successive primary variables at a node is less than this minimum specified value, the two values are deemed to be the numerically equivalent and the solution is converged without giving consideration to the significant figure criteria. For example, convergence at a node would be designated if the minimum difference was specified as 0.001 and the difference in the primary variable(s) between successive iterations was less than this value.

Consider two numbers such as 1.23×10^{-6} and 1.23×10^{-7} . These two numbers have the same number of significant digits but the difference (1.11×10^{-6}) is small and may have no physical meaning in the context of the analysis. The two numbers are consequently deemed to be equivalent within the tolerance.

8.2 Evaluating Convergence

GeoStudio provides several tools for judging or evaluating whether the computed results have converged to an acceptable solution.

Mesh view

View Preferences | Node Convergence paints the convergence state of the nodes when in Results. Figure 8-1 illustrates that an (X) is painted if the solution does not meet the significant figure requirement and a circle is painted on nodes that have a differences in the primary variable with iteration that is less than the minimum. The nodal convergence painting assists with identifying areas of the domain that are not meeting the convergence criteria. The solution in these regions can then be further inspected other features.

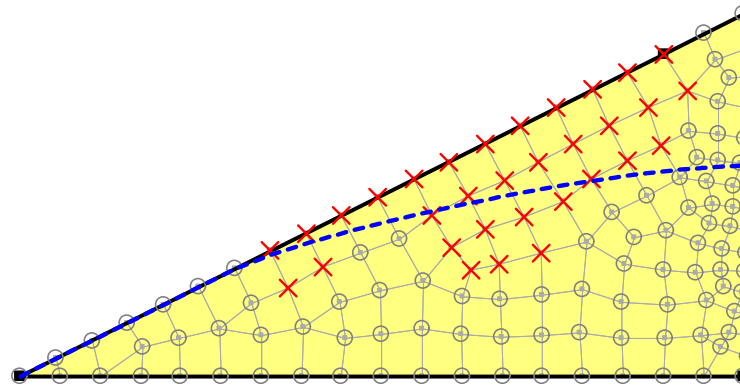


Figure 8-1 Nodes that have not achieved the convergence criteria

Graphs

A number of graphs can be generated to judge convergence based on Data from Nodes (Selected by the User) or from all nodes or Gauss regions within the entire domain. Figure 8-2, for example, shows the number of unconverged nodes versus iteration. The number of unconverged nodes steadily decreases towards 0 after 223 iterations. Graphs of this type are useful for examining the number of iterations required to achieve convergence, to detect whether the iterative process stopped at the specified maximum number of iterations and to detect whether there were oscillations during iteration.

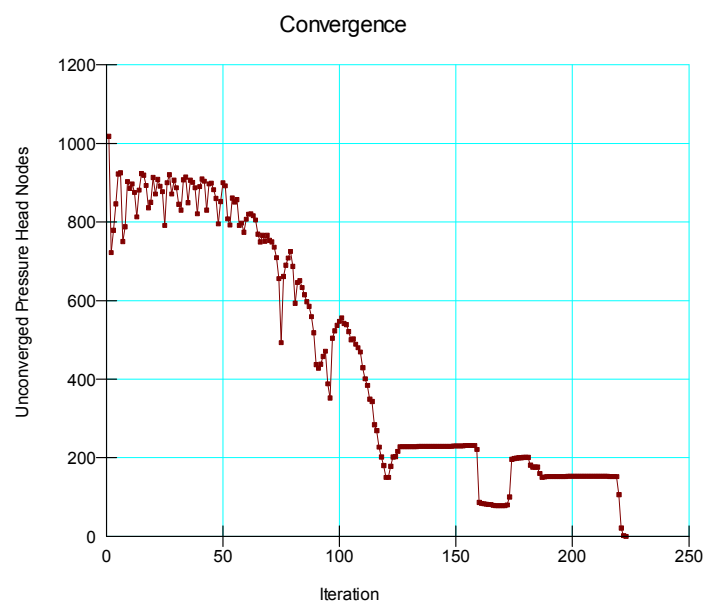


Figure 8-2 Unconverged nodes versus number of iterations

Figure 8-3 shows a graph of the hydraulic conductivity at every Gauss integration point with the entire domain that was used to obtain the solution versus the input function. The solution has not converged;

consequently the ‘Actual’ and input functions do not match. In contrast, Figure 8-4 shows a near match between the ‘Actual’ and input functions when convergence is obtained.

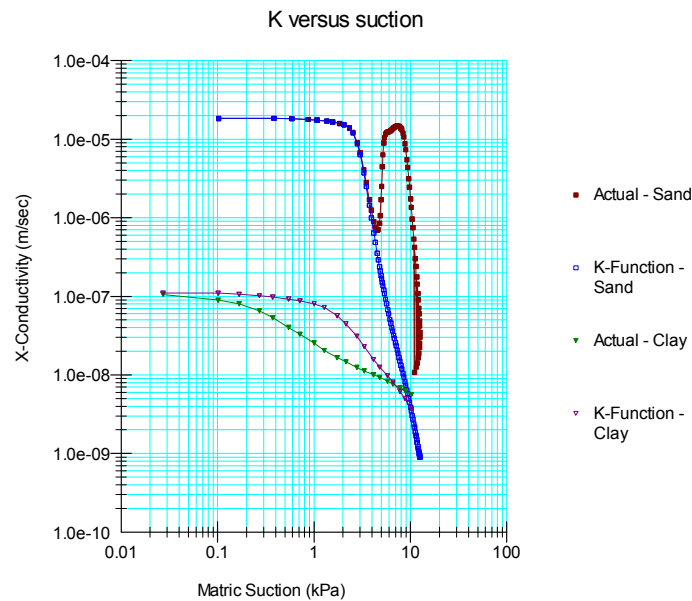


Figure 8-3 Conductivity versus suction illustrating non-convergence

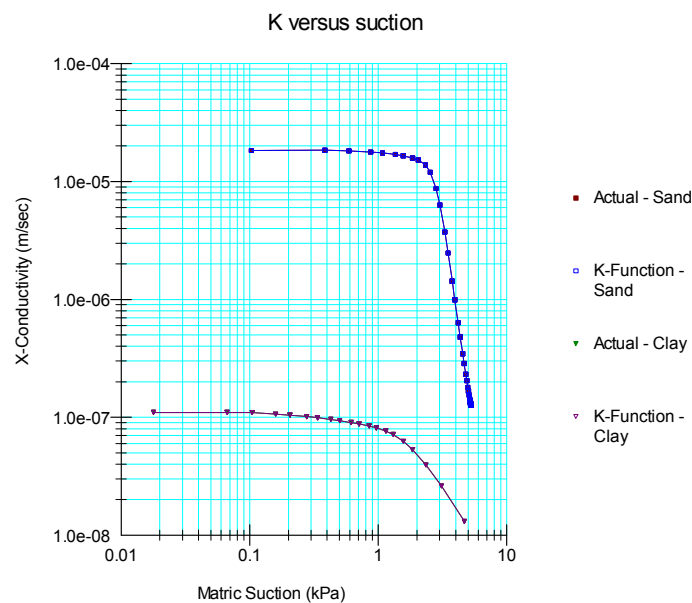


Figure 8-4 Conductivity versus suction graph illustrating a converged solution

Water balance error in a transient analysis

A useful tool for helping understand the reasonableness of a transient solution is to monitor the overall cumulative water balance error for the entire mesh. VADOSE/W reports and continually updates this value in the solver window at the end of each time step regardless of whether or not convergence is reached. The cumulative water balance error is simply the sum of all external boundary fluxes, minus the sum of the computed change in storage within all elements. Ideally, this value should equal zero – which would mean all water entering or leaving the problem domain is accounted for as a gain or loss within the domain.

Figure 8-5 is an example of a cumulative water balance error data generated by the VADOSE/W solver and saved to data file for subsequent graphing in the Results View. In this plot, the units of error are volume (e.g. m^3 or ft^3 depending on user set of units). It is clear there is an increase in error during the initial time steps, but it tapers out towards the end of the analysis. This type of chart can give some clue as to appropriate time step selection in early stages of an analysis, or at any point where there is a sudden change in cumulative water balance error.

As a rule, water balance errors are more likely to accumulate at the elements where there are boundary fluxes, as opposed to elements well within the domain and away from any edges. This is because it is quite easy to apply a boundary condition that is unrealistic (such as instant draw down of a reservoir) or that is too extreme, given the time step applied or the element size.

In VADOSE/W, the water balance error is reported as a cumulative volume of water, which means its magnitude must be considered relative to the size of the domain being modeled. For example, if you have a nearly saturated soil in a mesh that represents 100 meters across and 30 meters depth, it could have stored water equal to 1500 cubic meters (assuming a soil porosity of 50%: $100\text{m} * 30\text{m} * 1\text{m unit depth} * 0.5 = 1500 \text{ m}^3$). If the water balance error is reported as 2 cubic meters, this is a very small amount relative to the 1500 cubic meters in the system. On the other hand, for the same example if the error is two cubic meters and you only applied two cubic meters of water as a boundary flux, then the error is very significant.

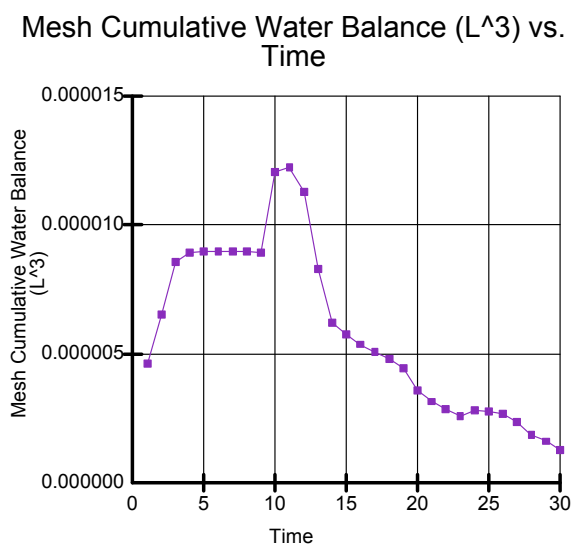


Figure 8-5 Water balance versus time results from VADOSE/W contour

VADOSE/W does not convert the water balance error to a percent error because the magnitude of the error depends on what you compare it to. In the previous example, the error would either be negligible or

extreme. It is up to you to determine if the error is significant given what you know about your problem and the boundary conditions you have applied.

In general, if the cumulative water balance error is low, the solution has proceeded quite well. It is useful, as a check, to see how the water balance error changes with time. There are cases where a large negative error on one time step can be reversed by a large positive error on another time step. If you do not see this pattern when you plot the error for all time steps, then you can increase your confidence in the overall solution.

Commentary

An unsaturated seepage analysis is a highly nonlinear process and consequently it can sometimes be difficult to obtain a converged solution. Evaluating the convergence in detail using the aforementioned techniques is highly advisable.

These tools are available at the end of a steady-state analysis or at the end of every *saved* time step in a transient analysis.

The degree of nonlinearity is dependent on the steepness of the conductivity function and volumetric water content function. Difficulties with convergence can be encountered when either of these material property functions becomes relatively steep.

How steep is steep? There is no single answer. In general, you can think of steepness in terms of two factors: how much the water content or conductivity will change for a small change in pressure; and, how fast will that pressure be changing? A steep soil property function can be used quite readily, but generally this requires smaller time steps in a transient analysis and smaller mesh element sizes. In an extreme case of non-convergence in a steady state analysis, you can try to use a long-term transient analysis to simulate the steady state. The transient analysis has the advantage in that you have to specify initial conditions and the solution can then march forward in time towards the steady state solution.

Coarse-grained materials can sustain a relatively small capillary zone and tend to de-saturate almost completely at small negative pore-water pressures. This behavior manifests itself in a very steep hydraulic conductivity function; that is, a function where the hydraulic conductivity varies greatly with small changes in negative pore-water pressure. A typical steep hydraulic conductivity function is shown in Figure 8-6.

Theoretically, the hydraulic conductivity function approaches a vertical line (infinitely steep) near the zero pressure axis when the material is very coarse. This is the case for sands and gravels that have virtually no capillary zone and are essentially dry above the water table.

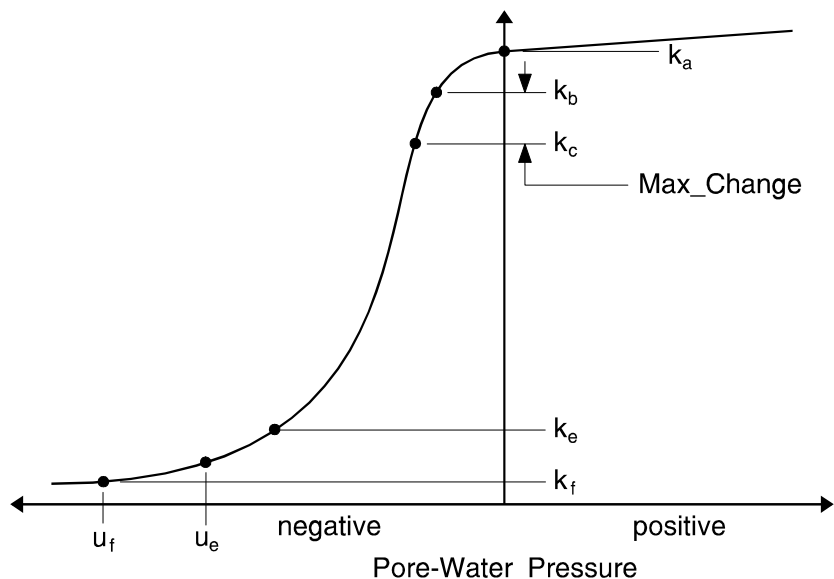


Figure 8-6 A typical steep hydraulic conductivity function

The first thing to do when you experience convergence problems is to re-evaluate the relevance of coarse materials. If a coarse material does not contribute to dissipation of the head, then you should try excluding the coarse material from the analysis. You can specify it to be a NULL element. In VADOSE/W this is done by setting the region material to None. The element will remain in the mesh, but will not be used in the solution. Not removing the element from the domain means you can try different things with the properties without having to use a unique mesh in each case. Removing coarse materials that do not contribute to head losses may simplify the problem and assist you in overcoming the convergence difficulties.

Very steep hydraulic conductivity functions can create difficulties with convergence. In fact, it may not be possible to obtain convergence when the hydraulic conductivity function approaches a vertical line. The solution will tend to diverge instead of converge and oscillate between two extreme solutions represented by the extremities of the hydraulic conductivity function.

Consider the function illustrated in Figure 8-6. Assume that for the first iteration all elements are assigned a saturated hydraulic conductivity corresponding to zero pressure. This hydraulic conductivity will allow for more flow than is required and will result in a highly negative pore-water pressure (Point k_f). For the next iteration, the hydraulic conductivity will be k_e . This value does not allow for enough flow, and the computed pressure will be positive. Once again, the hydraulic conductivity will be set to a value that is too high, resulting in a solution which oscillates between the extremities permitted by the function. Convergence could, in this case, be promoted by truncating the function or changing the steepness of the function. The results must be interpreted in light of the alterations of the functions.

Unnatural boundary conditions can also lead to convergence problems. For example, consider the case of filling a reservoir. Often, the reservoir is assumed to have been filled instantaneously. By modeling it this way, the initial flow gradients are so high that it can be difficult to get a solution. Applying a more realistic boundary condition that fills the reservoir over time can reduce convergence problems. Having unrealistic initial conditions in a transient analysis may also lead to convergence problems. In general, you should not try to model situations that cannot occur in reality.

8.3 Under-relaxation

The global assemblage of finite element matrices contains material properties that could be a function of the solution. A commonly used numerical procedure for coping with material non-linearity involves repeatedly solving the finite element equations and updating the material properties based on the solution at the end of an iteration. Convergence is obtained if successive solutions are equal within a specified tolerance. Unfortunately successive solutions can diverge and/or oscillate if the material properties are highly non-linear. In this case, some form of under-relaxation is required.

Under-relaxation procedures attempt to mitigate large variations in the material properties that are the source of the non-linearity. For instance, the conductivity parameter characterizing water transfer can vary by many orders of magnitude over a small pressure range. The inclusion of latent heat effects in an energy transfer analysis is another example of extreme material non-linearity. Divergence of the solution after two successive iterations can therefore be mitigated by limiting – under-relaxing – the variation of the material properties used to calculate the finite element matrices. This in turn exerts a control on the difference between successive solutions and produces a less chaotic progression towards a converged solution. The under-relaxation parameters are specified in the Convergence settings of the analysis definition and include:

1. Initial Rate (e.g. 1);
2. Minimum Rate (e.g. 0.1);
3. Rate Reduction Factor (e.g. 0.65);
4. Reduction Frequency (e.g. 10 iterations).

The Initial Rate essentially controls the allowable variation in the solution between successive iterations. A value of 1 corresponds to repeated substitution with no under-relaxation. The under-relaxation rate is reduced by multiplication of the Rate Reduction Factor once the Reduction Frequency is exceeded. For example, the under-relaxation rate would be 0.65 after the 10th iteration, 0.65² after the 20th iteration and so on until the under-relaxation rate is less than or equal to the minimum rate.

The default parameters may not be ideal for some numerically challenging problems. For example, it may be advantageous to immediately commence under-relaxation if the material properties are highly non-linear by specifying an Initial Rate that is less than 1 (e.g. 0.65). The Minimum Rate might also have to be reduced if the solution oscillates slightly around the solution (e.g. 0.01). Other variations on this strategy are possible, such as retaining the Initial Rate of 1 but reducing the Reduction Frequency (e.g. 5 iterations) and Minimum Rate (e.g. 0.01). Ultimately some form of numerical experimentation is required and convergence must be judged by using the previously mentioned techniques.

An under-relaxation rate is also specified for the thermal component of a VADOSE analysis. There are no other inputs except the under-relaxation rate.

8.4 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 8-1 gives the acceptable integration orders.

Table 8-1 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 that have secondary nodes. This is called a reduced integration order (see Bathe, 1982). Acceptable results can be obtained with reduced integration. For example, reduced integration is useful in saturated zones where the hydraulic gradient is low and the hydraulic conductivity is constant. Selective use of reduced integration can greatly reduce the required number of computations.

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 in an unsaturated zone where the hydraulic conductivity varies sharply with changes in pore-water pressure. 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 an unsaturated zone with hydraulic conductivity that varies sharply within an element, it is best to use quadrilateral elements with secondary nodes together with nine-point integration.

8.5 Equation solvers (direct or parallel direct)

VADOSE/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. VADOSE/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.

8.6 Time stepping

An incremental time sequence is required for all transient analyses and the appropriate time sequence is problem-dependent. In most cases, it will likely be necessary to try a reasonable sequence and then adjust the sequence as necessary in response to the computed results. For example, if the migration of the wetting front is too rapid, the time steps need to be decreased; if the migration is too slow, the time steps need to be increased.

The accuracy of the computed results is dependent to some extent on the size of the time step. Over the period of one time increment, the process is considered to be linear. Each time step analysis is equivalent to a mini steady-state analysis. The incremental stepping forward in time is, in reality, an approximation of the nonlinear process. For the same rate of change, large time steps lead to more of an approximation than small time steps. It follows that when the rate of change is high, the time steps should be small, and when the rate of change is low, the time steps should be large.

Many seepage processes related to the dissipation of excess pore-water pressures and infiltration follow an exponential form. The dissipation or infiltration is rapid at first and then decreases with time. A typical example is the consolidation of a soil. To model this situation, the time step sequence should approximately follow an exponential form. The time steps should be small at first and then progressively increase.

Automatic adaptive time stepping

VADOSE/W will permit you to activate an adaptive time stepping routine that will insert extra time steps between the users specified time steps. There are three methods of calculating adaptive time steps, plus a fourth scenario should the solution reach its maximum allowable iteration count without reaching convergence.

In the first two methods, the change in total nodal heads is used to determine an increase or decrease in time step between the allowable ranges specified. The first method checks each node to see if the heads between successive time steps are changing by more than the user-specified percentage. If the allowable percentage head change at any given node is too high, then the time steps will be reduced such that the percent change is upheld. In the second option, the vector norm of nodal heads is used as the criteria. The vector norm considers all heads simultaneously. Experience should show that the vector norm approach is faster for a large mesh with two-dimensional water flows. Analysis of a column study or a mesh with water flow primarily in one direction is better solved with the individual nodal head comparison. The time stepping scheme that compares head changes as adopted in VADOSE/W is that proposed by Milly (1982). As a general rule, nodal heads should not be allowed to vary more than 5 or 10 percent over any given time step. Keep in mind that this criterion depends somewhat on the actual heads being solved. For example, 5% of 1 meter is 0.05 meters. 5% of 100 meters is 5 meters. A tighter tolerance may be necessary for problems with an overall higher head range.

Regardless of the option to choose nodal heads or vector norm of nodal heads, the equation used to adjust the time step up or down is:

$$\text{MinMultFactor} = \frac{\text{Max Step}}{\text{Last Step}}$$

$$\text{MultFactor} = \text{abs} \left(\frac{\text{tolerance} \times H_0}{H_1 - H_0} \right)$$

The actual time step multiplication factor used to modify the existing time step is the lesser of the two values calculated in the above equation.

The third adaptive time stepping control routine does not consider nodal head change percentage. It continually tracks the total iteration count required to achieve convergence. If the iteration count exceeds 5, then time step adjustments are assessed. If the iteration count is less than 5, then no time step adjustment is made for the next solve step. When deciding how much to increase or decrease time steps, the solver compares the last converged iteration count with the current average iteration count. So, if the average number of iterations to converge is 8 and the last time step took 10 iterations, then the solver will reduce the time step by 8/10. Likewise, if the average count is 8 and the most recent count is 6, then the time steps will increase by 8/6.

In the adaptive scheme, the time steps are reduced for the first 2 iterations and are then held constant until convergence is reached. If the maximum number of iterations is reached without convergence, then the solver checks to see if the current time step is larger than the user-specified minimum allowable step. If the current step is larger, then the solver will reduce the current step by half and repeat the time step. If there is no room to reduce the step by half without reducing it below the user's minimum value, then the minimum value will be applied and the step repeated.

This multi-faceted time stepping logic can be quite powerful. Often you will find it quite useful to specify a lower number of allowable iterations to reach convergence rather than a higher number, because if the solver gets stuck on any given time step, it will reach the maximum allowable iterations more quickly and then try reducing the time step in half. The trade-off becomes repeating a time step or allowing more iterations. It is worth a simple trial and error test early on in a more lengthy analysis to see which option is better in the long run.

The adaptive scheme will always insert just enough time steps to return to the increments established by you. This way, no write out data steps are missed and you still have control over the general time stepping of the solution. In order to activate adaptive time stepping you must set up your time steps with preferred "save" time steps. Then you check the adaptive time stepping box and time step criteria as well as the maximum allowable change in nodal head per time step, the maximum adaptive step, and the minimum allowable time step. The time steps are entered in the same time units as the hydraulic conductivity.

Experience should show that the vector norm approach is faster for a large mesh with two-dimensional water flows. Analysis of a column study or a mesh with water flow primarily in one direction is better solved with the individual nodal head comparison.

An example with and without adaptive time stepping

Rapid drawdown of a reservoir is a good illustration of how adaptive time stepping can work to your advantage. In the first case, no adaptive time stepping was applied and 12 time steps of various increasing durations were set up such that the elapsed time was 1970 days. In the second case, one time step of 1970 days was used, but then the adaptive time stepping routine was engaged to allow a minimum step of 10

days, a maximum step of 50 days with a maximum 2.5% change in head per time step controlling the increase or decrease in time step between the max/min ranges.

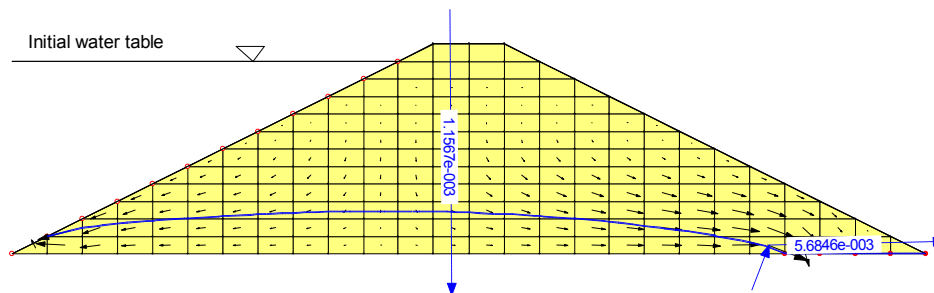


Figure 8-7 Drawdown without adaptive time stepping

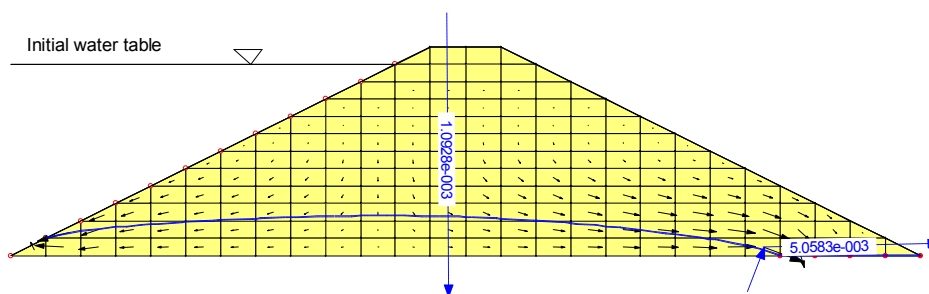


Figure 8-8 Drawdown with adaptive time stepping

In the first case, we have entered a time stepping scheme that will hopefully lead to a converged solution. We have entered 12 time steps with several "save" periods and a total elapsed time at the end of the simulation of 1970 days. Figure 8-7 shows the position of the water table 1970 days after drawdown of the reservoir. The cumulative water balance error in this analysis was $3.0 \times 10^{-3} \text{ m}^3$.

In the second case, we do not worry about appropriate time steps early on in the simulation and select, for convenience, a single "save" time at 1970 days. If we wanted more results at different times we could set up multiple steps of equal duration and still use the adaptive routine to control the step size within any user-specified step. Figure 8-8 shows the water table computed using the adaptive routine. The water balance in this case was also about $3.0 \times 10^{-3} \text{ m}^3$.

The results are similar for both cases. There are small differences, but not significant in the scope of this example. For problems where there are closed form "exact" solutions, the adaptive time stepping can yield more accurate results in some cases compared to a time stepping scheme that you must set up on a trial and error basis, in order to achieve reasonable results. In general, a combination of user AND adaptive time stepping should be used.

Time stepping and climate data

If a climate boundary condition is applied then it is critical to use time stepping that is appropriate for matching the change in climate parameters within any given day.

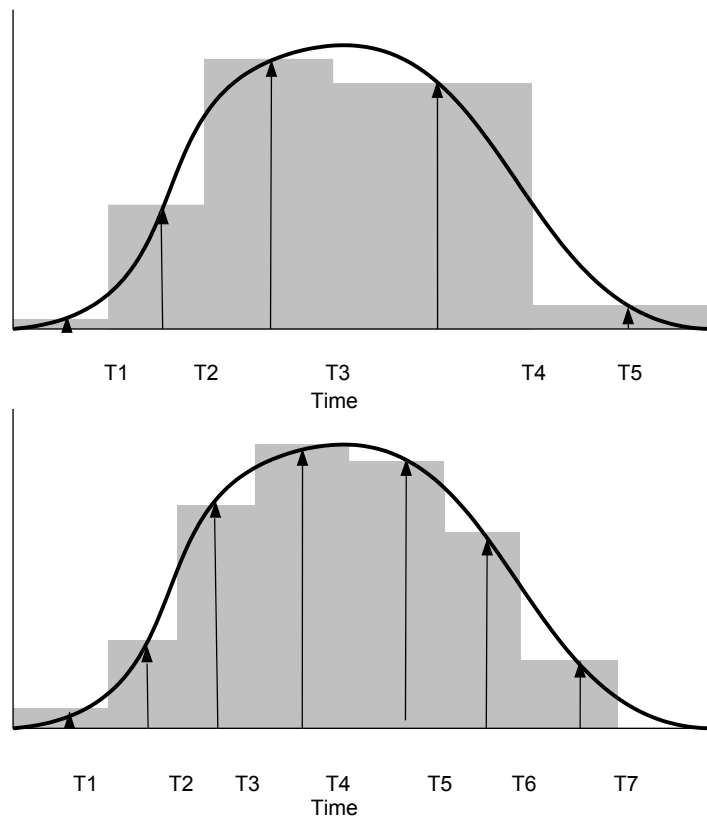


Figure 8-9 Less accurate and more accurate time stepping to fit climate data

Consider the illustrations in Figure 8-9 where two different time stepping schemes have been used to apply precipitation data throughout a single day. In the top illustration the time stepping scheme is not conducive to calculating the appropriate amount of rainfall. In this illustration, the total amount of rainfall is the area under the sinusoidal curve or the shaded step curve. If the time steps are too large, they can accurately represent this area. The shaded area in the figure is the applied amount of rainfall in the model. In order to get a more accurate solution, it is important to have small enough time steps. In the second figure there is much better agreement in the volume of water applied versus the actual rainfall.

In VADOSE/W, if you apply climate data with a sinusoidal distribution pattern then by default, the solver will limit the time step size to be less than 2 hours. HOWEVER, this 2 hour limit only applies if your rainfall is applied sinusoidally over a 24 hour period. If you have specified much short rainfall duration rates, then the solver will scale back the 2 hour maximum limit such that it breaks the curve into 12 or more smaller periods. The solver will make this adjustment for each day based on the specified rainfall periods. If there is no rainfall, then the 2 hour limit will be applied as there are still other climate parameters such as relative humidity and temperature that follow sinusoidal patterns throughout a day.

If you choose to apply climate data as a flat function, then the time step size in the solver will be limited to a full day. In either case, to use climate data, the adaptive time stepping scheme must be enabled.

9 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 must review various chapters in this book such as the Theory and Boundary Condition chapters.

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

9.1 *Transient versus steady state results*

The type of data you can view is somewhat dependent on the type of analysis you have completed. For example, if you do a steady state analysis, you can not interpret any data related to changes in time. You can view some instantaneous values such as water content, conductivity, total head, pressure head, temperature, concentration, gas flux, vapor pressure and gas diffusion coefficient. However, you can not see how these values may change with time because steady state, by nature, means things do not change with time. VADOSE/W steady state solutions limit the amount of data that is presented, compared with VADOSE/W transient solutions, for example. This is because VADOSE/W is primarily a transient program and only allows limited steady state results – enough to verify that the computed results are suitable for use as starting conditions for a detailed transient analysis.

In a steady state analysis, you are not required to define a volumetric water content function, because it is the slope of this function that is needed in the solution of the transient, not steady state, finite element equation. If you do not define a water content function, then it stands to reason that you cannot view water contents. Water contents can only be viewed in a steady state solution if you have defined a water content function that the solver can access to report water contents based on solved pressures. No water content function... no reported water contents!

In a transient analysis, you can look at how all of the various output data values change with respect to time and/or position, whereas in steady state analysis, you can only graph how the data changes with position.

9.2 *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. So, to recap, you set up the problem geometry, define material properties, and apply boundary conditions of either known head (or pressure) or flux. The solver assembles the soil property and geometry information for every Gauss point in every element and applies it to the flow equation that is written for every node. Therefore, at each node we have applied boundary data, 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 head 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.

In GeoStudio, all output data for nodes and gauss points anywhere in the model is accessible using the View Results Information command. With the command selected, you can click the mouse on any single node to view the output at the node. You can also hold down the shift key to multi-select many points. If

you click beside a node and within the element itself, you will get the Gauss point data at that location. You can multi-select Gauss point to see a table of data.

Figure 9-1 is an illustration of the type of information that can be viewed for each node in the finite element mesh. You can view the types of data in the list to see that there is a combination of heads, pressures, fluxes, velocities, gradients, conductivities and water contents. There is also a summary of the position of the node within the problem domain. In effect, the node information is a summary of the problem geometry, the soil material properties, and the boundary conditions – the three main parts of any finite element analysis.

One key point to note in the figure below is that the nodal Boundary Flux quantity is None. 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 water 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 fluxes at a node should equal zero and is reported as None – meaning there is no data at this point in time or space.

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

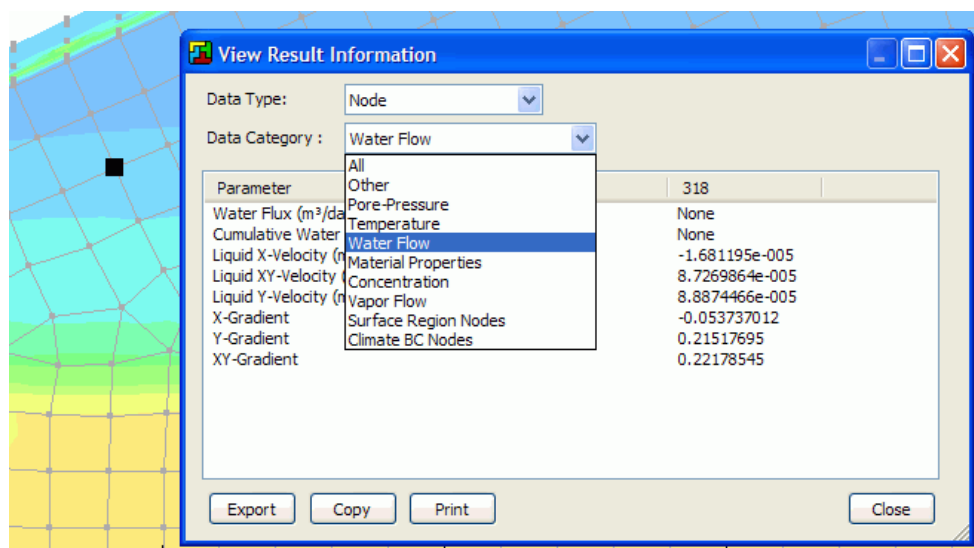


Figure 9-1 Visualization of node information

Figure 9-2 is the corresponding Gauss point information for the Gauss point located just below 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, this Gauss area is equal to one quarter 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 0.068%, 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 is not always easy and there is no sure quick or automatic method to make that happen.

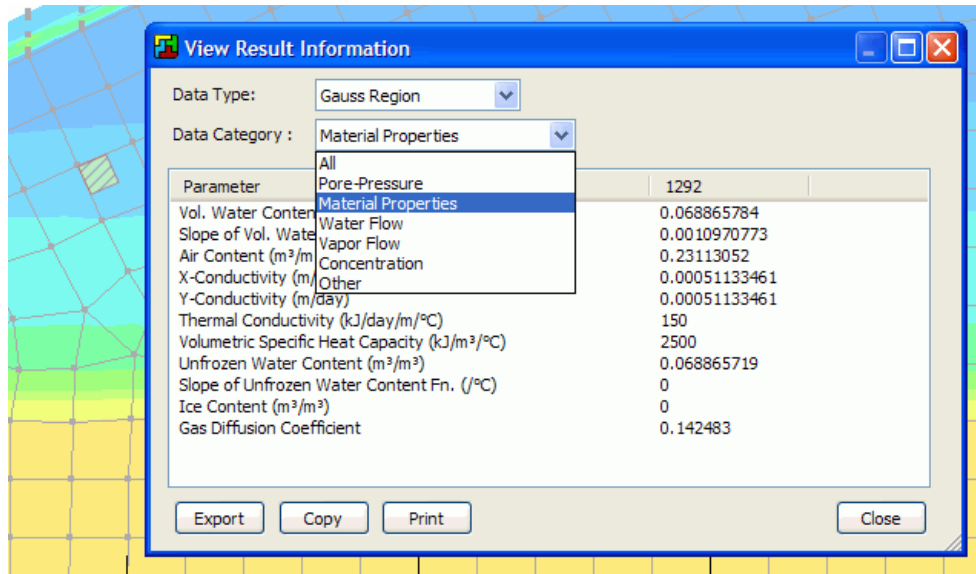


Figure 9-2 Visualization of element Gauss point information

9.3 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 9-3 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.

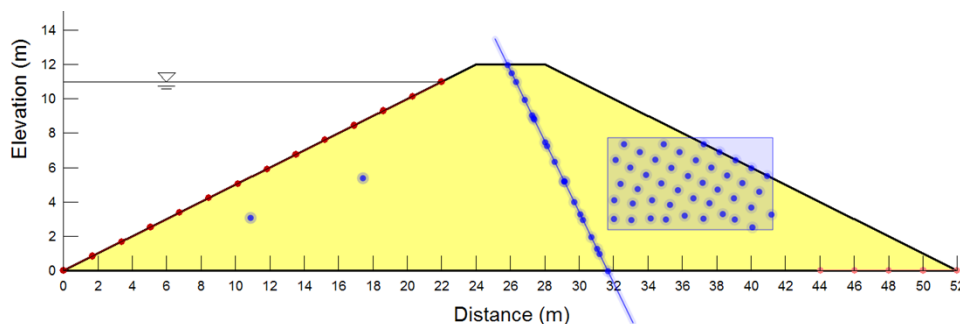


Figure 9-3 Graph data selection options (points, lines, planes)

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 9-4 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 9-4.

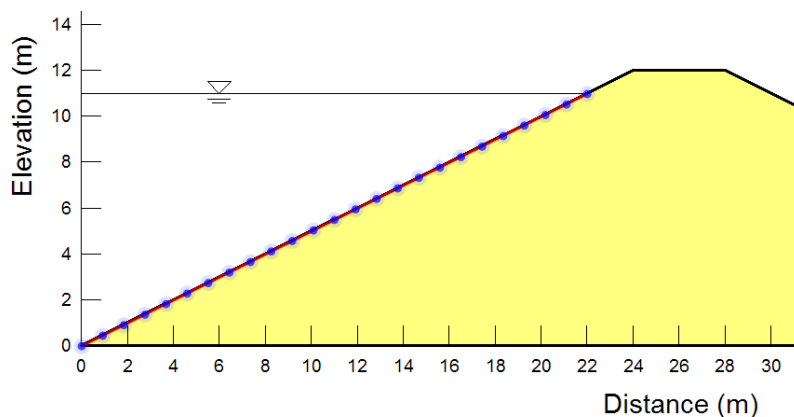


Figure 9-4 Graph selections based on geometry item (upstream region edge line)

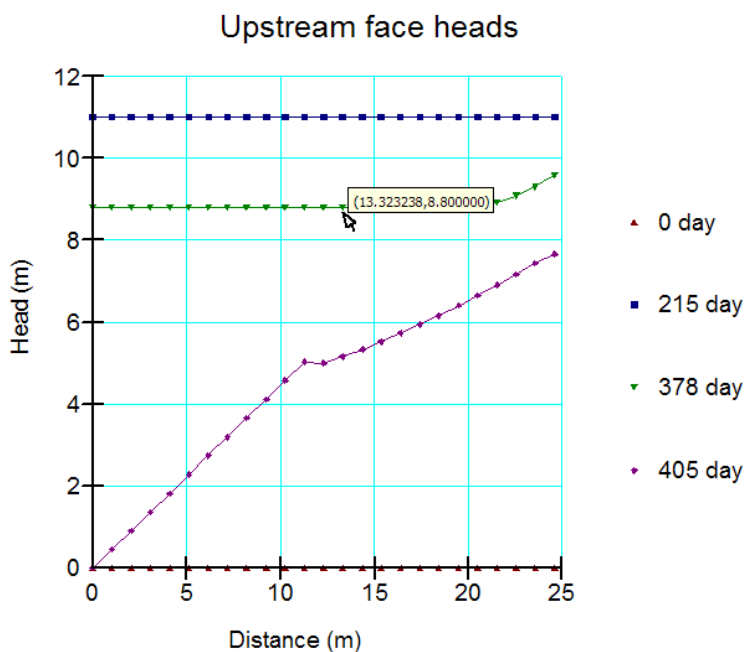


Figure 9-5 Upstream total head as a function of position for each time

9.4 “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. For example, in Figure 9-1 above, the node boundary flux values are set to “none”. This is because there are no nodal flows at internal, non boundary condition nodes.

“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.

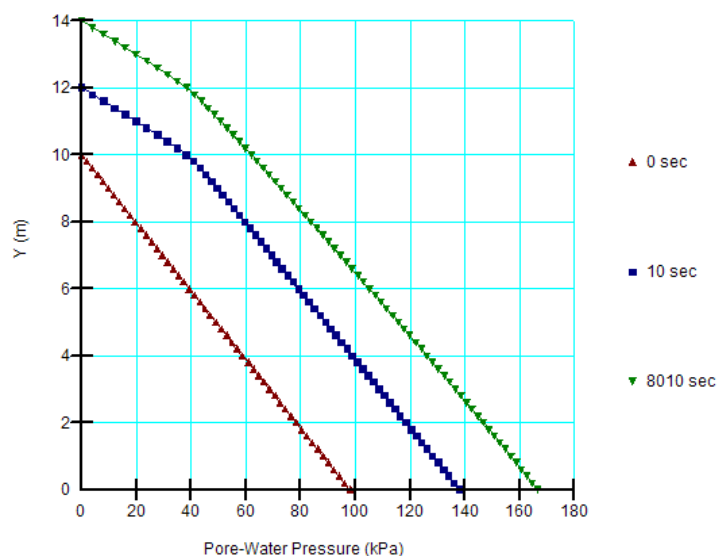


Figure 9-6 Graph showing how missing data is excluded and not printed as zero

Surface region node graphing

Because the surface region is a special engineering region, VADOSE/W creates output data for all nodes that make up the interfaces between soil types in the region. The types of data that can be graphed at any cover interface node are: cover node liquid flux, cover node vapor flux, cover node total flux, cover node cumulative liquid flux, cover node cumulative vapor flux, and cover node cumulative total flux. It should be noted that these values are either instantaneous values with units of volume/time or cumulative values with units of volume. If these values are to be converted back to a unit flux value, the actual spacing between nodes should be considered. For example, if the cover interface nodes are space 2 meters apart and the cover node total flux is $3\text{m}^3/\text{day}$, then the unit flux would be $3/2 = 1.5\text{ m}^3/\text{day}$ per square meter surface area.

One powerful use for this type of graph is to see where the water is getting through the cover system. While the total cover layer interface flux may be reported as 0.21 m^3 (see Figure 9-19 below), this does not indicate where the water is moving. Figure 9-7 is a graph of the cumulative nodal flux for all nodes across the bottom of the surface layer after two days in time and after 30 days in time. In this case, the two day results are for a period of time just after a heavy rainfall event. It can be seen that there is a large variation in infiltration or loss depending on the position across the soil profile (same profile as in Figure 9-17). The results for day 30 show much less variation in flux at these interface nodes, and this is due to the fact there were 29 consecutive days of evaporation after the heavy rainfall event. It is interesting to note however, that there is a small region of positive cumulative flux at the 1m x coordinate. This is

because there is still a small amount of ponded water infiltrating at this location, while the remaining soil surface is under a strong evaporation trend.

Surface region interface layer graphing

While the previous section deals with graphing data at any individual or group of surface region nodes, VADOSE/W is also capable of summing data at all of the nodes at any given interface and presenting a graph of the total flow across the interface, as illustrated in Figure 9-19. Data that can be plotted at any cover layer interface include: cover layer interface liquid flux, cover layer interface vapor flux, cover layer interface total flux, cover layer interface cumulative liquid fluxes, cover layer interface cumulative vapor fluxes and cover layer interface cumulative total fluxes.

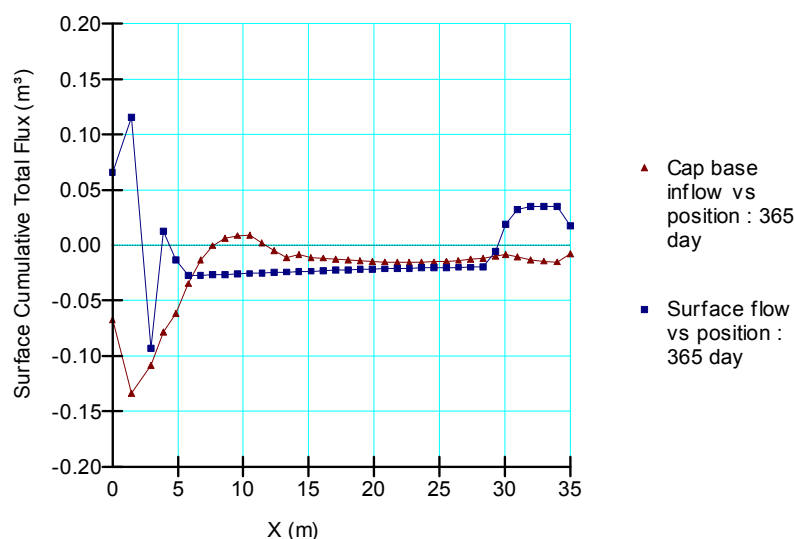


Figure 9-7 Cover node fluxes versus x coordinate after 365 days

Ground surface nodes data graphing

Climate data plays an important role in VADOSE/W input and output. It is important to be able to see that your specified climate input was used in the analysis and it is important to be able to see what types of results this climate data generated. If the surface nodes graphing category is selected, the following data can be accessed: node net radiation over time interval, node precipitation over time interval, node runoff over time interval, node infiltration over time interval, node potential evaporation over time interval, node actual evaporation over time interval, node actual transpiration over time interval, node cumulative radiation, node cumulative precipitation, node cumulative runoff, node cumulative infiltration, node cumulative potential evaporation, node cumulative actual evaporation, node cumulative actual transpiration, and node cumulative snow depth.

Figure 9-8 shows a graph of interval and cumulative infiltration at two locations of the model illustrated in Figure 9-17. Node 271 in the figure is at the top, right side of the mesh and node 133 is at the base of the trough in the center of the mesh where water has ponded due to the heavy rainfall on day one.

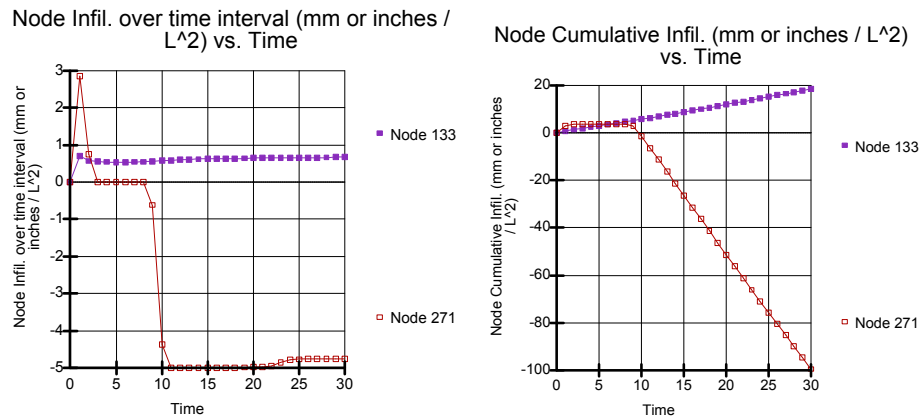


Figure 9-8 Surface node infiltration at two locations on mesh

It can be seen that there is a net cumulative loss from the system for the node at the higher elevation, and a net recharge for the node at the pond location. This agrees with expectations. It should be noted here that the term “interval flux” is not an instantaneous value, but a cumulative value, since the last data write out time step. The “cumulative flux” values are the sum of all “interval flux” values.

Water balance data graphing

Perhaps the most important graphing tool, from a “peace of mind” perspective, is the water balance category graphing. As a general rule, if the water balance of an analysis is reasonable, the results are reasonable. The types of data that can be accessed in this category include: mesh cumulative precipitation, mesh cumulative runoff, mesh cumulative boundary fluxes, mesh cumulative surface evaporation, mesh cumulative plant transpiration, mesh cumulative storage, and mesh cumulative water balance. A detailed discussion of how to use the water balance data for model checking is given in the chapter on Numerical Issues.

In Figure 9-9, the water balance line is shown to bounce around at times during the analysis, but the final water balance error volume of -0.12 cubic meters is less than 0.75% of the total applied precipitation value of 16 cubic meters.

This chart is a very helpful tool to interpreting when, during the simulation, the different surface fluxes are dominant. For example, the plant transpiration almost matches the change in storage data early in the simulation and then remains horizontal once the plants have shut down transpiring.

Surface evaporation remains influential until about day 175, when winter sets in and it shuts down. There is some precipitation during the winter months as evidenced by the slight gain in precipitation during the winter. However, this slight gain in precipitation is either due to snow melt or rainfall on non-freezing days. Most of the snowmelt is applied as precipitation in the later 40 days of the simulation.

Finally, the boundary flux series remains fairly flat during the year and only shows a real drop at the end, when the snowmelt that has infiltrated has reached and exited from the left end boundary of the slope.

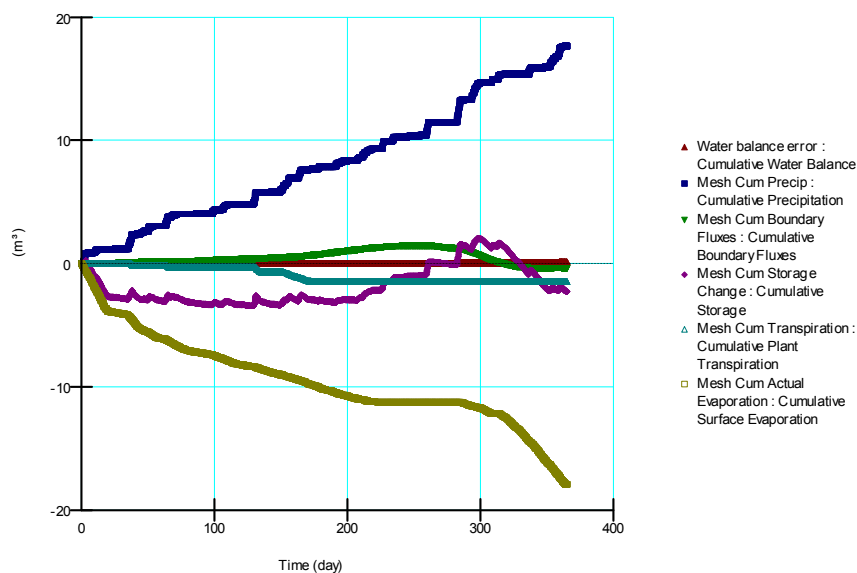


Figure 9-9 Sample water balance chart made in CONTOUR with VADOSE/W data

9.5 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 or matric suction. 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.

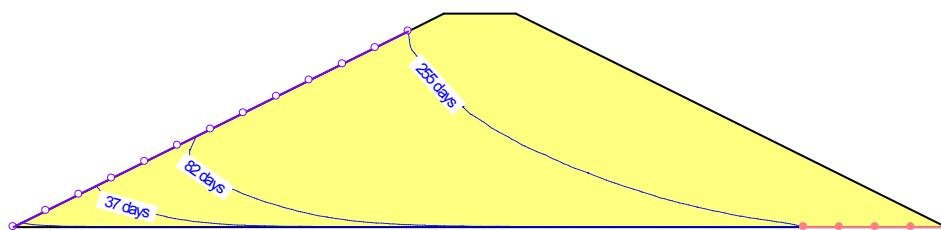


Figure 9-10 Water table (isolines) over time

9.6 Projecting Gauss point values to nodes

VADOSE /W performs contouring calculations based on parameter values at the nodes. Since the primary parameters, (total head, pressure, and pressure head), are computed at the nodes, these parameters can be contoured directly. However, secondary parameters, (velocity, gradient, conductivity, and volumetric water content), 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,
- $\langle N \rangle$ = 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 9-11 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 volumetric water content and that in some elements the water content at the Gauss points varies over the complete range of the volumetric water content function. Projecting such a large variation to the nodes can result in projected nodal water contents beyond the range of the volumetric 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.

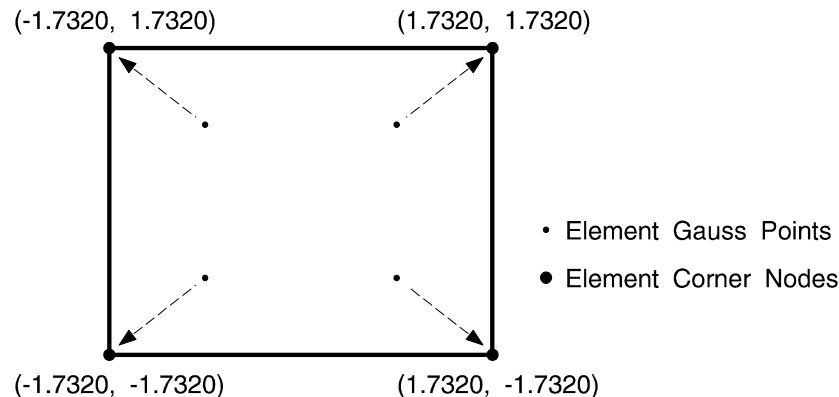


Figure 9-11 Local coordinates at the corner nodes of an element with four integration points

9.7 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 a section above we introduced isolines and showed how their relative positions give an indication of the change in a parameter over time

and space. In this section, we show that it is quite simple, and much more meaningful, to interpret parameters over space if we can view all values for a model at one time over the entire domain.

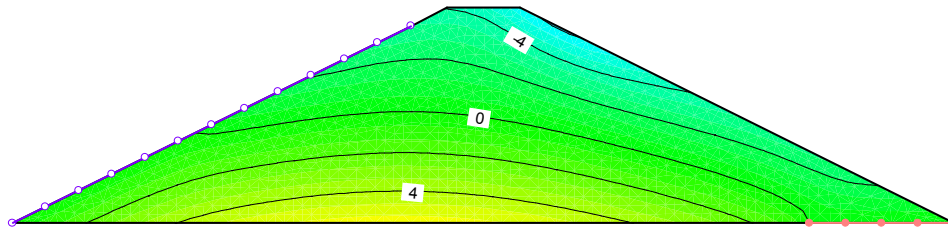


Figure 9-12 Contour of pressures at a fixed time

9.8 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.

9.9 Velocity vectors and flow paths

Calculating gradients and velocities

Once the solution has converged and the nodal heads are known, VADOSE /W computes the hydraulic gradients and Darcian flow velocities at each of the integration points within each element. The gradient at each Gauss or integration point is computed from the equation:

$$\begin{Bmatrix} i_x \\ i_y \end{Bmatrix} = [B]\{H\}$$

where:

i_x = the gradient in x direction,

i_y = the gradient in y direction,

[B] = the gradient matrix as defined in the theory chapter, and

{H} = the vector of total head at the nodes.

The Darcian velocities at each Gauss point are computed from the equation:

$$\begin{Bmatrix} v_x \\ v_y \end{Bmatrix} = [C][B]\{H\}$$

where:

v_x = the velocity in x direction,

v_y = the velocity in y direction, and
 [C] = the hydraulic conductivity matrix.

VADOSE /W stores the hydraulic conductivity at each Gauss point used in the formulation of the finite element equations in an array. The same hydraulic conductivity values are later used to compute the velocities.

The VADOSE /W velocity is actually the specific discharge, q , which is the total flux Q divided by the full cross-sectional area (voids and solids alike); it is not the actual speed with which the water moves between the soil particles. The actual microscopic velocity is:

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

where:

v = the average linear velocity,
 q = the specific discharge, and
 n = the soil porosity.

VADOSE /W does not compute the actual pore-channel velocity. Once the velocities and gradients are calculated, they are saved to a data file for later use in visualizing the node or Gauss point information, or for generating flow vectors and flow lines.

Velocity vectors

Velocity vectors are a useful way of seeing not only where the flow is occurring, but how much flow there is relative to other regions of the domain. VADOSE /W uses the magnitude of the actual velocity in its calculation of how large to display the vector so that you have a visual representation of where the velocities are high or low. For each element, the average x-velocity and average y-velocity from the Gauss point velocity values are computed and then vectorally summed to obtain an average velocity vector for the element. This average velocity vector is plotted with the tail of the vector at the center of the element.

When displaying vectors, VADOSE /W finds the maximum velocity vector and draws it at the length specified in the Draw Vectors dialog box. All other vectors are drawn in proportion to the element velocity relative to the maximum velocity. For example, if the element velocity is one quarter of the maximum velocity, then the length of the velocity vector is one-quarter of the length specified in the Draw Vectors dialog box.

You have the option of controlling the size of the vectors as they are displayed by controlling the magnification scale when you issue the command to create the vectors. Specifying a magnification value allows you to control the scale at which all vectors are drawn. When you type a value in the magnification edit box, the maximum length edit box is updated to display the length at which the maximum vector will be drawn. You can control the vector length either by specifying a magnification value or by specifying a maximum display length value. If you specify a length, the magnification value is computed by dividing the maximum length by the maximum velocity and adjusting the value for the scale of the page and engineering units.

Vectors are only drawn in element regions being viewed. Choose View Element Regions if you wish to view different materials or to not view infinite elements. If no elements are viewed, an error message appears when you choose Draw Vectors.

Flow paths

The VADOSE /W flow paths are not flow lines or stream lines as in a traditional flow net. In many cases the flow paths are a very good approximation of stream lines, but they are not the same. The flow paths are simply a line based on velocity vectors in an element that a drop of water would follow under steady-state conditions; and slight variations between a flow path and a flow line should not be of concern because they are computed in entirely different ways. At best, the VADOSE /W flow path should be viewed as a reasonable approximation of the flow lines within a flow net.

The flow paths will always be the most realistic in saturated zones where there is significant velocity. In zones where there is little or no flow, the VADOSE /W flow paths may not be realistic. Several cases are illustrated in Figure 9-13. In the upstream toe area where there is little flow, the flow path ends along the bottom boundary. This is not physically correct and therefore is not a realistic flow path. Within the unsaturated zone in the figure there is a flow path that ends within the dam section. The reason for this is that the path has reached an area where there is essentially no flow. Once again, such a flow path has no meaning. Since it is possible to click in an area with relatively no seepage and create an unrealistic flow path, some judgment is required by you when drawing flow paths. You should discard flow paths that you judge to be unrealistic.

When you create a flow path, a message will be displayed if you attempt to draw it in an area where there is little or no flow. After accepting the message, the flow path will be drawn, but it may not be complete; that is, the path will end inside the flow regime and not at an external mesh boundary. This message will also be displayed if the flow path encounters a no flow perimeter boundary.

Another important point is that in a saturated / unsaturated flow system, the phreatic line is not a flow line. It is simply a line of zero water pressure. Since water can flow from the saturated to the unsaturated zone, and vice versa, flow can take place across the phreatic surface. Consequently, a flow path may cross the phreatic surface as illustrated Figure 9-13. This is acceptable and realistic.

You can select any point to draw a flow path by clicking on a point within the flow domain. The path is drawn strictly on the basis of the velocity vectors within each element. The path is projected forward and backward incrementally within each element until the path encounters a boundary. The flow path is simply a graphical representation of the route a molecule of water would have traveled under steady-state conditions from the entrance to exit point within the flow regime.

Flow paths can only be drawn for steady-state conditions. Flow paths based on velocity vectors at an instant in time during a transient process have no physical meaning. For this reason, VADOSE/W does not permit you to draw flow paths for transient conditions

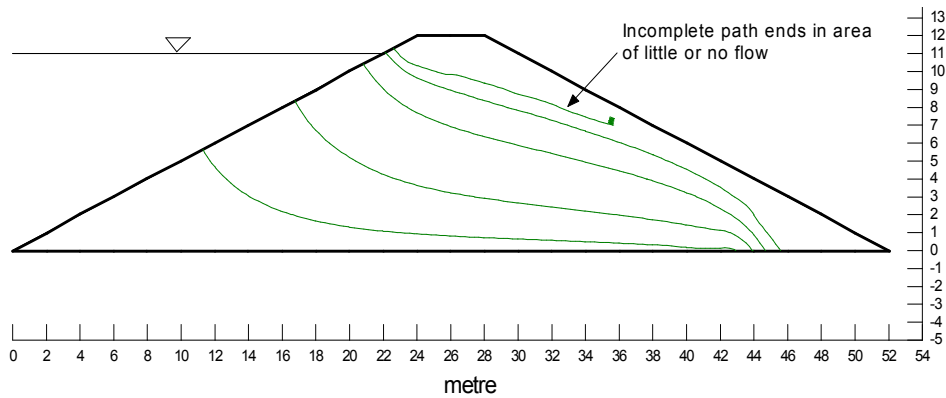


Figure 9-13 Illustration of flow lines in a steady state analysis before reservoir drained

9.10 Flux sections

VADOSE /W has the ability to compute the instantaneous seepage volume rate that flows across a user-defined section for either a steady state or transient analysis. This is a very useful tool for isolating flow volumes to specific regions of interest and it can save you manually adding up individual nodal flows in the case of a drain or seepage face that is comprised of many nodes.

Flux section theory

This value can be computed from the nodal heads and the coefficients of the finite element equation. For example, consider a mesh with only one element, as illustrated in Figure 9-14. The objective is to compute the total flow across a vertical section of the element.

In the Theory chapter, the full finite element form of the mass flow equation is presented. It can be re-written for just heads to illustrate how the flux value can be isolated on one side as follows:

$$[K]\{H\} + [M]\frac{\Delta H}{\Delta t} = \{Q\}$$

In a steady-state analysis, the storage term $[M]\frac{\Delta H}{\Delta t}$ becomes zero, and the equation can be reduced to:

$$[K]\{H\} = \{Q\}$$

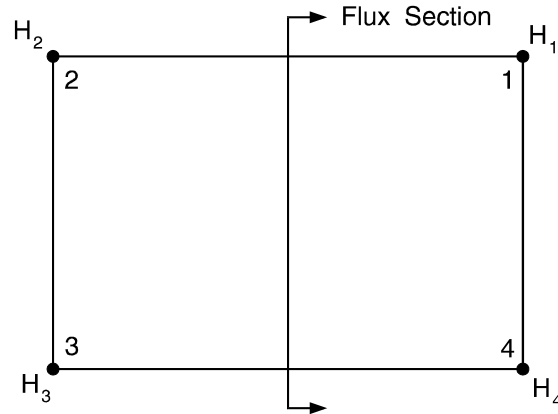


Figure 9-14 Illustration of a flux section across a single element

The global set of finite equations for one element is as follows:

$$\text{Equation 9-1} \quad \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \begin{Bmatrix} H_1 \\ H_2 \\ H_3 \\ H_4 \end{Bmatrix} = \begin{Bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{Bmatrix}$$

From Darcy's Law, the total flow between two points is:

$$\text{Equation 9-2} \quad Q = k A \frac{\Delta H}{l}$$

The coefficients, c , in Equation 9-1 are a representation of $\frac{KA}{l}$ in Equation 9-2. Therefore, the flow from Node i to Node j is:

$$Q_{ij} = c_{ij} (H_i - H_j)$$

In a transient analysis, because of material storage, the calculation of the total flow quantity must include the storage effect. The change in flow quantity due to the storage term can be expressed as:

$$\frac{1}{\Delta t} \begin{bmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{bmatrix} \begin{Bmatrix} \Delta H_1 \\ \Delta H_2 \\ \Delta H_3 \\ \Delta H_4 \end{Bmatrix} = \begin{Bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{Bmatrix}$$

where $\Delta H_{1,2,3,4}$ etc. are the changes of total head at the various nodes between the start and the end of a time step. In general, the average change of total head from Node i to Node j can be expressed as:

$$\Delta H_{ij} = \frac{\Delta H_i + \Delta H_j}{2}$$

Therefore, the change in flow quantity from Node i to Node j due to a change in storage is:

$$Q_{ij} = m_{ij} \frac{\Delta H_{ij}}{\Delta t}$$

The total flow quantity from Node i to Node j for a transient analysis then becomes:

$$Q_{ij} = c_{ij} (H_i - H_j) + m_{ij} \frac{\Delta H_{ij}}{\Delta t}$$

The total flow quantity through the flux section shown in Figure 9-14 is:

$$Q = Q_{21+} + Q_{24} + Q_{31} + Q_{34}$$

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

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 that an influx is equal to an out flux such as illustrated in Figure 9-15; or you may want to know the total drain flux as illustrated in Figure 9-16.

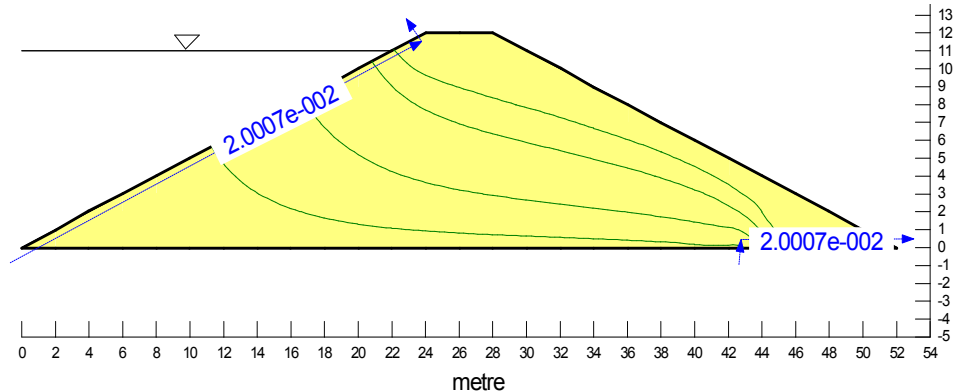


Figure 9-15 Flux section used to check balance of inflow and outflow

Flux sections do not have to be drawn as single straight lines. They can be made of continuous attached segments as illustrated in both figures 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 drain nodes in Figure 9-16, 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.

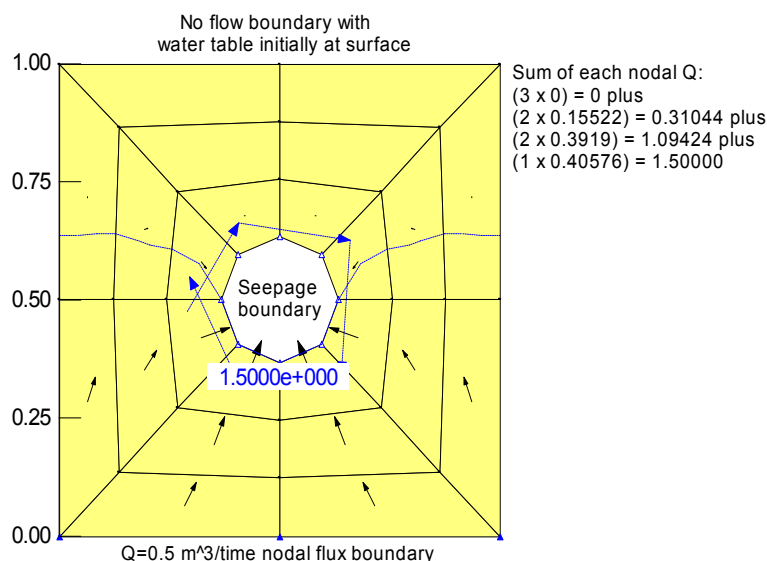


Figure 9-16 Flux section used around series of drain nodes to check flow

9.11 Surface region flux sections

VADOSE/W has a very powerful automatic algorithm that tracks instantaneous and cumulative flux data across the interface of any soil layers constructed as part of a surface region. This makes it possible to track actual fluxes through each layer of a thinly spaced layered strata, without having to manually draw flux sections. The algorithm lets data be graphed for the entire soil interface or any individual (or group of) nodes at any soil layer interface.

Figure 9-17 is a figure of two manually drawn flux sections on each side of a surface regions interface layer (the mesh is turned off but the interface exists between the two illustrated flux sections). The flux section values shown in VADOSE/W are both instantaneous (left of “/” mark) and cumulative (right of “/” mark). You can see that there are very different values of cumulative flux on either side of the soil interface layer. The flux section above shows 0.247 m³ of water passing the section, while the value below shows only 0.067 m³ of water passing the interface. In many cases, the correct value is an average of the two values, but in this case, that is not so. The reason neither flux section is accurate enough is that there is some change in storage between the two flux sections that is affecting the results. Figure 9-18 shows a zoom in of the element that the two flux sections pass through, and it can be seen that the lower flux section passes through a larger element. This larger element is storing some water so the two flux sections are not agreeing. For a non-critical mesh location (other than at the interface between layers in a soil cover / cap system) this discrepancy may not be critical. In this case, it is and another more guaranteed method of finding the percolation is needed.

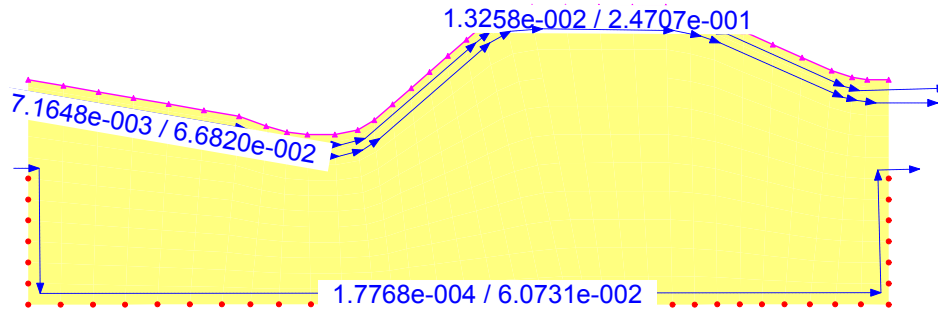


Figure 9-17 Manual flux sections on each side of a cover interface layer

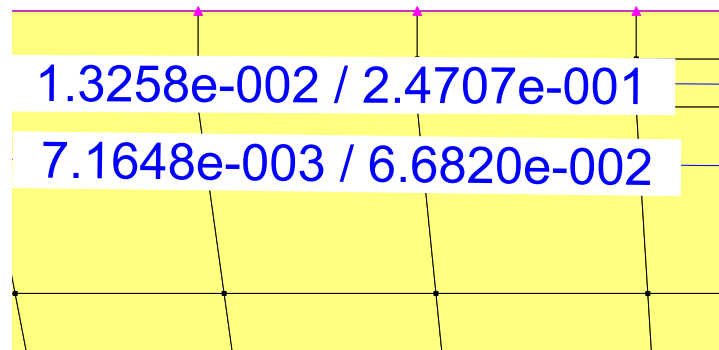


Figure 9-18 Zoom in on flux sections showing different element size above / below soil interface

Figure 9-19 is a VADOSE/W generated graph of the cumulative cover layer interface flux versus time. This graph shows both the ground surface flux (a net loss in the figure as it is a boundary location with a negative value) and the base of each surface layer cumulative flux (the positive value indicates an upward flow at internal positions of the mesh). This data is obtained directly at each node that makes up the interface between surface region soil layers, and it is exact for that point. Each node's values are summed to arrive at the total flow across a layer.

Another key advantage of using the surface layer graphing of fluxes, is that the direction of flow is always known by the sign of the value displayed. User drawn flux sections are all presented as positive values, as their sign depends on which direction they were drawn in (e.g., right to left, or down to up). You must manually use other data to determine the net flow direction if relying on flux section data.

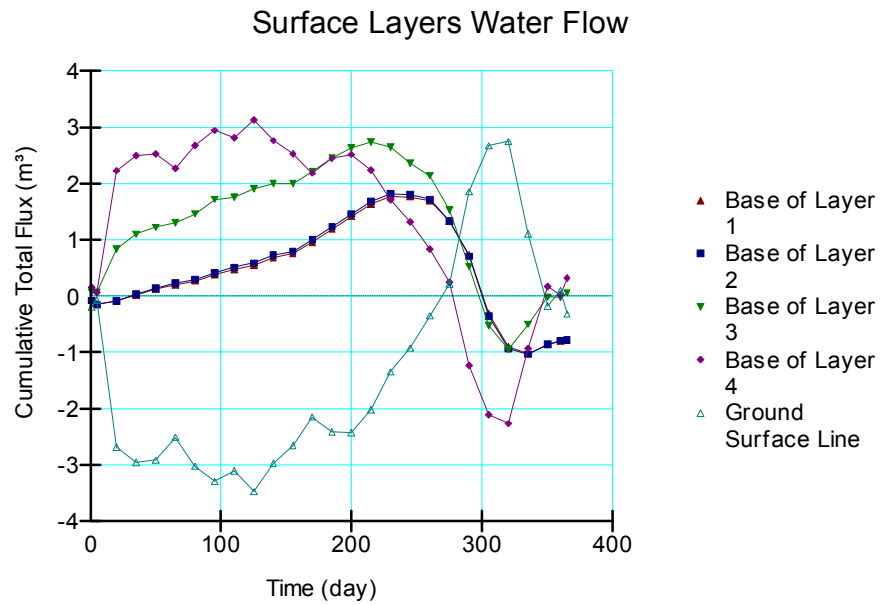


Figure 9-19 Automatic surface mesh interlayer flux data

It is not recommended that you try to draw a manual flux section for flow through surface region layers. Use the automatic flux section feature available through the CONTOUR graphing command.

10 Modeling Tips and Tricks

10.1 Introduction

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

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 they will also enhance 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!

10.2 Modeling progression

One of the most important rules to follow in finite element modelling 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. Determining what causes unrealistic results can be difficult if all of the possible complexities are included at the start of the problem analysis. Furthermore, in finite element modelling, it is important that the results obtained are of a form similar to results obtained from simple hand calculations. It is easier to make this judgment if you start with a simplified version of the problem.

In VADOSE/W you can make the process "simple" by initially using soil functions that are not excessively steep. You can use simple cover designs with only one or two materials, and you can scale climate data to minimize extreme rain events if there are any or apply the rainfall over a 24 hour period to minimize the shock loading of high rainfall in a short period of time. Once you are confident in the set ups, you can add complexity.

10.3 Evaporation analysis tips

An evaporative flux analysis is quite different from a general seepage analysis because there is a strong possibility that the soil water pressures near the surface will become extremely negative, as much as several hundred thousand kPa negative. Numerical analysis of this phenomenon is quite difficult because of the extreme pressure gradients over very thin distances near the surface. The objective of the check list presented below is to help reduce common evaporative flux analysis methodology errors and to increase the confidence in the results that are generated.

It is strongly suggested that you review the check list laid out below when you set up a simulation. Due to the lengthy solving times for a typical 365 day analysis, it is a good idea to apply the following prior to your simulation, not after you have waited a few hours to discover errors.

Many of the items in the following check list are discussed in more detail elsewhere in this chapter. You may want to print out the table and manually check each item if it is relevant to your analysis.

Table 10-1 Checklist for VADOSE/W analysis

Item	Category	Comments and Questions	Check
1	Material properties	Do the time units of the hydraulic and thermal conductivity functions match those you have set in the Set Scale menu? Do they match the time units of your time steps?	
2	Material properties	Did you use the closed form equation for the volumetric water content function? You should use this or else define a clear splined function over the full pressure range from zero to minus 1 million kPa (or minus 20.8 million PSF).	
3	Climate data	Do the units of climate data match those of your problem geometry and time step (i.e., imperial versus metric)? Climate units will be mm of precipitation even though you have meters distance units. Just ensure climate units are not inches of precipitation if distance units are meters.	
4	Time steps	You must have time steps that fall on even day increments. You do not have to write out data every day but the time steps you generate can not be more than a day. It is reasonable to write out results data every 10th day or so. If you observe high infiltration periods you may want to manually add a write out day just following the infiltration event. You should take advantage of the adaptive time stepping option. Is it turned on?	
5	Vegetation functions	Did you specify a leaf area index function AFTER you imported or set up climate data? The function estimation routine needs to know how many days of climate data you have so do not increase the simulation dates without redefining vegetation functions that are dependent on date.	
6	Vegetation functions	Does your root depth function have depths from surface that are greater than the total cover thickness you have drawn? If yes, the solver will limit root depths to the cover elements only.	
7	Cover mesh and surface soil layer	<p>Did you enter too many elements for a cover mesh? A good rule of thumb is to have cover elements be about 5 or 6 cm thick (2 to 3 inches). They can be up to 2 meters long (6 feet) but should not be too thin with the exception being the ground surface elements (see next paragraph).</p> <p>Does your ground surface hydraulic conductivity function have values that drop over 10 orders of magnitude across the suction range? This will make numerical convergence very difficult during infiltration events into dry ground. Consider specifying a unique soil type for the top 2 to 4 cm of soil such that the hydraulic function only drops 2 or 3 orders of magnitude over the full pressure range. The water content and thermal functions can be the same as the main surface layer soil but the K function in the top few cm should be relaxed. This has a physical basis in that the surface of a soil is often roughed up and loose due to drying and desiccation effects. It does not make sense to say that hydraulic conductivity is shut down to almost zero when</p>	

		a surface soil is dry.	
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8	Main mesh	Do you have too many small elements in places where there will be little change in pressure over time? If yes, you are slowing down the solving time and not necessarily gaining accuracy.	
9	Initial conditions	Are your initial conditions causing the problem to have poor water balance error on the first few days? Perhaps add a few data write out days at the start so you can stop the simulation in the first few days to see what is happening. It's easier to make changes after a few days than to wait 365 days to make a change back on day 1.	
10	Boundary conditions	<p>Do you have any up stream or down stream boundary conditions other than the surface climate boundary? If yes, you may be creating an infinite source of water that feeds your ground surface. If no, you are modeling a bath tub that only drains and fills through the ground surface. Careful thought must be given to boundary condition application. 33% of all model problems are due to poor choice of boundary conditions.</p> <p>If you have a down stream seepage face boundary condition that is applied to nodes beneath a cover node where those nodes may be root uptake nodes, then just be advised that the vegetation will be turned off at the review node. Generally this is not going to affect the results in any significant way as this situation would only likely occur at the edge of a mesh and this is not the main region of climate influence on your problem.</p>	
11	Control options - vegetation	If you entered vegetation functions and applied them to the surface climate nodes, did you also turn on the vegetation option in the Keyin Analysis Settings Control Tab? This control option exists so you can toggle on / off vegetation analysis without having to redraw the cover boundary conditions each time.	
12	Control options - freezing	Even though you have a few climate days with freezing air temperatures, do you really need to analyse freezing in the ground. This slows the solution down and may not provide useful information to you. Ground temperatures will still solve to values below freezing if you do not select the freezing option. The freezing option enables the addition of latent heat of phase change to be added during the process as well as the build up of ice which can restrict infiltration of snow melt in the spring. The freezing option does not prevent the calculation and accumulation of snow.	
13	Convergence - solver	If you have less than a couple thousand elements, it is likely the Direct Solver will be more efficient. It is the default solver. Did you de-select it in error?	
14	Water Balance	You should watch the water balance in the solver window for the first few days of the simulation. If it increases to a value near 1.0 in a short period of time this means you have issues that must be dealt with. Try writing out data for each of the first few days and then re solve the model. In Contour, plot the water balance versus time to see if there is a continually changing balance error or if it jumps up on a given day. Investigate to resolve the issues before re solving an entire year.	

15	Surface water runoff	Have you observed "negative" runoff? Negative runoff is water generated by a review boundary that is ponded and re-infiltrates on a subsequent time step.	
16	Convergence graphing	If you have water balance problems, check the convergence graphs. Press the SOLVE button but do not start the solve. Use the GRAPH button in the solve window to view all convergence data from the previous solve session. You should check for instances where maximum iterations were reached and where the maximum number of seepage reviews was reached. Compare these days with climate data days to see if there are extreme conditions being applied to the model. Also perhaps add data write out days at this point and re-start the analysis on the days just prior to the problem period.	

10.4 Problem engineering units

In all GeoStudio products except VADOSE/W any system of units can be used for a seepage analysis; the only requirement is that you must be consistent. 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. In VADOSE/W, however, the solver needs to know what the various unit sets are so that it can convert standard format climate data to the appropriate values. Therefore, three sets of compatible units are available to choose from. Table 10-2 to Table 10-4 present sets of consistent units you can choose from but it is strongly recommend that you choose the set detailed in Table 10-3 as time units of “days” are very convenient for setting up a long term analysis, both from a data input perspective but also from an results interpretation perspective.

Table 10-2 Consistent SI Units (J, m, sec, C)

Parameter	Symbol	Units
Length	L	meters
Time	t	seconds
Force	F	kN
Pressure	F/L^2	kN/m^2
Unit Weight of Water	F/L^3	kN/m^3
Hydraulic conductivity	L/t	m/sec
Total / Pressure head	L	m
Nodal Flux (Q)	L^3/t	m^3/sec
Boundary Flux (q)	L/t	m/sec
Flux Section	L^3/t	m^3/sec
Volume	L^3	m^3
Temperature	-	Celsius
Heat	-	Joules

Table 10-3 Consistent SI Units (kJ, m, day, C)

Parameter	Symbol	Units
Length	L	meters
Time	t	day
Force	F	kN
Pressure	F/L^2	kN/m^2
Unit Weight of Water	F/L^3	kN/m^3
Hydraulic conductivity	L/t	m/day
Total / Pressure head	L	m
Nodal Flux (Q)	L^3/t	m^3/day
Boundary Flux (q)	L/t	m/day
Flux Section	L^3/t	m^3/day
Volume	L^3	m^3
Temperature	-	Celsius
Heat	-	kilo Joules

Table 10-4 Consistent Imperial Units (BTU, ft, hours, F)

Parameter	Symbol	Units
Length	L	feet
Time	t	hours
Force	F	lbs
Pressure	F/L^2	psf
Unit Weight of Water	F/L^3	pcf
Hydraulic conductivity	L/t	ft/hr
Total / Pressure head	L	ft
Nodal flux	L^3/t	ft ³ /hr
Boundary Flux (q)	L/t	ft/hr
Flux Section	L^3/t	ft ³ /hr
Volume	L^3	m ³
Temperature	-	Fahrenheit
Heat	-	BTU

10.5 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.

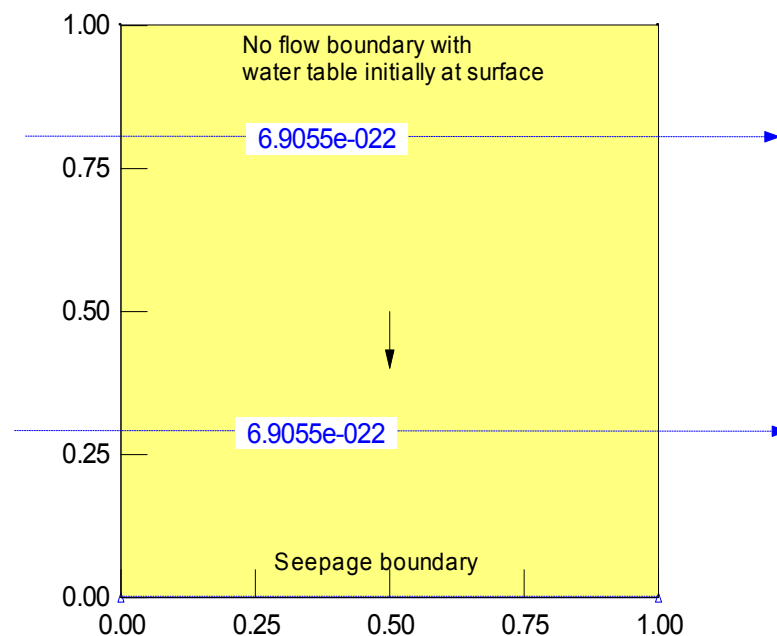


Figure 10-1 Test to check flux section locations

10.6 Drain flux values

Question: What is the best way to compute a total drain flux?

Answer: You can sum each individual nodal flux, or, draw a flux section around the nodes.

The figure below shows a total flux into the system through the three bottom nodes of 1.5 m^3 per time unit (each node contributing a total nodal flux of 0.5 m^3). This example also shows that with no other place for the water to flow except the drain, the flux into the base equals the flux out of the drain nodes.

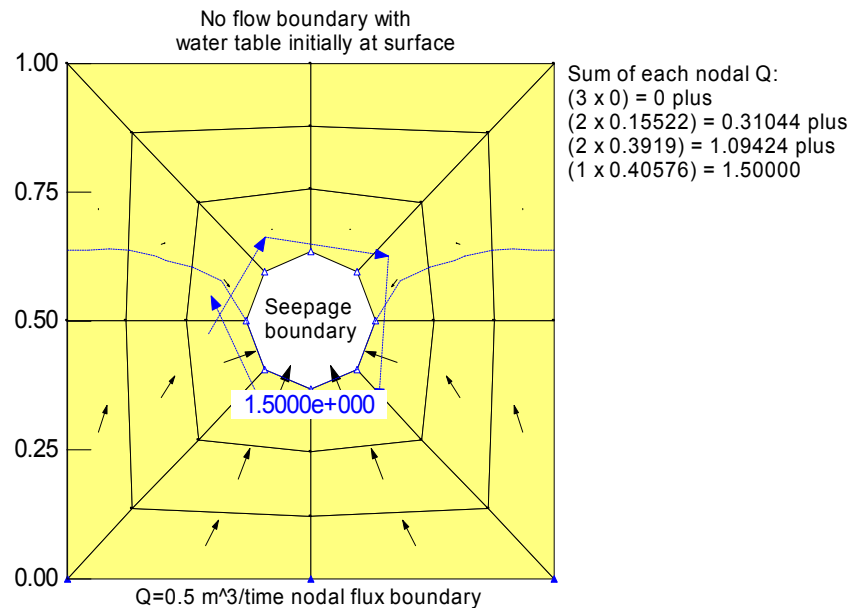


Figure 10-2 Test to see best method for observing drain flux

10.7 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 $1 \text{ m}^3 / \text{time} / \text{meter edge length}$ has been applied to the bottom of the element. The top is a seepage face which will let the water out. The flux sections drawn in the element confirm that the total edge flux of $1 \text{ m}^3 / \text{time}$ has been converted by the solver into two equal total nodal fluxes of $0.5 \text{ m}^3 / \text{time}$ each.

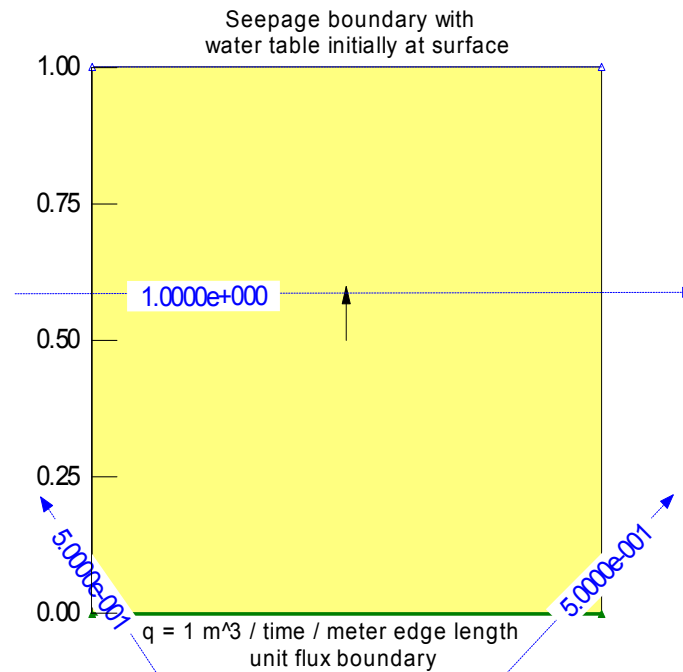


Figure 10-3 Test to compare unit flux and total flux

10.8 Flow above phreatic line

Question: Is there really flow above a water table?

Answer: The amount of flow through the unsaturated zone depends on its conductivity value as a function of how saturated the ground is. If the conductivity is quite high in a partially saturated state, the flow can be quite high.

In the numerical test below, there is a head gradient from right to left and the water table sits at the mid point of the mesh. You can see from the flux section values that 45% of the total flow passes through the soil ABOVE the phreatic surface in the unsaturated zone.

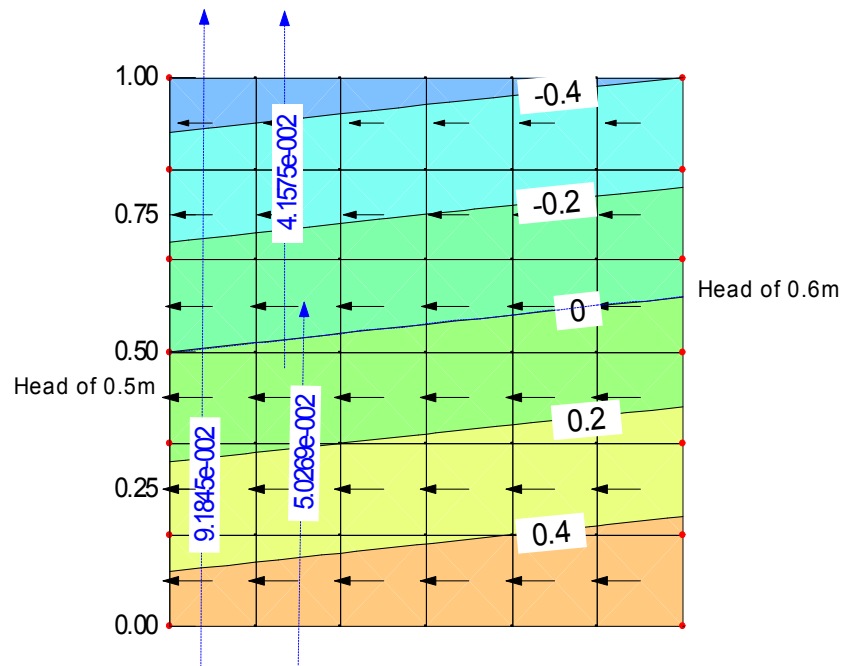


Figure 10-4 Test to see flow above phreatic line with pressure head contours shown.

10.9 Pressure boundary with depth

Question: If I know the pressure boundary with depth, do I have to put a different pressure value at each node?

Answer: If the pressure change is hydrostatic, simply specify a total head of a constant value along the entire edge and let the solver figure out the pressure at each node. The total constant head value should be equal to the elevation of the water table along that edge.

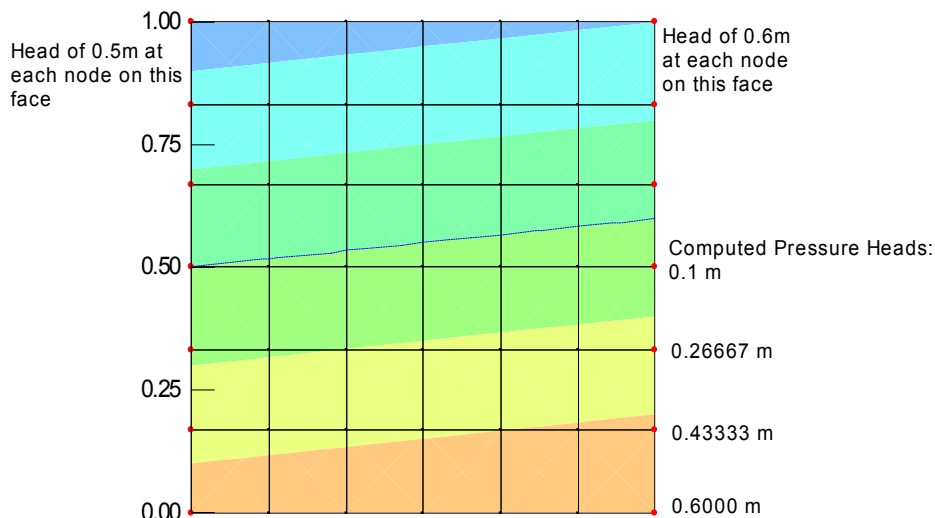


Figure 10-5 Test to see how pressure boundary can be applied as constant total head value along entire edge

10.10 Summing graphed data

In some cases you may want to know the total flow that crosses a boundary or the total change in stored water within the system. There is a trick you can do with the graphing feature to aid in this task.

The graphing feature has a check box that will “Sum(y) vs Average(x)” values. This option will result in all the “y” data points being added together and plotted versus the average of the “x” value each data point. If the “x” category is time, then there is no averaging and the resulting graph is a sum of all “y” values versus time.

Figure 10-6 shows the nodes selected for graphing on the upstream face of a reservoir during the filling stage. The objective is to know how much water crossed this boundary over time. One option is to draw a flux section but this is not the most accurate way in a transient analysis because the flux section is drawn through the elements and there is change in storage within the element. The most accurate way is to plot cumulative flow at each boundary node.

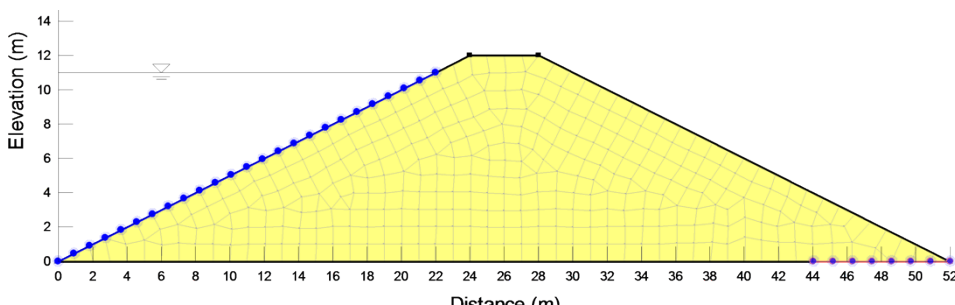


Figure 10-6 Graphing nodes selected on upstream dam face

The figure below shows the individual nodal flows at each selected node. You can see that each node has a different flow value. The second figure is much easier to interpret. In that graph, the check box for Sum(y) vs Average(x) was selected. This second graph is the cumulative total flow across the entire face.

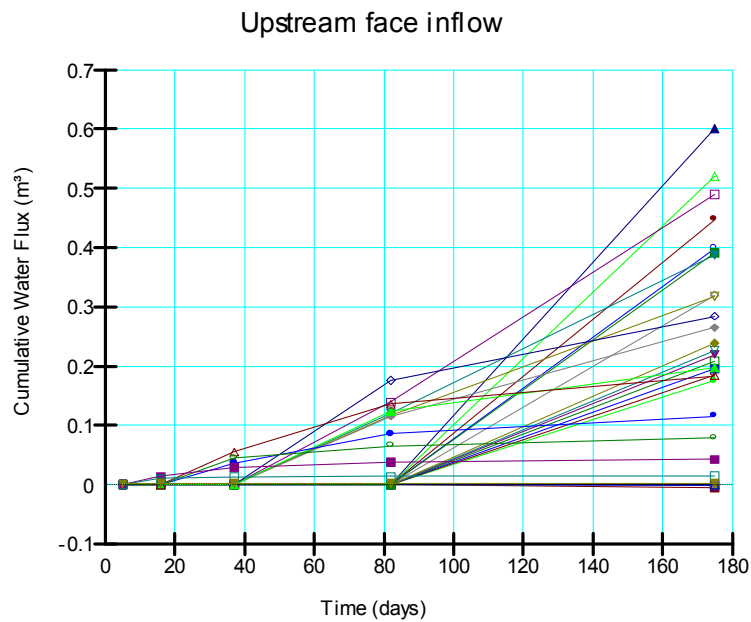


Figure 10-7 Individual nodal flow on upstream face

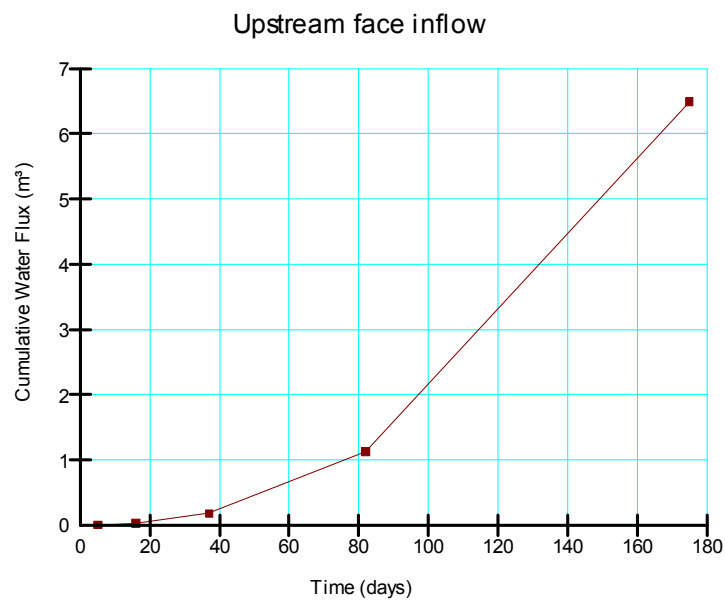


Figure 10-8 Sum of all nodal flow on upstream face

Suppose now we wanted to look at the change in stored water in the dam throughout a filling and draining cycle. We could select ALL the nodes in the mesh and use the Sum option as shown next.

11 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.

12 Theory

This chapter describes the theoretical engineering basis for the VADOSE/W program. The first part deals specifically with coupling ground response with atmospheric forcing from a practical and theoretical perspective.

The second part deals with the fundamental flow laws for steady state and transient flow of water, heat, vapor and gas and it shows how these laws are represented in numerical form. This chapter is not a study of groundwater and flow in porous media. For advanced discussion of these topics the reader is referred to the textbooks *Groundwater*, by Alan Freeze and John Cherry (Prentice Hall, 1979); and *Unsaturated Soil Mechanics*, by Del Fredlund and Harianto Rahardjo (John Wiley & Sons, 1995).

12.1 *Atmospheric coupling*

The key to geotechnical modeling of the vadose zone is the ability to accurately predict the surface boundary condition. The most significant variable to quantify is the magnitude of surface infiltration and actual evaporation, or in modeling terms, the surface unit flux boundary. VADOSE/W determines this value by coupling the moisture and heat stress states at the ground surface with climate conditions present above the ground surface.

Traditionally, evaporative flux modeling has been limited to methods that predict the unit flux evaporation rate based on a potential evaporation (PE) value. This PE value is computed based on some form of a Dalton type equation, such that PE is a function of a turbulence mixing parameter multiplied by the difference between the saturation vapor pressure at the ground surface and that in the air above the ground. This approach forms the basis for the widely used Penman (1948) method, which assumes the ground surface is always saturated. Other methods, such as the temperature based Thornthwaite (1948) and energy based Priestly-Taylor (1972) methods, also predict PE, but they are site specific and again make the fundamental assumption that the ground surface is saturated.

It is now well known that the rate of actual evaporation (AE) is only equal to the potential evaporation (PE) rate when the soil is saturated; and that the AE rate starts to decrease relative to PE as the soil desaturates at its surface. The question becomes, what is the relationship between AE and PE? Wilson (1990, 1994) showed that if the ratio AE/PE is plotted versus various soil surface parameters an interesting observation is made. Wilson (1990, 1994) plotted AE/PE versus time, water content and soil water pressure for three very different soil types (silt, sand and plastic clay) under the same atmospheric climate conditions (using a climate controlled laboratory chamber). When AE/PE is plotted versus time or soil water content, there is no correlation between the AE/PE rate for any of the soil types. When AE/PE is plotted versus soil suction (negative water pressure), all AE / PE curves for all soil types plot directly on top of each other. Figure 12-1 is a comparison of results for these cases.

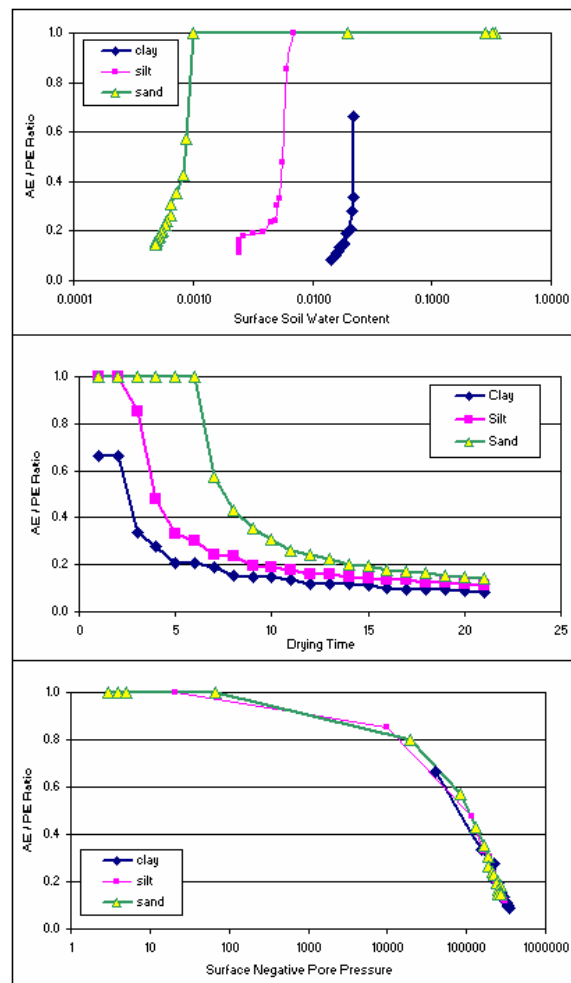


Figure 12-1 Comparison of AE to PE ratio for various soils and various criteria

This is a significant result because it shows that the rate of actual evaporation is not dependent on a measured soil parameter (i.e., water content or temperature or time of exposure to drying), but on the soil stress state (i.e., negative water pressure). Thus, in order to accurately determine AE, it is first necessary to know the water pressure, not water content, in the soil - regardless of whether the soil is sand, silt or clay.

This data is only valid for the specific climatic conditions used in the test and applied equally to all soils in the model. VADOSE/W can be used to determine similar comparisons based on any combination of soil and climate data.

Figure 12-2 shows how the vapor pressure in the soil directly controls the ability of the soil to release water to the atmosphere. As the curvature of the menisci decreases, the lower the energy state of the water molecules become, and the less likely they are to push through the tensile skin to the atmosphere.

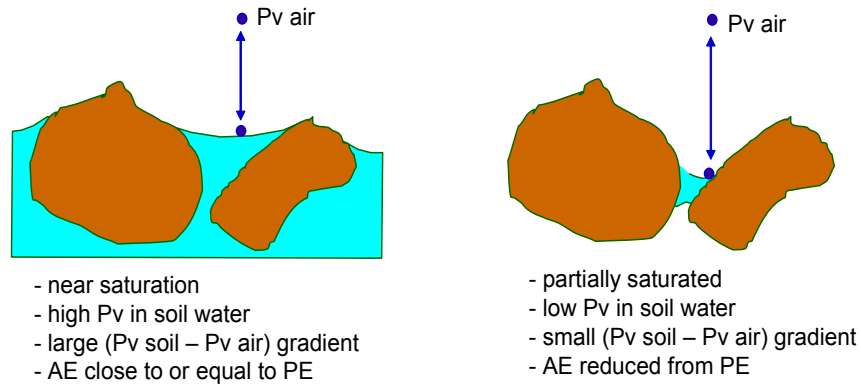


Figure 12-2 Schematic of vapor pressure gradient influence on actual evaporation

The finite element equations for coupled heat and mass flow (with vapor flow) are absolutely necessary to solve this boundary condition. The soil suction can be computed independently based on knowledge of soil temperature but in order to compute the saturated vapor pressure at the soil surface which is needed for application of the modified Dalton type evaporation rate equation, it is necessary to know the temperature at the surface and the relative humidity of the air in the soil pores at the surface.

VADOSE/W uses the Penman-Wilson (1990) method for computing AE at the soil surface such that AE is computed as a function of PE or net solar radiation for all soil moisture conditions, independent of soil type and drying history. The coupled heat and mass equations with vapor flow in VADOSE/W permit the necessary parameters at the soil surface to be available for use in the Penman-Wilson method.

VADOSE/W uses the State of the Art formulation first presented in the 1-D SoilCover model and modified for 2D analysis.

Actual evaporation

Atmospheric coupling is achieved by calculating the soil evaporative flux based on the Penman-Wilson formulation (1990) as follows:

$$AE = \frac{\Gamma Q + \nu E_a}{\nu A + \Gamma}$$

where:

- | | | |
|----------|---|--|
| AE | = | actual vertical evaporative flux (mm/day), |
| Γ | = | slope of the saturation vapor pressure versus temperature curve at the mean temperature of the air (kPa/oC), |
| Q | = | net radiant energy available at the surface (mm/day), |
| u | = | psychrometric constant, |
| Ea | = | f(u)Pa(B - A), |
| f(u) | = | function dependent on wind speed, surface roughness, and eddy diffusion, |
| | = | 0.35(1 + 0.15Ua), |
| Ua | = | wind speed (km/hr), |
| Pa | = | vapor pressure in the air above the evaporating surface (kPa), |
| B | = | inverse of the relative humidity of the air = 1/hA |

A = inverse of the relative humidity at the soil surface = 1/hr.

The Penman-Wilson formulation accounts for net radiation, wind speed, and the relative humidity of both the air and soil surface while calculating the evaporation from an unsaturated soil surface. The Penman-Wilson formulation reduces to the conventional Penman method (Penman, 1948) when the surface is saturated as the soil will have a relative humidity equal to 100% and "A" in the above equation will equal unity. The relative humidity of the soil surface is evaluated by simultaneously solving the rigorously coupled moisture and heat flow equations. The addition of the vapor flow component in VADOSE/W ensures that all moisture flow is not shut down when the hydraulic permeability decreases due to drying. Thus, vapor flow can supply water to the soil surface and the Penman-Wilson formulation can account for its removal to the atmosphere.

If the user does not have measured or estimated net surface radiation data but does have measured potential evaporation data, then the actual evaporative flux applied in the model is determined based on the current time steps potential evaporation value according to the relationship:

$$AE = PE \left(\frac{h_r - \frac{V_{p.sat.air}}{V_{p.sat.soil}} h_A}{1 - \frac{V_{p.sat.air}}{V_{p.sat.soil}} h_A} \right)$$

where:

PE = user supplied Potential Evaporation (mm/day).

Ground surface temperature

No snow present

Temperatures within the soil profile are required for the solution of the moisture and heat flow equations. The surface temperature may be estimated (for conditions where no snow pack is present) with the following relationship (Wilson, 1990):

$$T_s = T_a + \frac{1}{vf(u)}(Q - E)$$

where:

Ts = temperature at the soil surface (oC),

Ta = temperature of the air above the soil surface (oC),

v = psychrometric constant,

Q = net radiant energy (minus transpiration energy) available at the surface (mm/day), and

AE = actual vertical evaporative flux (mm/day),

This equation is basically stating that the ground temperature is increased by energy that was not consumed in the evaporation or transpiration process.

With snow pack

If there is snow cover, then snow accumulation / melt and ground temperatures are based on an energy balance approach adopted from various methods presented in the following references: SNTHERM89 model, Bras (1990), Liang, et al (1994), and Flerchinger (1989).

Full details of how VADOSE/W determines snow accumulation and melt as well as ground temperatures will not be given here as there are many physical and empirical equations and an entire book could be written on the subject. In general, the snow routine in VADOSE/W should balance user supplied precipitation data with applied snow melt during the freshet. The computed snow depths and ground temperatures are affected by many variables so exact correlation with field data may be hard to obtain. However, the intent of the snow routine in VADOSE/W is not to predict snow drifting or frost heaving. The intent is to enable year round analysis that does not force the user to neglect what happens during winter months or during snow melt when it comes to applying a temperature or water flux boundary at the surface.

When the climate routine is called the following activities occur:

The relative humidity, air temperature and precipitation are computed at the elapsed time of the day. If a sinusoidal climate distribution option is selected, the air temperature is assumed to be at its minimum value at sunrise and at its maximum value at 12:00 pm (noon). The relative humidity is assumed to be at its maximum at sunrise and its minimum at 12:00 pm. Both the air temperature and relative humidity are distributed sinusoidally between their minimum and maximum times. The daily precipitation is assumed to follow a sinusoidal distribution over the user specified hours of the day, with the peak rainfall (or snowfall) occurring at the mid point of the specified interval.

If the user selects to have climate data applied as a constant value over the day then the temperature and relative humidity are fixed for the day and the amount of precipitation will be the daily total, divided by the duration of the day, multiplied by the current solver time step. If the user selects to have climate data be averaged from day to day, then the previous days and next days average values are assumed to occur at mid day and then a function is created to look up any value based on the elapsed time since the previous mid day.

If there is precipitation and the air temperature is cold enough then the albedo of the ground surface is set to be that for fresh snow. If there is no new snow or there is old snow, the albedo is computed accordingly based on techniques in the references cited above.

The net radiation for the time of day is computed using the albedo and other climate parameters as discussed in the references. The net radiation is assumed to be at its peak value at 12:00 pm and is assumed to be zero prior to sunrise or after sunset. It is possible to have a maximum radiation value that is negative. This occurs if the incoming long and short wave radiation is less than the reflected and surface emitted radiation.

Using the data calculated above, the snow accumulation or melt routine is called.

The heat storage capacity of any existing snow pack and any fresh snow is determined.

The snow surface temperature is assumed to be at the freezing point and then an energy balance is carried out to determine if there is a net surplus of energy or an energy deficit. Ground heat flux, sensible heat flux, and latent heat flux are included in the energy balance as is the ground surface temperature at the last time step.

If the net energy balance across the snow is positive, then some snow is melted to balance the equation. If the net energy is negative, then an iterative scheme is called to compute the correct snow surface

temperature to balance the equation. If the energy balance returns zero, then the assumed ground surface temperature is correct.

Once the snow surface temperature is calculated, the snow water equivalent and snow heat storage capacities are updated.

Using the new snow parameters the snow density is updated as is the snow depth. The snow density of the main snow pack is assumed to be a function of time and is set to increase as the snow season increases or as the duration since the last snow fall increases. The maximum snow density is assumed as 500 kg per cubic meter. The snow depth is a function of the snow density and the snow water equivalent.

Once the snow layer parameters are established, the temperature beneath the snow pack is computed by using the fixed snow surface temperature and iteratively solving for a new ground surface temperature such that the ground heat flux into the bottom layer of the snow pack will balance with the heat storage capacity of the snow pack.

12.2 Actual transpiration

Vegetation plays a significant and dynamic role in the overall evapotranspiration process (Saxton, 1982). VADOSE/W incorporates these affects using a nodal vegetative uptake source term that is combined with a surface energy term based on canopy cover (Tratch, 1996). The amount of actual nodal root uptake depends also on root depth and density, and water stress (negative pore water pressure).

Lack of available plant water and/or high evaporative demands will cause most plants to biologically react by closing stoma, reducing transpiration, and reducing metabolic reactions (Saxton, 1982). Under continued and increasing stress the plant will reach its wilting point. The wilting point results in leaf drop and tissue death (Saxton, 1982). In VADOSE/W the user must implement a Plant Moisture Limiting function which determines the percentage decrease in the plants ability to draw water as the negative water pressure increases in the unsaturated ground.

A typical Plant Moisture Limiting function is given in Figure 12-3. In this function the plant reaches a wilting point at a negative pore water pressure of about -100 kPa and is completely unable to draw water if the pressure reaches -1500 kPa.

Figure 12-4 illustrates a typical leaf area index function. The leaf area index is used by VADOSE/ w to reduce the amount of net radiation intercepting the soil surface, which in turn reduces the computed actual evaporation. In other words, the leaf area index controls how the energy at the surface is partitioned between that available for direct evaporation from the soil and that which is available to the plants in their attempt to transpire water.

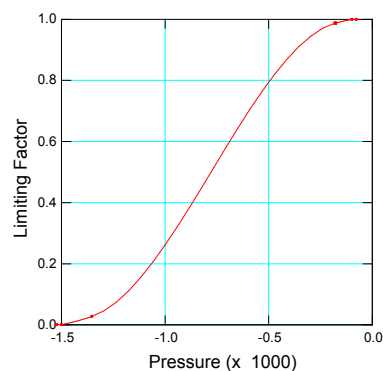


Figure 12-3 Plant moisture limiting factor function

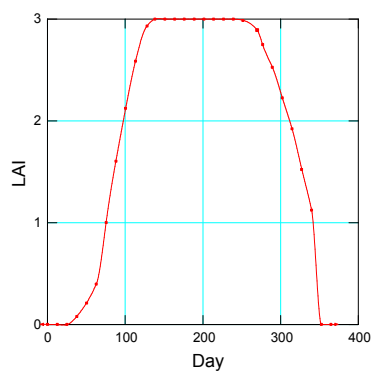


Figure 12-4 Typical leaf area index function for excellent grass coverage

You are required to enter the anticipated root depth profile for the duration of the growing season. This specifies the depth over which the vegetative cover will extract water from the soil profile. It is important to note that your root depth function can not exceed the total thickness of the cover nodes you included in your mesh. This function should be based on site specific knowledge of plant species growth patterns as well as knowledge of the climate data applied in the model. An example of a root depth function is illustrated in Figure 12-5.

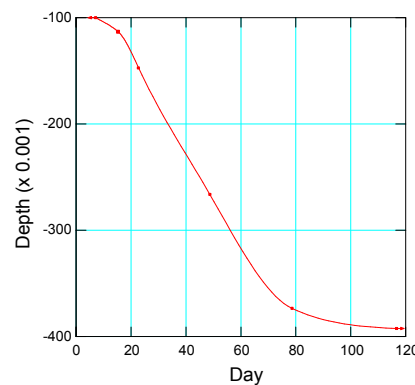


Figure 12-5 User specified root depth versus growing season function

Once all the functions are defined and applied to a climate surface node, they are used in the following way.

The Actual Evaporation (AE) is computed as described above. This value is then modified by the equation below such that a portion of the available energy is to be partitioned to the plants.

$$AE = AE * \left\{ 1 - (-0.21 + 0.7 * \sqrt{LAI}) \right\}$$

where:

LAI = the user specified leaf area index for the day in question.

The modified evaporation value is set equal to zero if the LAI is greater than 2.7 and is set to its full value if the LAI is less than 0.1 (based on Tratch, 1996).

Next it is necessary to determine the potential transpiration (PT). This value is related to the potential evaporation and will be equal to the potential evaporation value if the LAI is greater than 2.7. The PT is calculated using:

$$PT = PE * (-0.21 + 0.7 * \sqrt{LAI})$$

where:

PE = the potential evaporation (mm/day).

The PT value is that energy that is now available to the plant. If the soil is saturated, the full amount of this energy will be applied to the roots according to the root depth and root shape functions. If the soil is partially saturated, then the actual transpiration value is further reduced according to the plant moisture limiting function entered by the user as follows:

$$AT = PRU * PML$$

where:

AT = the actual nodal transpiration,

$$PRU = \frac{2PT}{R_T} \left(1 - \frac{R_n}{R_T} \right) A_n$$

RT	=	total thickness of root zone,
Rn	=	the depth to the node in question,
An	=	the nodal contributing area of the node in question,
PML	=	user entered plant moisture limiting function value at the current nodal soil negative pore water pressure.

In VADOSE/W any nodal root uptake beneath a cover node is recorded as actual transpiration at the surface node, EVEN THOUGH the actual water leaving the mesh is applied at the nodes beneath the surface node. This is done for bookkeeping convenience.

One final point that should be made is the sum of any actual evaporation and any actual transpiration can never be greater than the potential evapotranspiration at the surface node. This criterion meets the conservation of energy requirement.

12.3 Infiltration and runoff

On days where there is no precipitation, then it is likely that an evaporative flux will be computed for all surface climate nodes based on one of the methods described above. If there is precipitation, then several possible scenarios exist.

If the precipitation over the next time step to be solved is less than the anticipated actual evaporation over the next time step, then the applied surface flux boundary condition will be equal to the precipitation value minus the actual evaporation and a negative flux will be applied will be applied to the node.

If the precipitation minus any actual evaporation is a positive value, then a positive (infiltrative) surface flux will be applied as a boundary condition.

If the positive flux boundary condition is such that the solved pressures at the surface become positive, then the solution is allowed to converge to this positive pressure condition and subsequently the surface node is changed to a head boundary condition and the time step is REPEATED. After it has converged with its new head boundary condition, the solver checks to see if the computed flux is more or less than that which was applied when the original flux boundary was used. If the nodal flux is less than the original amount, then runoff is calculated as:

Runoff = Precipitation - AE - Infiltration.

Runoff should not be a negative value UNLESS previously runoff surface water is stored down slope and reapplied as infiltration on a subsequent time step. The reapplied surface water is negative runoff.

Runoff can be handled in two ways, depending on the user preference set in the Analysis Settings. One option is to ignore the volume of water that seeps out or does not infiltrate. In this case, the water leaving the system is not available for re-infiltration. NOTE: runoff will not be reapplied if the analysis type is Axisymmetric. The user can only choose to reapply runoff if the analysis type is set to be 2-dimensional.

The second option is to have the volume of generated surface water accumulated and applied down slope in any troughs or depressions where it is ponded and applied as infiltration on subsequent time steps. If water is ponded, the solver will determine, based on the volume of water and the volume of the depression it is sitting in, how much head to apply as a boundary condition on the next time step.

There are several assumptions inherent in the surface water runoff routine that the user should be aware of.

Water that seeps out of the ground or that does not infiltrate is assumed to flow overland to the lowest point on the mesh where it is available for re-infiltration. The duration of the overland flow and the depth of flow are ignored.

If the slope of the ground at the left or right end extents of the mesh is downward, no ponding can occur. Water will be assumed to flow out of the extents of the mesh. Ponding will occur at the mesh extents if they are flat or inclined upwards as one moves to the extents of the mesh. The solver will calculate the volume of any ponds and determine the elevation that water will fill the ponds to. This elevation is the subsequent head boundary value. If a pond overflows, the excess water will be applied as a source at the next node down slope from the overflow point.

Water will not pond on a flat mound located within the bounds of the mesh. Any water that "runs off" at these nodes will be applied as a source flux at the top node of any adjacent slope during the next time step.

The following figures illustrate these rules (the head of the arrow indicates the point at which the surface water is reapplied as a source or ponded head value):

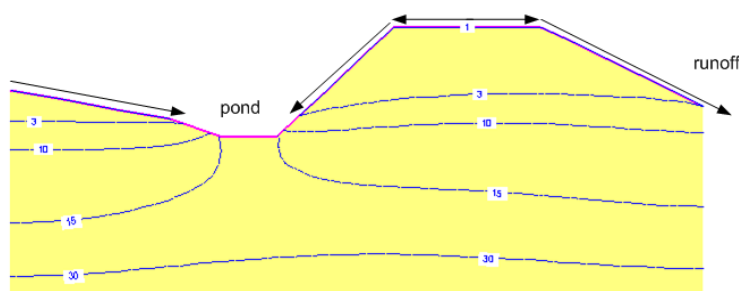


Figure 12-6 No ponding on right slope. Ponding only in center trough.

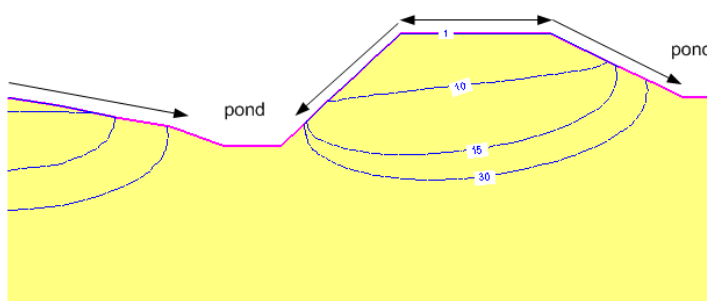


Figure 12-7 Ponding on right slope - serves to recharge lower pond over time.

12.4 Freeze - thaw

Ground freezing is incorporated into VADOSE/W in a manner similar to that in TEMP/W with the exception being how the material properties are defined and how the unfrozen water content function is obtained. VADOSE/W does not require you to enter an unfrozen water content versus temperature function. Instead, the necessary function is obtained using the required volumetric water content versus

pressure curve (water storage function) and converting pressures to negative temperatures using the Clausius Clapeyron equation for phase equilibrium.

VADOSE/W uses the concept of "apparent" specific heat to incorporate the latent heat of phase change into the heat balance equation. The capacity to store heat is composed of two parts. The first part is the volumetric heat capacity of the material (either frozen or unfrozen) and the second part is the latent heat associated with the phase change. In equation form:

$$\lambda = c + L \frac{\partial \Theta_u}{\partial T}$$

where:

c	=	volumetric heat capacity (material property),
L	=	latent heat of water,
θ	=	total unfrozen volumetric water content, and
T	=	temperature.

The term $L \frac{\partial \Theta_u}{\partial T}$ represents the rate of change of the latent heat added to the heat storage component in the heat balance equation.

Assumptions in the freezing routine

Detailed ground freezing analysis where heat and mass flow is coupled is very complex and the theory is not fully understood. VADOSE/W is not intended to be a fully rigorous ground freezing program and as such, certain assumptions are made to facilitate numerical stability and execution time during the solving process. VADOSE/W will give relatively good estimates of the depth of frost penetration if accurate material properties are used. The following items discuss some of the assumptions the user should be aware of before interpreting ground freezing results.

convective heat transfer: Convective heat transfer is included.

cryogenic suction: As water turns to ice the negative pressures (or suction) in the ground can be quite significant which can lead to moisture redistribution towards a freezing front. This is a primary cause of frost heave in fine grained soils. VADOSE/W does not allow negative pressures to increase in frozen ground, however, it does approximate (based on temperature and the Clausius Clapeyron equation) what these pressures would be in order to compute a reduced hydraulic conductivity as ice replaces liquid water in frozen pores.

frost heave: VADOSE/W limits the amount of ice that can exist in soil pores to be equal to the porosity of the soil. In other words, frost heave can not exist.

snow melt infiltration: Snow depth is accumulated during the winter period and melted during the spring. During snow accumulation, any user data precipitation is stored and only released as snow melt. As it is released, it can either infiltrate the soil or runoff the surface. VADOSE/W will check to the soil temperature and ice content in order to determine the hydraulic conductivity. If the conductivity is high enough to allow snow melt to infiltrate, then that will occur. If ice is restricting infiltration at depth, then the surface water pressures will build up and become positive which will automatically result in a seepage face boundary condition and potential runoff. In other words, infiltration is based on the hydraulic conductivity of the ground and the storage potential.

atmospheric coupling: If there is a snow cover, actual evaporation from the ground surface is shut down. Any precipitation is applied to calculating the snow depth and is later applied to the ground as snow melt. The ground surface temperature calculation across the snow pack is quite complex and the adopted approach is described in the Ground Surface Temperatures topic

sublimation: Sublimation is included in the formulation but is not output as a result variable. It can manually be computed as Precipitation – evaporation – transpiration – runoff – change in storage – boundary flow – water balance error.

12.5 General flow law

VADOSE/W is formulated on the basis that the flow of water, heat, vapour and gas through both saturated and unsaturated soil follows an appropriate form of a Darcy type flow law which states that:

$$q = ki$$

where:

q = the specific flux,
 k = the conductivity, and
 i = the gradient of potential.

Darcy's Law for water flow was originally derived for saturated soil, but later research has shown that it can also be applied to flow through unsaturated soil (see Richards, 1931 and Childs & Collins-George, 1950). The only difference is that under conditions of unsaturated flow the hydraulic conductivity is no longer a constant but varies with changes in water content and indirectly varies with changes in pore-water pressure. In the case of heat flow, the thermal conductivity is a function of soil water, air and ice content; while for vapour and gas flow the coefficient of diffusion is a function of degree of saturation.

Darcy's Law is often written as:

$$v = ki$$

where:

v = the Darcian velocity.

Note that the actual average velocity at which water moves through the soil is the linear velocity which is equal to Darcian velocity divided by the porosity of the soil. In unsaturated soil, it is equal to Darcian velocity divided by the volumetric water content of the soil. VADOSE/W computes and presents only the Darcian velocity.

12.6 Partial differential water and heat flow equations

The general governing differential equation for two-dimensional seepage can be expressed as:

Equation 12-1

$$\begin{aligned} & \frac{1}{\rho} \frac{\partial}{\partial x} \left(D_v \frac{\partial P_v}{\partial x} \right) + \frac{1}{\rho} \frac{\partial}{\partial y} \left(D_v \frac{\partial P_v}{\partial y} \right) + \\ & \frac{\partial}{\partial x} \left(k_x \frac{\partial \left(\frac{P}{\rho g} + y \right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial \left(\frac{P}{\rho g} + y \right)}{\partial y} \right) \\ & + Q = \lambda \frac{\partial P}{\partial t} \end{aligned}$$

where:

- P = pressure,
 P_v = vapor pressure of soil moisture,
 m_v = slope of the volumetric water content function,
 K_x = hydraulic conductivity in the x-direction,
 K_y = hydraulic conductivity in the y-direction,
 Q = applied boundary flux,
 D_v = vapor diffusion coefficient as described by Wilson (1990),
 y = elevation head,
 ρ = density of water,
 g = acceleration due to gravity, and
 t = time.

For heat transfer:

Equation 12-2

$$\begin{aligned} & L_v \frac{\partial}{\partial x} \left(D_v \frac{\partial P_v}{\partial x} \right) + L_v \frac{\partial}{\partial y} \left(D_v \frac{\partial P_v}{\partial y} \right) + \\ & \frac{\partial}{\partial x} \left(k_{tx} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{ty} \frac{\partial T}{\partial y} \right) + Q_t \\ & + \rho c V_x \frac{\partial T}{\partial x} + \rho c V_y \frac{\partial T}{\partial y} = \lambda_t \frac{\partial T}{\partial t} \end{aligned}$$

where:

- ρc = volumetric specific heat value,
 K_x = thermal conductivity in the x-direction,
 K_y = thermal conductivity in the y-direction and assumed equal to K_{tx} ,
 V_{xy} = the Darcy water velocity in x and y directions,
 Q_t = applied thermal boundary flux, and
 L_v = latent heat of vaporization.

The equations state that the difference between the flow (liquid or vapor flux) entering and leaving an elemental volume at a point in time is equal to the change in the volumetric water content or heat capacity. More fundamentally, it states that the sum of the rates of change of flows in the x and y directions plus the external applied flux is equal to the rate of change of the volumetric water or heat contents with respect to time.

The mass transfer equation can be derived directly from the Richards equation for transient flow in unsaturated soils with adaptations for vapor flow added by Wilson (1990) with a modification proposed by Milly (1982). The driving force for Darcian liquid flow is total head but the equations have been re-written as functions of pressure so that the heat and mass equations can be fully coupled. The heat transfer equation is a standard Fourier equation for conductive heat transfer with modifications for the inclusion of vapor transfer and convective heat transfer due to flowing water.

Under steady-state conditions, the flux entering and leaving an elemental volume is the same at all times. The last term of the equation consequently vanishes and the equation for mass transfer, neglecting vapor flow for clarity, reduces to:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial \left(\frac{P}{\rho g} + y \right)}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial \left(\frac{P}{\rho g} + y \right)}{\partial y} \right) + Q = 0$$

Similar dropping of terms can be carried out for the heat transfer equation under steady state conditions. VADOSE/W does include the vapor flux component in its steady state formulation which is used to determine initial conditions for the subsequent transient climate coupled analysis.

12.7 Coupling heat and mass equations

Examination of the governing heat and mass transfer equations reveals that there are three unknown parameters, namely pressure (P), temperature (T), and vapor pressure (Pv). In order to solve the equations, a third relationship between these parameter is necessary.

Edlefsen and Anderson (1943) presented the relationship:

$$P_v = P_{vs} (e^{\frac{-P \cdot w}{R \cdot T}}) = P_{vs} h_{rair}$$

which Joshi (1993) reformed as:

$$\nabla P_v = d_1 \nabla(-P) + d_2 \nabla T$$

where:

P_{vs}	=	saturated vapor pressure of pure free water,
w	=	molecular mass of water vapor,
R	=	universal gas constant,
T	=	temperature (K) for the term in the exponent, and
h_{rair}	=	relative humidity of air.

12.8 Gas transfer analysis

VADOSE/W solves the partial differential equations describing oxygen or radon gas transfer that are described in the subsequent sections. The formulations do not account for gas transfer due to advection in the air phase. The inherent assumption is that the air phase is always at atmospheric pressure; consequently, gas movement through the soil is only by diffusion in the air phase.

The units of concentration and flux differ depending on the type of gas transfer analysis. Oxygen is tracked by its mass so it has concentration units of mass per volume and flux units of mass per time. Radon is tracked by its activity level so it has concentration units of Becquerel's per volume or Becquerel's per time. In the Contour program, all gas fluxes are referred to as mass values for convenience. The user should be aware that radon mass flux values are actually units of activity.

Oxygen transfer

VADOSE/W is formulated to solve the governing equation for oxygen transport through reactive variably saturated soils (e.g. tailings). The governing differential equation is a modified form of Fick's second law given by (written for a one-dimensional domain; Mbonimpa et al. 2003):

$$\frac{\partial}{\partial t}(\theta_{eq}C) = \frac{\partial}{\partial y}\left(D_{eff}\frac{\partial C}{\partial y}\right) - K_rC$$

where:

C	=	the concentration of oxygen in pore air (Mass/Volume),
θ_{eq}	=	the equivalent diffusion porosity defined $\theta_a + H\theta_w$ (Aubertin et al., 2000),
θ_a	=	the volumetric air content,
θ_w	=	the volumetric water content,
H	=	dimensionless form of Henry's equilibrium constant (0.028 at 25 degrees Celsius),
D_{eff}	=	the effective diffusion coefficient (L ² /time), and
K_r	=	effective reaction rate coefficient (1/time)

The dimensionless form of Henry's equilibrium constant H is equal to the ratio C_w/C_a , where C_a is the O₂ concentration in the air phase and C_w is the O₂ concentration in the dissolved phase. The equilibrium constant varies linearly with temperature from the zero origin to the concentration of oxygen in water adjacent to oxygen saturated air at a given temperature and atmospheric pressure (i.e. solubility). The concentration of oxygen in water at the reference temperature T_1 of 25 degrees Celsius is approximately 8.32 mg oxygen per liter water for the case where the air is saturated with oxygen (approximately 20.9% oxygen by mass). The ratio $H = C_w/C_a$ for this condition is denoted as S_1 . The ratio $H = S_2$ at different a different temperature (T_2) can be computed using the Clausius-Clapeyron phase equilibrium relationship as follows:

$$\log \frac{S_1}{S_2} = \frac{\Delta H}{2.303R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

where:

ΔH	=	enthalpy of dissolution of gas (= -3500 cal for oxygen),
------------	---	--

- R = universal gas constant,
 $T_{1,2}$ = reference and unknown temperatures respectively (K), and
 $S_{1,2}$ = reference and unknown oxygen concentration in water respectively (mg/L).

The effective diffusion coefficient (D_{eff}) is obtained internally by the solver using the method proposed by Colin and Rasmuson (1988). Their model accounts for the diffusion of oxygen through the air phase as well as through the water phase and is computed as follows:

$$D_{eff} = D_a (1-S)^2 [n(1-S)]^{2Xa} + HD_w S^2 (nS)^{2Xw}$$

where:

- D_a = the diffusion coefficient of oxygen in air (1.8e-5 m²/s),
 S = the degree of saturation,
 n = the soil porosity (volume of voids / volume total),
 X_a = an empirical parameter,
 D_w = the diffusion coefficient of oxygen in water (2.2e-9 m²/s), and
 X_w = an empirical parameter.

The two empirical parameters in the above equation are determined by the an algorithm that iteratively solves the following set of equations for the two unknowns:

$$[n(1-S)]^{2Xa} + [1-n(1-S)]^{Xa} = 1$$

$$(nS)^{2Xw} + (1-nS)^{Xw} = 1$$

The effective reaction rate coefficient K_r is the user input that characterizes consumption rates due to oxidation. The value of K_r is a highly non-linear function of water content; however, some studies indicate the coefficient becomes nearly constant over a relatively large range of saturations (Gosselin et al. 2011). There are relatively few studies to confirm the generality of this statement and it may therefore prove more general to input the coefficient as a splined data point function of volumetric water content; however, the current implementation assumes characterization of the consumption rate by a single constant.

Radon transfer

VADOSE/W is formulated to solve the governing equation for radon transport through variably saturated soils based on a method proposed by Claus E. Andersen (Riso, 2000). The governing differential equation used in VADOSE/W incorporates the effects of radon mass loss from the air phase into the water phase due to dissolution as well as decay and is written for two dimensions as:

$$\frac{\partial (\Theta_{air} + \Theta_w L) C}{\partial t} = D_{eff} \frac{\partial^2 C}{\partial x^2} + D_{eff} \frac{\partial^2 C}{\partial y^2} - \lambda \Theta_{air} C - \lambda L \Theta_w C$$

where:

- L = Ostwald solubility coefficient (Bq gas/ Liter water) based on the temperature, and
 λ = the decay constant for Radon (3.825 days = 1.0479e-2 years).

Note that some of the units are specified above. This is for reference only as the user is not required to enter these parameters. The concentration units will depend on the user input set of units (i.e., metric or imperial). Unlike for oxygen concentration values, the concentration of Radon gas is specified in units of Bequerels per volume (Bq/m3 for example).

The Ostwald solubility, L is a ratio of the volume of gas dissolved versus the volume of water. The Ostwald solubility coefficient is a function of temperature that ranges between values of 0.5 at the freezing point to 0.1 at 70 degrees C (after Clever, 1985). A curve fit equation representing the decay of this function is used by VADOSE/W to determine the correct coefficient for any given temperature.

The effective diffusion coefficient for Radon is computed internally by the solver using the method proposed by Rogers and Nielson (1991). The model accounts for the diffusion of radon through the air phase in a variably saturated soil and is computed as follows:

$$D_{eff} = D_a n \exp^{(-6nS - 6S^{14n})}$$

12.9 Finite element water flow equations

Applying the Galerkin method of weighed residual to the governing differential equation the finite element for two-dimensional seepage equation with vapour coupling can be derived as:

$$\begin{aligned} & \int_v ([B]^T [C] [B]) dv \{P\} + \int_v ([B]^T [D_2] [B]) dv \{T\} + \\ & \int_v ([B]^T [K] [B]) dv \{y\} + \int_v (\lambda \langle N \rangle^T \langle N \rangle) dv \{P\}, t \\ & = q \int_A (\langle N \rangle^T) dA \end{aligned}$$

where:

- $[B]$ = gradient matrix,
 $[C]$ = element stiffness matrix = $[K/\rho g + D1]$,
 $D1$ = $Dvd1 / \rho$ □
 $[D2]$ = $[Dvd2 / \rho]$ □
 $\{P\}$ = vector of nodal pressures,
 $\{y\}$ = vector of elevation heads,
 $[K]$ = element hydraulic conductivity matrix,
 λ = $m_w \lambda_w$,
 $\langle N \rangle^T \langle N \rangle$ = $[M]$, the mass matrix,
 $\{P\}, t$ = change in pressure with time,
 q = unit flux across the side of an element, and
 $\langle N \rangle$ = vector of interpolating function.

For a VADOSE/W two-dimensional analysis the thickness of the element is considered to be constant over the entire element. The finite element equation can consequently be written as:

$$\begin{aligned} & t \int_A ([B]^T [C] [B]) dA \{P\} + t \int_A ([B]^T [D_2] [B]) dA \{T\} + \\ & t \int_A ([B]^T [K] [B]) dA \{y\} + t \int_A (\lambda \langle N \rangle^T \langle N \rangle) dA \{P\}, t \\ & = qt \int_L (\langle N \rangle^T) dL \end{aligned}$$

where t is the element thickness.

When t is a constant the integral over the volume becomes the integral over the area and the integral over the area becomes the integral over the length from corner node to corner node.

In an axisymmetric analysis the equivalent element thickness is the circumferential distance about the symmetric axis. The complete circumferential distance is 2π radian times R . Since VADOSE/W is formulated for one radian, the equivalent thickness is R . The finite element equation for the axisymmetric case is:

$$\begin{aligned} & \int_A ([B]^T [C] [B]R) dA \{P\} + \int_A ([B]^T [D_2] [B]R) dA \{T\} \\ & + \int_A ([B]^T [K] [B]R) dA \{y\} + \int_A (\lambda \langle N \rangle^T \langle N \rangle R) dA \{P\}, t \\ & = q \int_L (\langle N \rangle^T R) dL \end{aligned}$$

The radial distance R is not a constant as is the thickness t for a two-dimensional analysis within an element; consequently, R is a variable in the integration.

In abbreviated form, the finite element equation for mass transfer is:

$$[Kw] \{P\} + [Kwt] \{T\} + [M] \{P\}, t = \{Q\}$$

The corresponding two-dimensional heat transfer finite element equation can be written as:

$$\begin{aligned} & t \int_A ([B]^T [C_t] [B]) dA \{T\} + t \int_A ([B]^T [L_v D_1] [B]) dA \{P\} \\ & + t \int_A (\lambda_t \langle N \rangle^T \langle N \rangle) dA \{T\}, t = qt \int_L (\langle N \rangle^T) dL \end{aligned}$$

where:

- $[Ct]$ = element thermal stiffness matrix = $[Kt + LvD2]$,
- $\{T\}$ = vector of nodal temperatures,
- $\{T\}, t$ = change in temperature with time, and
- qt = unit heat flux across the side of an element.

In abbreviated form, the finite element equation for heat transfer is:

$$[Kt] \{T\} + [Ktw] \{P\} + [Mt] \{T\}, t = \{Qt\}$$

Finally, the combined coupled equations can be written in abbreviated form as:

$$\begin{bmatrix} \frac{K_w}{K_{tw}} & \frac{K_{wt}}{K_t} \end{bmatrix} \left\{ \frac{P}{T} \right\} + \begin{bmatrix} M & 0 \\ 0 & M_t \end{bmatrix} \left\{ \frac{P_{time}}{T_{time}} \right\} = \left\{ \frac{Q}{Q_t} \right\}$$

12.10 Temporal integration

The finite element solution for a transient analysis is a function of time as indicated by the $\{P\}_t$ term in the finite element equation. The time integration can be performed by a finite difference approximation scheme.

Writing the finite element mass transfer equation (leaving vapor flow out for the moment) in terms of finite differences leads to the following equation (Segerlind, 1984):

$$\left(\omega \Delta t \left[\frac{K}{\rho g} \right] + \left[\frac{M}{\rho g} \right] \right) \{P_1\} = \Delta t ((1-\omega)\{Q_0\} + \omega\{Q_1\}) + \left(\left[\frac{M}{\rho g} \right] - (1-\omega)\Delta t \left[\frac{K}{\rho g} \right] \right) \{P_0\} - [K]\{Y\}\Delta t$$

where:

- Δt = time increment,
- ω = a ratio between 0 and 1,
- $\{P_1\}$ = head at end of time increment,
- $\{P_0\}$ = head at start of time increment,
- $\{Q_1\}$ = nodal flux at end of time increment,
- $\{Q_0\}$ = nodal flux at start of time increment,
- $[K]$ = element characteristic matrix, and
- $[M]$ = element mass matrix.

VADOSE/W uses the Backward Difference Method, a method that sets ω to 1.0, the finite element equation is then simplified to:

Equation 12-3

$$\left(\Delta t \left[\frac{K}{\rho g} \right] + \left[\frac{M}{\rho g} \right] \right) \{P_1\} + \Delta t [D_2] \{T_1\} = \Delta t Q_1 + \left[\frac{M}{\rho g} \right] \{P_0\} - [K]\{Y\}\Delta t$$

The heat transfer transient finite equation for Θ equal to 1.0 with the vapor flow term added but the convective heat transfer term omitted for clarity is:

$$(\Delta t [K_t] + [M_t]) \{T_1\} + \Delta t [L_v D_1] \{P_1\} = \Delta t Q_1 + [M_t] \{T_0\}$$

As indicated by Equation 12-3, in order to solve for the new head at the end of the time increment, it is necessary to know the head at the start of the increment. Stated in general terms, the initial conditions must be known in order to perform a transient analysis.

12.11 Numerical integration

VADOSE/W uses Gaussian numerical integration to evaluate the element characteristic matrix $[K]$ and the mass matrix $[M]$. The integrals are evaluated by sampling the element properties at specifically defined points and then summed together for the entire element.

Using the characteristic matrix $[K]$ as an example, the following integral

$$[K] = \tau \int_A ([B]^T [C] [B]) dA$$

can be replaced by:

$$[K] = \tau \sum_{j=1}^n [B_j]^T [C_j] \det|J_j| W_{1j} W_{2j}$$

where:

- j = an integration point,
- n = the number of integration points,
- $[C_j]$ = the element hydraulic conductivity matrix at the integration point,
- $[B_j]$ = the element matrix at the integration point,
- $\det|J_j|$ = the determinant of the Jacobian matrix, and
- $W_{1j} W_{2j}$ = a weighting factors.

The number of sample (integration) points required in an element depends on the number of nodes and the shape of the elements. The tables below contain the number and location of sampling points that are used by SEEP/W.

Table 12-1 Sample point locations and weightings for four point quadrilateral element

Point	r	s	w1	w2
1	+0.57735	+0.57735	1.0	1.0
2	-0.57735	+0.57735	1.0	1.0
3	-0.57735	-0.57735	1.0	1.0
4	+0.57735	-0.57735	1.0	1.0

Table 12-2 Sample point locations and weightings for nine point quadrilateral elements

Point	r	s	w1	w2
1	+0.77459	+0.77459	5/9	5/9

2	-0.77459	+0.77459	5/9	5/9
3	-0.77459	-0.77459	5/9	5/9
4	+0.77459	-0.77459	5/9	5/9
5	0.00000	+0.77459	8/9	5/9
6	-0.77459	0.00000	5/9	8/9
7	0.00000	-0.77459	8/9	5/9
8	+0.77459	0.00000	5/9	8/9
9	0.00000	0.00000	8/9	8/9

Table 12-3 Sample point locations and weighting for one point triangular element

Point	r	s	w1	w2
1	0.33333	0.33333	1.0	0.5

Table 12-4 Sample point locations and weightings for three point triangular element

Point	r	s	w1	w2
1	0.16666	0.16666	1/3	1/2
2	0.66666	0.16666	1/3	1/2
3	0.16666	0.66666	1/3	1/2

One-point integration for a triangular element results in a constant gradient throughout the element. The number of integration points is denoted as the integration order. 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 12-5 gives the acceptable integration orders.

Table 12-5 Acceptable element integration orders

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

It is also acceptable to use four-point integration for quadrilateral elements that have secondary nodes. This is called a reduced integration order (see Bathe, 1982, p. 282). Acceptable results can be obtained with reduced integration. For example, reduced integration is useful in saturated zones where the hydraulic gradient is low and the hydraulic conductivity is constant. Selective use of reduced integration can greatly reduce the required number of computations.

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 in an unsaturated zone where the hydraulic conductivity varies sharply with changes in pore-water pressure. 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 one point integration in triangular elements with secondary nodes is not acceptable.

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 unsaturated zone with hydraulic conductivity varies sharply within an element, it is best to use quadrilateral elements with secondary nodes together with nine-point integration.

12.12 Hydraulic conductivity matrix

The general form of the VADOSE/W element conductivity matrix is:

$$[C] = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

where:

$$\begin{aligned} C_{11} &= k_x \cos^2 \alpha + k_y \sin^2 \alpha \\ C_{22} &= k_x \sin^2 \alpha + k_y \cos^2 \alpha \\ C_{12} &= k_x \sin \alpha \cos \alpha + k_y \sin \alpha \cos \alpha \\ C_{21} &= C_{12} \end{aligned}$$

The parameters k_x , k_y and α are defined in Figure 12-8.

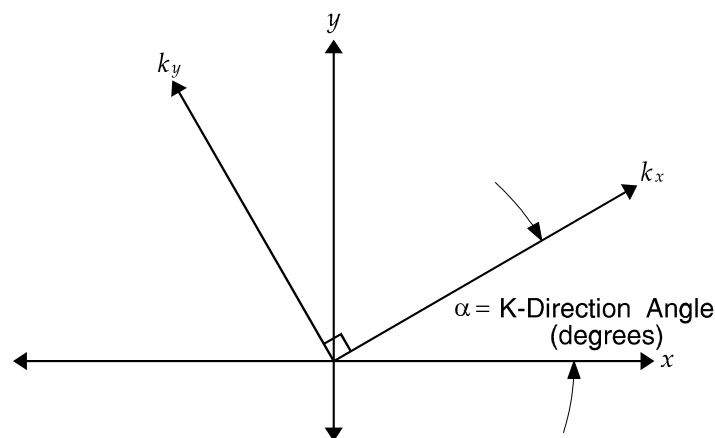


Figure 12-8 Definition of hydraulic conductivity matrix parameters

When α is zero, $[C]$ is reduced to:

$$[C] = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix}$$

The parametric k_x is always determined from the hydraulic conductivity function. Parameter k_y is then computed as k_x multiplied by k_{Ratio} . In equation form,

$$k_y = k_x \times k_{Ratio}$$

12.13 Mass matrix

As first presented above, the element mass (or storage) matrix for a two-dimensional analysis is defined as:

$$[M] = \tau \int_A (\lambda < N >^T < N >) dA$$

Similar to the element characteristic matrix, the mass matrix is also evaluated by numerical integration as shown below:

$$[M] = \tau \sum_{j=1}^n \lambda_j < N >^T < N > \det |J_j| W_{1j} W_{2j}$$

When the mass matrix is evaluated, VADOSE/W uses a lumped formulation to lump the off-diagonal coefficients in the mass matrix to the diagonal terms. For higher order elements, diagonal scaling is also used. The lumped formulation, together with diagonal scaling, is adopted to improve stability in transient analysis. The detail of the lumped formulation is given by Segerlind, 1984, pp. 178-182.

To evaluate λ , VADOSE/W obtains a m_w value from the volumetric water content function (the storage function) for each integration point in one of two ways. In most cases it computes m_w from the slope of a straight line between the old and new pore-water pressures at a Gauss point, as illustrated in Figure 12-9. The slope of this straight line can be viewed as the average rate of change during one increment of time. This is considered to be a more realistic value than taking the derivative of the function at a specific point. An exception to this procedure is when the old and new pore-water pressures are nearly identical. In this case, SEEP/W computes m_w by calculating the slope of the function at the average of the old and new pore-water pressures.

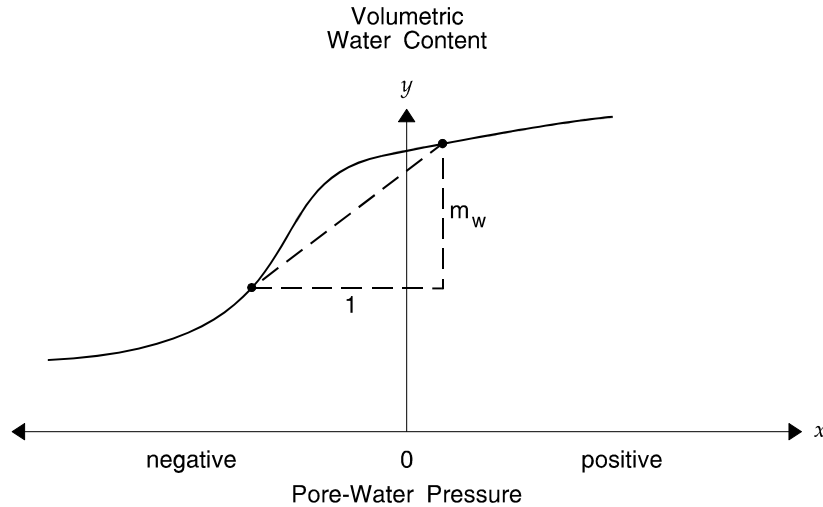


Figure 12-9 Computation of storage term, m_w

12.14 Flux boundary vector

The nodal flux boundary vector $\{Q\}$ for a two-dimensional analysis is defined as:

$$\{Q\} = q\tau \int_L \left(\langle N \rangle^T \right) dL$$

or for an axisymmetric analysis as:

$$\{Q\} = q \int_L \left(\langle N \rangle^T R \right) dL$$

and for a plan view analysis as:

$$\{Q\} = q \int_A \left(\langle N \rangle^T \langle N \rangle \right) dA$$

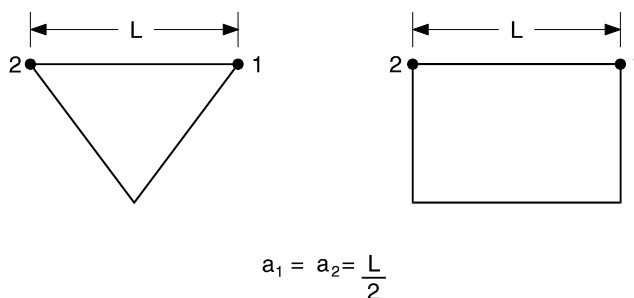
where:

- q = the unit flux across the side of an element,
- τ = the element thickness,
- A = the area of the element in plan view, and
- R = the radial distance from the symmetric axis to the element corner nodes.

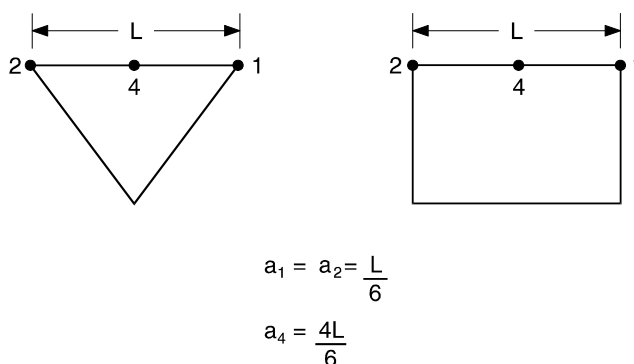
Solutions to the integrals are dependent on the analysis type and on the presence of secondary nodes. For two-dimensional (i.e., vertical section) and axisymmetric analyses, the integrals are solved by closed form solutions as illustrated in Figure 12-10 and Figure 12-11. However, for plan view analysis, the contributing area of a node is computed by numerical integration in the same way as forming the mass matrix. In other words, the contributing area per node in a plan view depends on the partial contributing areas of all elements surrounding that node, and this must be computed using the Gauss region area integration scheme for each element, not standard shape relationships as discussed here.

Two types of flux boundaries may be specified in VADOSE/W namely: a nodal flux boundary (Q) and a unit flux boundary (q). A nodal flux boundary (Q) can be specified directly on the boundary nodes. A unit flux boundary (q) must be specified along the boundary edges of the elements, except for a plan view analysis where the unit flux is applied per unit area on the plan view. When you set up a boundary condition, you identify the edges of the elements across which a q boundary should be applied. Based on this specific element edge information, the solver performs the integration and determines the applied flux Q at the nodes. The solver needs Q, not q, to solve the finite element equations.

For two-dimensional (i.e., vertical section) and axisymmetric analyses, the nodal flux Q computed by the solver is dependent on the specified element thickness. For plan view analysis, since the surface area is independent of the element thickness, the nodal flux Q is also independent of the element thickness.

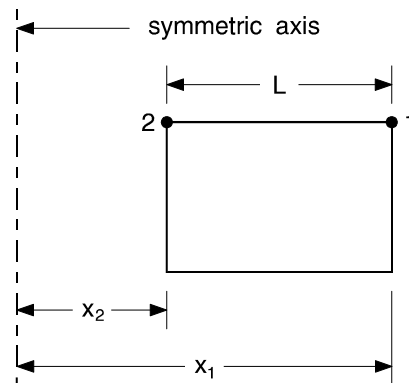


(a) No intermediate node



(b) With an intermediate node

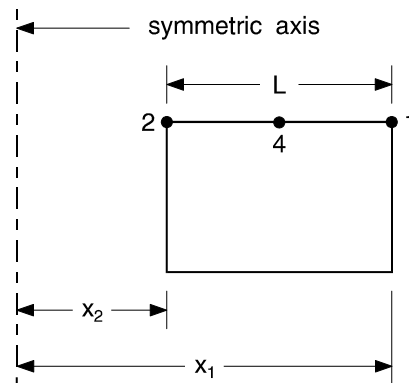
Figure 12-10 Contributing area for section view elements with unit thickness



$$a_2 = \frac{L}{6} (2x_2 + x_1)$$

$$a_1 = \frac{L}{6} (x_2 + 2x_1)$$

(a) No intermediate node



$$a_2 = \frac{L}{6} (x_2)$$

$$a_4 = \frac{2L}{6} (x_2 + x_1)$$

$$a_1 = \frac{L}{6} (x_1)$$

(b) With an intermediate node

Figure 12-11 Contributing area for axisymmetric elements over unit Radian thickness

13 Appendix A: Interpolating Functions

13.1 Coordinate systems

The global coordinate system used in the formulation of VADOSE/W is the first quadrant of a conventional x y Cartesian system.

The local coordinate system used in the formulation of element matrices is presented in Figure 13-1. Presented as well in Figure 13-1 is the local element node numbering system. The local coordinates for each of the nodes are given in Table 13-1.

Table 13-1 Local element node numbering system

Element Type	Node	r	s
Quadrilateral	1	+1	+1
	2	-1	+1
	3	-1	-1
	4	+1	-1
	5	0	+1
	6	-1	0
	7	0	-1
	8	1	0
Triangular	1	0	0
	2	1	0
	3	1	1
	4	—	—
	5	$\frac{1}{2}$	0
	6	$\frac{1}{2}$	$\frac{1}{2}$
	7	0	$\frac{1}{2}$
	8	—	—

SEEP/W uses the fourth node to distinguish between triangular and quadrilateral elements. If the fourth node number is zero, the element is triangular. If the fourth node number is not zero, the element is quadrilateral.

In the case of quadrilateral elements, Nodes 5, 6, 7, and 8 are secondary nodes. In the case of triangular elements, Nodes 5, 6, and 7 are secondary nodes.

The local and global coordinate systems are related by a set of interpolation functions. SEEP/W uses the same functions for relating the coordinate systems as for describing the variation of the field variable (head) within the element. The elements are consequently isoperimetric elements.

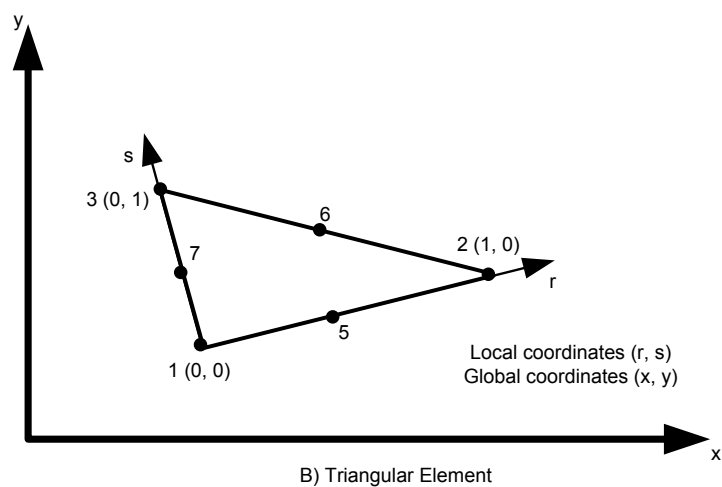
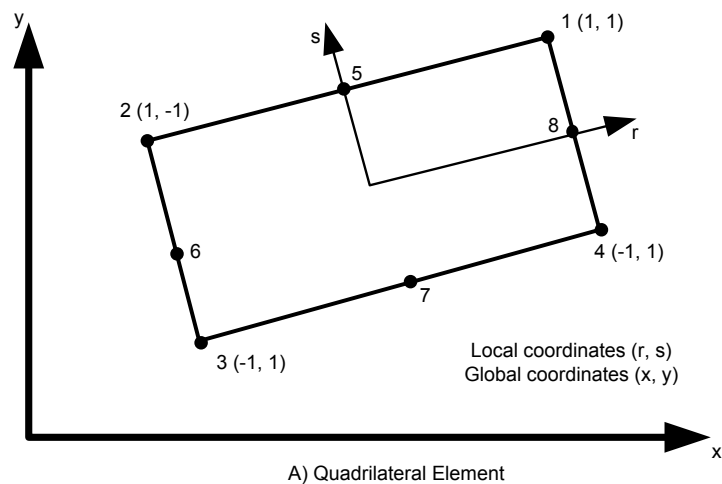


Figure 13-1 Global and local coordinate system

The x- and y-coordinates anywhere in the element are related to the local coordinates and to the x- and y-coordinates of the nodes by the following equations:

Equation 13-1

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

$$y = \langle N \rangle \{Y\}$$

where:

- $\langle N \rangle$ = is a vector of interpolating shape functions,
- $\{X\}$ = the global x-coordinates of the element nodes, and
- $\{Y\}$ = the global y-coordinates of the element node.

The interpolating functions are expressed in terms of local coordinates. Therefore, once a set of local coordinates (r,s) have been specified, the corresponding global coordinates can be determined by Equation 13-1.

13.2 Interpolating functions

VADOSE/W uses a general set of interpolating functions presented by Bathe (1982). These general functions are suitable for elements which have none, some, or all of the secondary nodes defined. This allows for considerable versatility in the types of elements that can be used.

The interpolating functions in terms of local coordinates r and s for quadrilateral and triangular elements are given in Table 13-2 and Table 13-3, respectively.

The functions represent a linear equation when the secondary nodes are missing, and a quadratic (nonlinear) equation when the secondary nodes are included.

Table 13-2 Interpolation functions for quadrilateral elements

Function	Include in function if node is present			
	5	6	7	8
$N1 = \frac{1}{4}(1+r)(1+s)$	$-\frac{1}{2}N5$	—	—	$-\frac{1}{2}N8$
$N2 = \frac{1}{4}(1-r)(1+s)$	$-\frac{1}{2}N5$	$-\frac{1}{2}N6$	—	—
$N3 = \frac{1}{4}(1-r)(1-s)$	—	$-\frac{1}{2}N6$	$-\frac{1}{2}N7$	—
$N4 = \frac{1}{4}(1+r)(1-s)$	—	—	$-\frac{1}{2}N7$	$-\frac{1}{2}N8$
$N5 = \frac{1}{2}(1-r^2)(1+s)$	—	—	—	—
$N6 = \frac{1}{2}(1-s^2)(1-r)$	—	—	—	—
$N6 = \frac{1}{2}(1-s^2)(1-r)$	—	—	—	—
$N7 = \frac{1}{2}(1-r^2)(1-s)$	—	—	—	—

Table 13-3 Interpolation functions for triangular elements

Function	Include in function if node is present		
	5	6	7
$N1 = 1-r-s$	$-\frac{1}{2}N5$		$-\frac{1}{2}N7$
$N2 = r$	$-\frac{1}{2}N5$	$-\frac{1}{2}N6$	
$N3 = s$		$-\frac{1}{2}N6$	$-\frac{1}{2}N7$
$N5 = 4r(1-s)$			
$N6 = 4rs$			
$N7 = 4s(1-r-s)$			

Field variable model

To formulate a finite element analysis, it is necessary to adopt a model for the distribution of the field variable within the element. Since the field variable in the seepage analysis is the total head (H), it is necessary to adopt a model for the distribution of H within the element.

VADOSE/W assumes that the head distribution within the element follows the adopted interpolating functions. This means that the head distribution is linear when the secondary nodes are missing, and the head distribution is nonlinear when the secondary nodes are present.

In equation form, the head distribution model is:

Equation 13-2 $h = \langle N \rangle \{H\}$

where:

$$\begin{aligned} h &= \text{the head at any local coordinate,} \\ \langle N \rangle &= \text{a vector of interpolation function, and} \\ \{H\} &= \text{a vector of heads at the nodes.} \end{aligned}$$

Interpolation function derivatives

The constitutive relationship for a seepage analysis is Darcy's Law. The equation is:

$$q = ki$$

The gradient i is one of the key parameters required in the finite element formulation. The following presents the procedure used by VADOSE/W to compute the gradient.

From the adopted head distribution model, the head at any point within the element in terms of the nodal heads is obtained from Equation 13-2

The gradients in the x and y directions are then known by:

Equation 13-3

$$\begin{aligned} i_x &= \frac{\partial h}{\partial x} = \frac{\partial \langle N \rangle}{\partial x} \{H\} \\ i_y &= \frac{\partial h}{\partial y} = \frac{\partial \langle N \rangle}{\partial y} \{H\} \end{aligned}$$

The interpolating functions are written in terms of r and s and not in terms of x and y . The derivatives must consequently be determined by the chain rule of differentiation, as follows:

$$\frac{\partial \langle N \rangle}{\partial s} = \frac{\partial \langle N \rangle}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial \langle N \rangle}{\partial y} \frac{\partial y}{\partial s}$$

This can be written as:

$$\begin{Bmatrix} \frac{\partial \langle N \rangle}{\partial r} \\ \frac{\partial \langle N \rangle}{\partial s} \end{Bmatrix} = [J] \begin{Bmatrix} \frac{\partial \langle N \rangle}{\partial x} \\ \frac{\partial \langle N \rangle}{\partial y} \end{Bmatrix}$$

where $[J]$ is the Jacobian matrix and is defined as:

Equation 13-4

$$[J] = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{bmatrix}$$

The derivatives of the interpolation function with respect to x and y is called the B matrix and can be determined by inverting the Jacobian matrix and rewriting the equations as:

$$[B] = \begin{Bmatrix} \frac{\partial \langle N \rangle}{\partial x} \\ \frac{\partial \langle N \rangle}{\partial y} \end{Bmatrix} = [J]^{-1} \begin{Bmatrix} \frac{\partial \langle N \rangle}{\partial r} \\ \frac{\partial \langle N \rangle}{\partial s} \end{Bmatrix}$$

Recalling Equation 13-1 and taking their derivative with respect to s and r as follows:

$$\frac{\partial x}{\partial r} = \frac{\partial \langle N \rangle}{\partial r} \{X\}$$

$$\frac{\partial x}{\partial s} = \frac{\partial \langle N \rangle}{\partial s} \{X\}$$

$$\frac{\partial y}{\partial r} = \frac{\partial \langle N \rangle}{\partial r} \{Y\}$$

$$\frac{\partial y}{\partial s} = \frac{\partial \langle N \rangle}{\partial s} \{Y\}$$

then substituting these values into Equation 13-4, the Jacobian matrix becomes:

$$[J] = \begin{bmatrix} \frac{\partial(N_1, N_2, \dots, N_8)}{\partial r} \\ \frac{\partial(N_1, N_2, \dots, N_8)}{\partial s} \end{bmatrix} \begin{bmatrix} X_1 & Y_1 \\ X_2 & Y_2 \\ \vdots & \vdots \\ X_8 & Y_8 \end{bmatrix}$$

The derivatives of the interpolation functions with respect to r and s are required to compute the Jacobian matrix and to compute the flow gradients (Equation 13-3).

The derivatives of the interpolation functions with respect to r and s used by VADOSE/W for quadrilateral and triangular elements are given in Table 13-4 and

Table 13-5 respectively.

Table 13-4 Interpolation function derivatives for quadrilateral elements

Derivative of Function	Include in derivative if node is present			
	5	6	7	8
$N1,r = \frac{1}{4}(1+s)$	$-\frac{1}{2}(N5,r)$	—	—	—
$N2,r = -\frac{1}{4}(1+s)$	$-\frac{1}{2}(N5,r)$	$-\frac{1}{2}(N6,r)$	—	—
$N3,r = -\frac{1}{4}(1-s)$	—	$-\frac{1}{2}(N6,r)$	$-\frac{1}{2}(N7,r)$	—
$N4,r = \frac{1}{4}(1-s)$	—	—	$-\frac{1}{2}(N7,r)$	$-\frac{1}{2}(N8,r)$
$N5,r = -\frac{1}{2}(2r+2sr)$	—	—	—	—
$N6,r = -\frac{1}{2}(1-s^2)$	—	—	—	—
$N7,r = -\frac{1}{2}(2r-2sr)$	—	—	—	—
$N8,r = \frac{1}{2}(1-s^2)$	—	—	—	—
$N1,s = \frac{1}{4}(1+r)$	$-\frac{1}{2}(N5,s)$	—	—	$-\frac{1}{2}(N8,s)$
$N2,s = \frac{1}{4}(1-r)$	$-\frac{1}{2}(N5,s)$	$-\frac{1}{2}(N6,s)$	—	—
$N3,s = -\frac{1}{4}(1-r)$	—	$-\frac{1}{2}(N6,s)$	$-\frac{1}{2}(N7,s)$	—
$N4,s = -\frac{1}{4}(1+r)$	—	—	$-\frac{1}{2}(N7,s)$	$-\frac{1}{2}(N8,s)$
$N5,s = \frac{1}{2}(1-r^2)$	—	—	—	—
$N6,s = -\frac{1}{2}(2s-2sr)$	—	—	—	—
$N7,s = -\frac{1}{2}(1-r^2)$	—	—	—	—
$N8,s = -\frac{1}{2}(2s+2sr)$	—	—	—	—

Table 13-5 Interpolation function derivatives for triangular elements

Derivative of Function	Include in derivative if node is present		
	5	6	7
$N1,r = -1.0$	$-\frac{1}{2}(N5,r)$	—	—
$N2,r = 1.0$	$-\frac{1}{2}(N5,r)$	$-\frac{1}{2}(N6,r)$	—
$N3,r = 0.0$	—	$-\frac{1}{2}(N6,r)$	$-\frac{1}{2}(N7,r)$
$N5,r = (4-8r-4s)$	—	—	—
$N6,r = 4s$	—	—	—
$N7,r = -4s$	—	—	—
$N1,s = -1.0$	$-\frac{1}{2}(N5,s)$	—	—
$N2,s = 0.0$	$-\frac{1}{2}(N5,s)$	$-\frac{1}{2}(N6,s)$	—
$N3,s = 1.0$	—	$-\frac{1}{2}(N6,s)$	$-\frac{1}{2}(N7,s)$
$N5,s = -4r$	—	—	—
$N6,s = 4r$	—	—	—
$N7,s = (4-4r-8s)$	—	—	—

The following notation is used in the preceding tables:

$$N_{i,r} = \frac{\partial N_i}{\partial r}$$

$$N_{i,s} = \frac{\partial N_i}{\partial s}$$

The Jacobian matrix is a 2x2 matrix:

$$[J] = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix}$$

The inverse of [J] is:

$$[J]^{-1} = \begin{bmatrix} J_{22} & -J_{12} \\ -J_{21} & J_{11} \end{bmatrix}$$

The determinant of [J] is:

$$\det[J] = J_{11} \times J_{22} - J_{21} \times J_{12}$$

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Consistent Sets of Units

Parameter	Symbol	Metric	Metric	Imperial
Length	L	meters	meters	feet
Time	t	seconds	day	hours
Force	F	kN	kN	lbs
Pressure	F/L^2	kN/m^2	kN/m^2	psf
Unit Weight of Water	F/L^3	kN/m^3	kN/m^3	pcf
Hydraulic conductivity	L/t	m/sec	m/day	ft/hr
Total / Pressure head	L	m	m	ft
Nodal Flux (Q)	L^3/t	m^3/sec	m^3/day	ft^3/hr
Boundary Flux (q)	L/t	m/sec	m/day	ft/hr
Flux Section	L^3/t	m^3/sec	m^3/day	ft^3/hr
Volume	L^3	m^3	m^3	m^3
Temperature	-	Celsius	Celsius	Fahrenheit
Heat	-	Joules	kilo Joules	BTU