Golder Associates Ltd.

500 – 4260 Still Creek Drive
Burnaby, British Columbia, Canada V5C 6C6
Telephone (604) 296-4200
Fax (604) 298-5253

Golder Associates

REPORT ON

APPROACHES AND METHODS FOR EVALUATION OF UNSATURATED ZONE CONTAMINANT TRANSPORT PROCESSES AND EFFECTS ON GROUNDWATER

"HYDROGEOLOGICAL ASSESSMENT TOOLS PROJECT"

Submitted to:

Science Advisory Board for Contaminated Sites in British Columbia
Department of Chemistry
University of Victoria
PO Box 3065 Stn C
Victoria, British Columbia V8W 3V6
Canada

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1.0 INTRODUCTION

This report prepared for the Science Advisory Board for Contaminated Sites (SABCS) in British Columbia evaluates approaches and methods that could be used by practitioners to evaluate unsaturated soil zone fate and transport of chemicals at contaminated sites in British Columbia. The objective of this evaluation is to identify a suite of tools, ranging from relatively simple to complex models, that could be used to evaluate the significance of unsaturated zone contamination and possible effects on groundwater quality.

The scope of this review is relatively limited and is intended to provide an overview of selected issues for prediction of unsaturated soil fate and transport processes with a particular emphasis on approaches that can be easily incorporated into the Screening Level Risk Assessment (SLRA) Level 2 Soil and Groundwater Modules. The review addresses fundamental aspects relating to the soil-water characteristic curve and unsaturated zone hydraulic conductivity. A range of models for water movement and organic and inorganic solute transport within the unsaturated porous media are evaluated. The evaluation of unsaturated zone processes is limited to consideration of porous media.

The primary focus of this evaluation involves the leaching of chemicals from contamination sources within the unsaturated soil zone and the migration of dissolved chemicals to the saturated zone, where the chemicals may adversely influence groundwater quality. Other potentially relevant pathways such as volatilization and vapour inhalation or direct contact with contaminated soil are not considered as part of this review. In addition, the migration of separate-phase non-aqueous phase liquids (NAPL) is not addressed.

The fundamental physical processes governing contaminant transport in saturated soils are also valid and applicable for unsaturated soils. The key unsaturated soil properties describing fluid migration; however, can no longer be considered as soil constants. In unsaturated soils the transport soil parameters take on a nonlinear mathematical relationship with the negative pore-water pressure (or the equivalent matric suction), or the water content of the soil. The character of the unsaturated soil property functions are of particular importance to the evaluation of solute transport in the unsaturated soil zone. While the focus of this assessment involves the leaching and migration of dissolved solutes, the theories and models in this review have broad application to geoenvironmental problems.

The report begins with an overview of unsaturated zone transport fundamentals, including a description of common water retention or soil-water characteristic curve models and methods that can be used to estimate unsaturated hydraulic conductivity. Next, several relatively simple modeling concepts and approaches that could be used to evaluate water movement (i.e., advection) and solute transport through the unsaturated soil zone are described. The report concludes with an evaluation of several more complex, but commonly used numerical models that can be used for the simulation of these processes in the unsaturated soil zone.

2.0 UNSATURATED SOIL ZONE TRANSPORT FUNDAMENTALS

The fundamental physical concepts, constitutive relations and mathematical formulations are briefly summarized in the following sections. The mathematical formulations describe the basic elements of physics of unsaturated zone transport for a Representative Elemental Volume (i.e., REV). The end result is one or more partial differential equations that satisfy conservation of mass and can be solved subject to a set of boundary conditions. While there are some closed-form analytical solutions, it is becoming more common to use numerical modeling techniques such as finite element and finite difference methods. Numerical models are useful for the evaluation of more complex contaminant transport scenarios. As for all solutions of these partial differential equations, the models require an adequate description of: 1) the surface geometry and the subsurface stratigraphy, 2) the saturated and unsaturated soil properties, and 3) initial conditions and boundary conditions.

2.1 Overview of Vadose Zone Processes

The vadose zone is defined as the geologic media between the land surface and the regional water table (API, 1996). The upper part of the vadose zone commonly includes the plant root zone and weathered soil horizons. Within the vadose zone, soils and bedrock are usually unsaturated; meaning that the pores are only partly filled with water. The vadose zone is typically the first subsurface environment encountered by contaminants. As a result, all subsequent groundwater and surface water concentrations, and any resulting environmental impacts are influenced by the complex and dynamic processes that occur within the vadose zone.

The main source of water in the vadose zone is the atmosphere. Precipitation falls on the ground surface and enters the vadose zone through the process of infiltration. In this way, the climatic conditions at the ground surface are translated into a moisture flux that largely drives what happens below the ground surface. The downward flow of water, aided by gravitational forces is termed percolation. Figure 1 is a schematic of a water balance model that illustrates the fundamental components of the surface hydrology for precipitation, snow melt, run-off, potential evaporation, actual soil evaporation, plant transpiration, changes in shallow soil moisture and finally net infiltration or percolation.

The water balance near the ground surface is also a function of surface runoff, evaporation and transpiration. The physical model that embraces the processes occurring at ground surface is called a soil-atmosphere model. Numerous physical models have been proposed to predict “potential evaporation” (i.e., pan evaporation). However, the actual evaporation from a ground surface, which is generally less than the potential evaporation, is of greater relevance to the modeling process. Long-term predictions of moisture and contaminant movement require that the "upward" and "downward" movement of water (and water vapour) across the ground surface be assessed in a reasonable manner. Adequate characterization of the surface hydrology to determine the net infiltration is an important aspect of solute transport modeling in unsaturated soil since the seepage fluxes are controlled solely by the surface flux boundary.

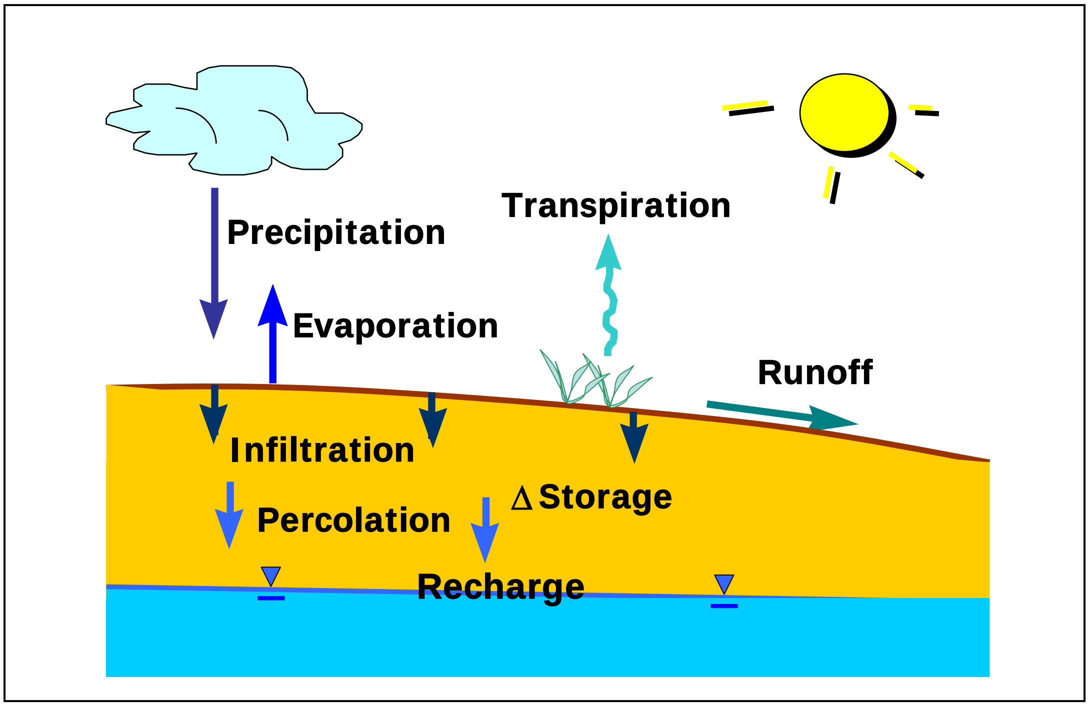


FIGURE 1: Conceptual Water Balance Model

As in saturated aquifers, the downward flow of water through the vadose zone is impeded by the solid grains. Unlike saturated flow, however, interactions between air, water, and the soil matrix lead to capillary effects. Capillary forces affect the moisture state within the vadose zone as well as the rate that water moves. The amount of water that infiltrates through the sub-surface, in turn, has a direct impact on the quantity of chemical mass that is transported in the aqueous phase toward groundwater.

2.2 Capillary Effects and Water Retention Characteristics

2.2.1 Introduction

The multiphase nature of the vadose zone gives rise to capillary effects which cause each fluid phase to have differing local fluid pressures. The capillary effects largely determine the static fluid distributions in the vadose zone. In the remainder of this report, it is assumed that there is one liquid, water in the pores. In this situation, the fluid pressure of the soil water is less than atmospheric pressure. The relationship between the amount of water in a soil and the negative pore-water pressure is an important factor in analyzing unsaturated soil behavior. The theory must be understood along with the means of obtaining this relationship. For example, even in the simple-to-apply HELP model (Section 3.1.1), key input parameters are required to describe the soil water retention characteristics.

2.2.2 Definitions

The ratio of the volume of voids to the total volume of a porous medium sample is known as the porosity, n. The interconnected or effective porosity largely determines the volume of fluid that can be contained in a given volume of soil. The soil void spaces can be filled with one or more fluids. In the vadose zone, a gas phase is generally present in the pores along with a liquid water (aqueous) phase. At contaminated sites, a NAPL, such as a chlorinated solvent or hydrocarbon fuel may also form an immiscible third fluid phase that is present in the pore space.

Several measures are commonly used to define the amount of water in a soil. Gravimetric water content, w, is the term most commonly used in geotechnical engineering and is defined on a mass fraction or weight fraction basis (i.e., mass or weight of water divided by mass or weight of oven-dried soil). Volumetric water content, θ_w, has been commonly used in agriculture and hydrology-related disciplines to describe the amount of water in a soil and is equal to the product of the degree of water saturation and the porosity of the soil, $\theta_w = n\ S_w$. The degree of saturation, S_w, is defined as the percentage of the voids of a soil that is filled with water. All three measures of the amount of water in a porous medium are used in the literature when defining the relationship between the amount of water and soil suction.

2.2.3 Soil-Water Characteristic Curve

The relationship between water content and soil water pressure (or soil suction) is commonly referred to as the soil-water characteristic curve (or the water retention curve) and forms the basis for the evaluation of all unsaturated soil properties. The water flow and storage characteristics of an unsaturated soil are closely related to the amount of water contained in the pores. The amount of water in a soil can be related to the negative pore-water pressure (i.e., soil suction) in the soil. There are two components to soil suction; namely, matric suction and osmotic suction. The sum of the matric suction and the osmotic suction is called total suction. The term “soil suction” is a more general term for either matric suction, osmotic suction or total suction (Fredlund and Rahardjo, 1993). The constitutive relationship used to define the relationship between soil suction and water content is called by several names such as: 1) the soil-water characteristic curve, SWCC, 2) the water retention curve, WTC, or 3) the capillary pressure curve. In the soil suction range up to 1,500 kPa, the matric suction is plotted versus the amount of water in the soil. For soil suction values beyond 1,500 kPa, the total suction is plotted versus the amount of water in the soil. In the reminder of this report, the term soil-water characteristic curve, SWCC, is used when referring to the constitutive relationship between soil suction and the amount of water in a soil.

The SWCC defines the water storage capacity of a soil. The SWCC divides soil behaviour into three distinct stages of desaturation as shown in Figure 2. The stages of desaturation are referred to as the “boundary effect stage” at low soil suction, the “primary and secondary transition stages” at intermediate soil suctions, and the “residual stage” at high soil suctions that extend to 1,000,000 kPa. There are two defining breaks along most SWCC and these are referred to as the “air entry value” of the soil and the “residual value” of the soil. These points are illustrated in Figure 3. The air entry value is the point at which the difference between the air and water pressures (i.e., the capillary pressure) becomes sufficiently large such that water can be displaced by air from the largest pore spaces in the soil. The residual degree of saturation is the point at which a further increase in capillary pressure fails to displace a significant amount of water. The residual degree of saturation is usually associated with the smallest pores in the system and with adsorbed water films.

The relationship between soil suction and water content depends upon whether the soil is in a drying (desorption) mode or a wetting (adsorption) mode. In other words, the wetting and drying of any porous media exhibits non-unique characteristics known as hysteresis, as shown in Figure 4. Therefore, when using the SWCC, the modeler must be aware of whether a wetting or drying process is being simulated and the corresponding curve must be used. It should also be noted that there can be intermediate scanning curves that traverse between the drying and wetting bounding SWCC curves.

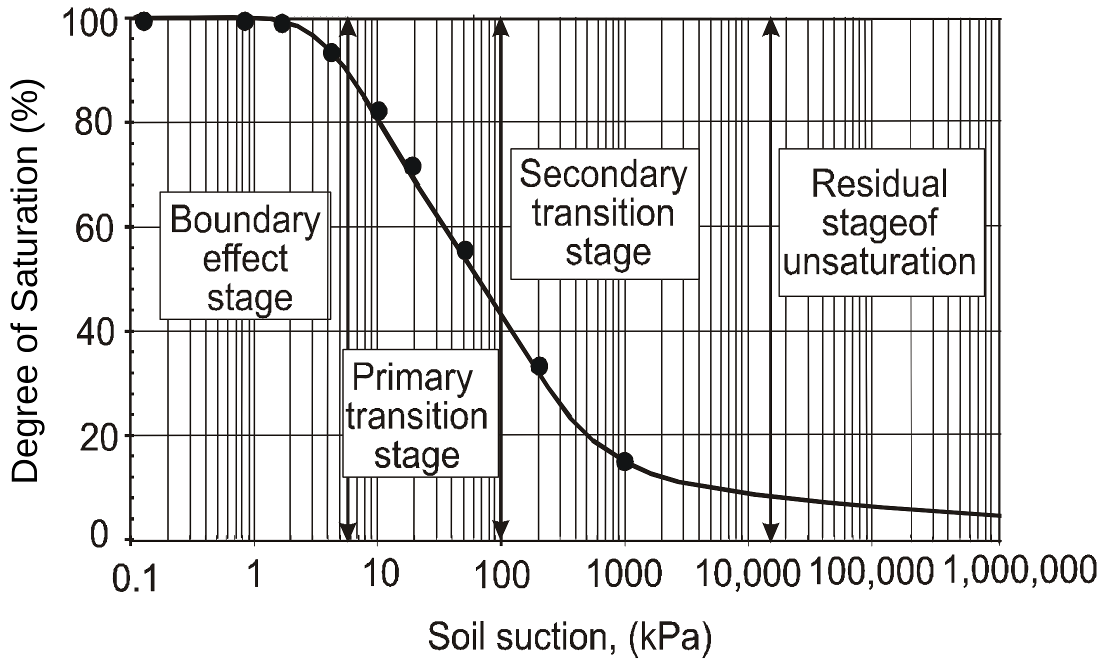


FIGURE 2: Soil-Water Characteristic Curve Showing the Stages of Desaturation of a Soil.

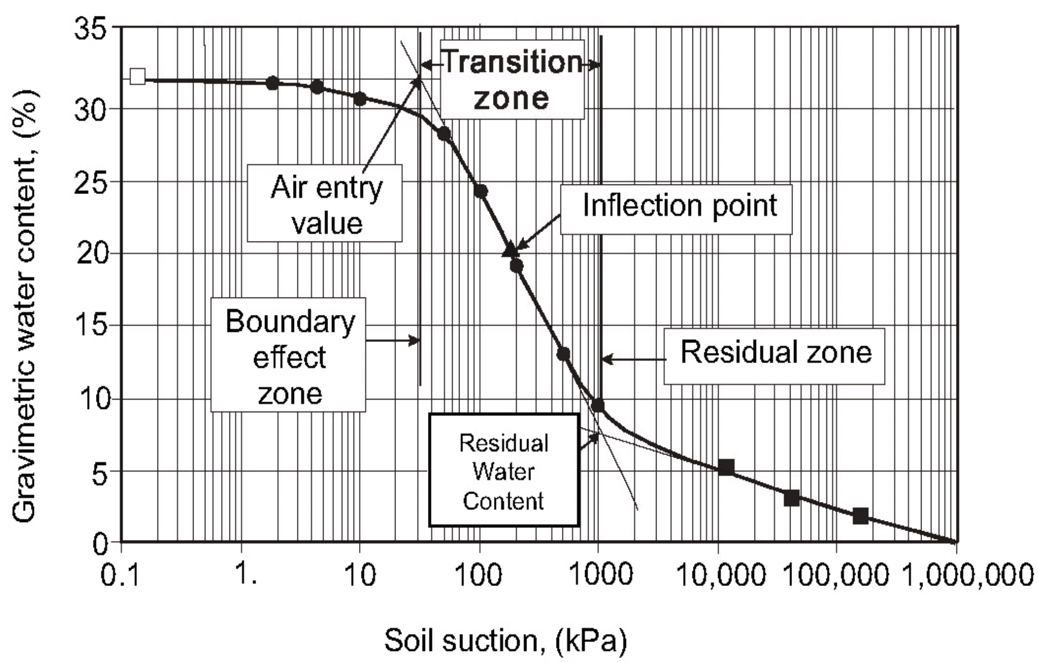


FIGURE 3: Soil-Water Characteristic Curve Illustrating the Air Entry Value and the Residual Value for a Soil.

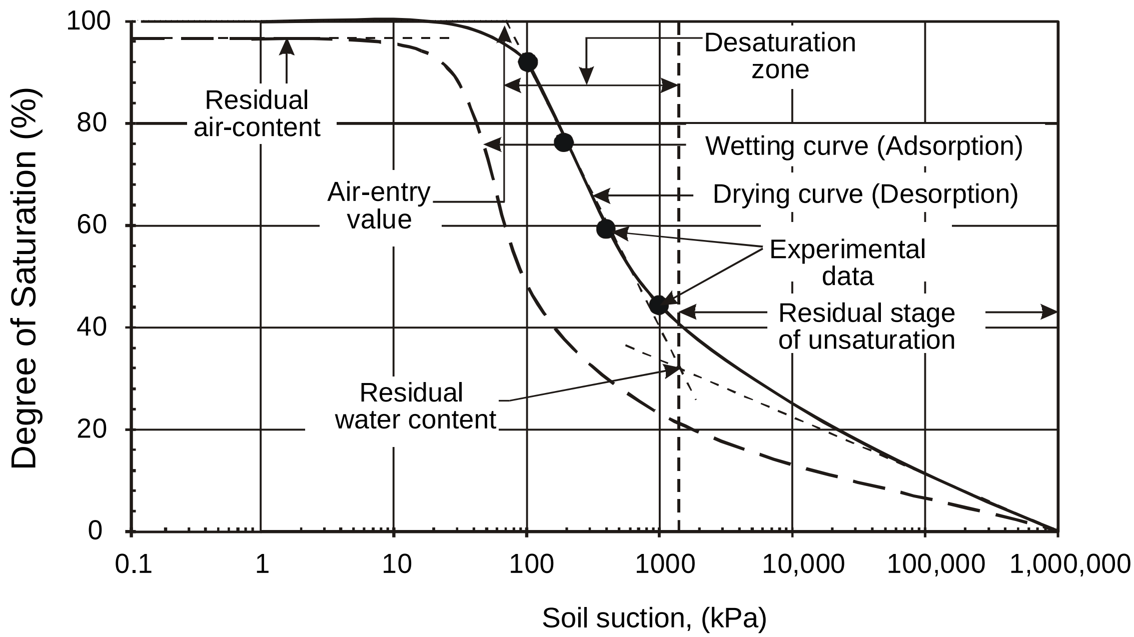


FIGURE 4: Illustration of the non-uniqueness of the Soil-Water Characteristic Curve due to hysteretic effects.

The physical meaning of the SWCC can be visualized through use of the capillary pressure concept or the capillary tube model. The SWCC from the laboratory can be translated to the vadose zone in the field and used to assist in the visualization of *in situ* processes.

Under an assumption of steady state infiltration, the pore-water pressure in the soil is nearly constant in the upper portion of the vadose zone, but the pore-water pressure increases with depth until the capillary zone is reached. When there are coarse-grained soil zones or preferential pathways (e.g., fractures, macropores), the water holding capacity (retention) of the soil is limited (i.e., low residual saturation). Two types of behaviour become possible. The localized coarse-grained zones may become preferential conduits of flow or the coarse-grained soil might also function as a capillary barrier to flow.

2.2.4 Equations for the Soil-Water Characteristic Curve

Determination of the capillary parameters for the SWCC is an important component of unsaturated soil hydrogeology. Mathematical functions by Brooks and Corey (1964), Campbell (1974) and van Genuchten (1980) have historically been widely adopted to describe soil-water characteristic curves. In these functions, the water content has often been normalized between saturation and residual water content conditions. This alternate expression of water content is referred to as effective saturation, $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$, where θs and θr indicate saturated and residual volumetric water content values, respectively. One view of residual water content is that it represents the water content where unsaturated hydraulic conductivity approaches zero (Mualem, 1976). The mathematic equations for soil-water characteristic curves by Brooks and Corey (1964), Campbell (1974) and Van Genuchten (1980) are shown in Table 1. The Brooks and Corey (1964) and Campbell (1974) equations contain two empirical soil parameters. The van Genuchten (1980) equation contains three soil parameters.

More recently, Fredlund and Xing (1994) proposed an alternate mathematical function for the SWCC that directs all curves to a soil suction value of 1,000,000 kPa at a water content of zero percent. In this way, the water content conditions lower than the residual water content are more accurately defined than by previous equations. The Fredlund and Xing (1994) equation for the SWCC is written as follows:

$$w(\psi) = C(\psi) \frac{w_s}{\ln\{e + [\frac{\Psi}{\Psi_{aev}}]^n\}^m} \qquad [1]$$

where: $w(\psi)$ = water content at any soil suction, Ψ,

Ws = gravimetric water content saturated soil,

$C(\psi)$ = correction factor directing all SWCC curves to 1,000,000 kPa at zero water content,

Ψ = soil suction, namely matric suction, $(u_a - u_w)$, up to 1,500 kPA and total suction above 1,500 kPa,

Ψ_{aev} = soil parameter indicating the inflection point that bears a relationship to the air entry value,

n = soil parameter related to the rate of desaturation, and

m = soil parameter related to the curvature near residual conditions.

Equation [1] can be written either in terms of gravimetric water content, volumetric water content or degree of saturation. The *n* and *m* parameters defined in Equation [1] are not the same as the van Genuchten *n* and *m* parameters.

TABLE 1: Common Water Retention Models and Methods for Estimating Unsaturated Hydraulic Conductivity

Hydraulic Soil Characteristics	Parameters	Parameter Correspondence
Brooks and Corey (1964)		
Soil water retention	λ = pore-size index	λ = λ
$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left(\frac{h_b}{h}\right)^{\lambda}$$	h_b = bubbling capillary pressure	$h_b = h_b$
	θ_r = residual water content	$\theta_r = \theta_r$
Hydraulic conductivity	θ_s = saturated water content	$\theta_s = \theta_s$
$$\frac{K(\theta)}{K_s}=\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{n}=(S_e)^n$$	K_s = fully saturated conductivity ($\theta = \theta_s$)	$K_s = K_s$
	N = $3 + \frac{2}{\lambda}$	
Campbell (1974)		
Soil water retention	θ_s = saturated water content	$\theta_s = \theta_s$
$$\frac{\theta}{\theta_s}=\left(\frac{H_b}{h}\right)^{1/b}$$	H_b = scaling parameter with dimension of length	$H_b = h_b$
Hydraulic conductivity	b = constant	b = $\frac{1}{\lambda}$
$$\frac{K(\theta)}{K_s}=\left(\frac{\theta}{\theta_s}\right)^{n}$$	n = $3 + 2b$	
Van Genuchten (1980)		
Soil water retention	θ_s = saturated water content	$\theta_s = \theta_s$
$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\left[\frac{1}{1+(\alpha h)^n}\right]^m$$	θ_r = residual water content	$\alpha = (h_b)^{-1}$
	α = constant	$n = \lambda + 1$
	n = constant	
	m = constant	$m = \frac{\lambda}{\lambda+1}$
Hydraulic conductivity		
$$\frac{K(\theta)}{K_s}=\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{1/2}\left\{1-\left[1-\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{1/m}\right]^m\right\}^2$$		

θ = volumetric water contant; h = matric suction, cm; $K(\theta)$ = hydraulic conductivity for given water content , cm/h

2.2.5 Measurement of Soil-Water Characteristic Curve

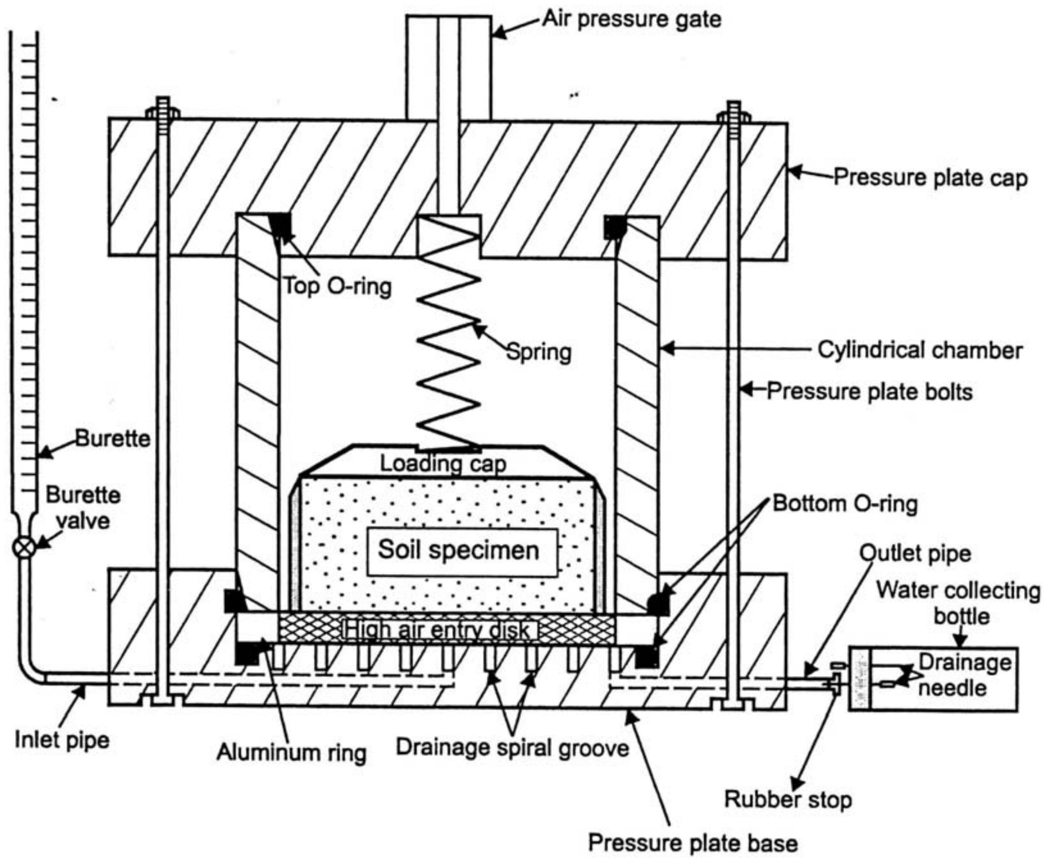


FIGURE 5: Five-bar pressure plate cell used at the University of Saskatchewan (1998)

There are a series of methodologies that have been proposed for the measurement of the soil-water characteristic curves in the laboratory. ASTM Designation D6836-02 describes five methods; namely, 1) the Hanging Column (up to 80 kPa), 2) Pressure Chamber (Volumetric measurement), 3) Pressure Chamber (gravimetric measurement), 4) Chilled Mirror Hygrometer, and 5) Centrifuge method (ASTM, 2002). There are a number of pressure plate devices that have been developed, and these are the most common methodology for measuring the soil-water characteristic curve for a soil.

Pressure plate extractors commonly referred to as "Tempe" cells are used to apply suctions of less than 100 kPa (or 10 m of water). Other more robust pressure cells have been designed and built for higher matric suctions (Wang and Benson, 2004; Fredlund, 1998). Figure 5 shows a pressure plate cell that has been designed and built at the University of Saskatchewan for applied suctions up to 500 kPA (Fredlund, 1998). If possible, a relatively undisturbed soil sample from a Shelby tube should be obtained for testing. Alternately, a disturbed soil sample can be re-compacted to its approximate *in situ* density. The SWCC data can be analyzed to determine the best-fit soil parameters for any of the proposed empirical equations for the SWCC (e.g., van Genuchten et al., 1991; Fredlund and Xing, 1994; Sale, 2001). The RETC computer code (van Genuchten et al., 1991) can be used to analyze the SWCC for the determination of the best-fit parameters that can then be used for estimation of the hydraulic conductivity function.[1] The SoilVision Knowledge-Based[2] database can also be used to provide best-fit parameters to a wide range of soil-water characteristic curve equations. The SoilVision software can also be used to compute a wide range of unsaturated soil property functions for most unsaturated soil processes. Examples are functions for hydraulic conductivity, water storage and contaminant transport.

A typical set of SWCCs for three pressure-plate tests on a silt soil are shown on Figure 6. Both the drying and wetting curves were measured, in this case illustrating the consistent results that can be obtained.

[1] This software is available on a CD with documentation free of charge from the U.S. Salinity Laboratory, USDA, Agricultural Research Service, Riverside, CA 92501 (http://www.ussl.ars.usda.gov/models/hydrus2d.htm)

[2] SoilVision Knowledge-Based System, SoilVisions Systems Ltd., Saskatoon, Saskatchewan, Canada. (http://www.soilvision.com/)

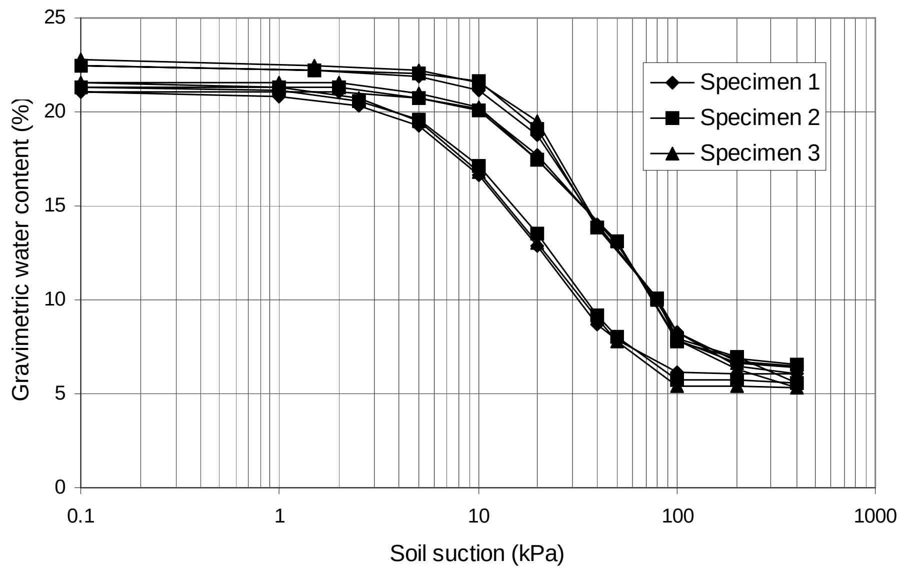


FIGURE 6: Typical measured drying and wetting SWCCs for a processed silt.

2.2.6 Estimation of the Soil-Water Characteristic Curve

The soil-water characteristic curve has long been an important soil property in agriculture-related disciplines. A large volume of soil-water characteristic curve data has been collected in these disciplines. For many engineering problems it is sufficient to have an estimate of the SWCC. This is particularly true for preliminary studies. A compiled database can be of great assistance in selecting an approximate soil-water characteristic curve. In addition, pedo-transfer functions (predictive functions of certain soil properties that may be obtained from more readily available or cheaply measured properties) have been proposed to estimate the SWCC. Several different methods for estimating the SWCC are described below.

Predicting the SWCC From the Grain-size Distribution Curve

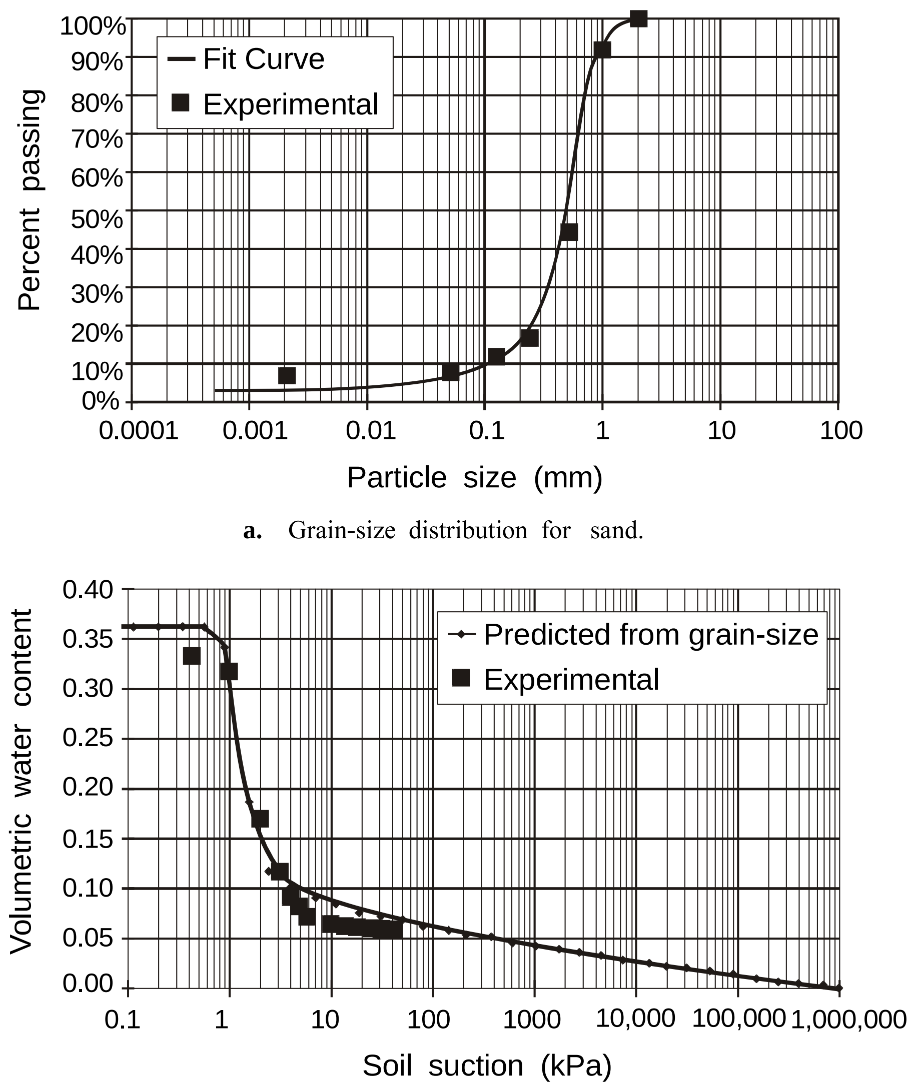
If direct measurements of the SWCC are not feasible, the SWCC can be estimated using the grain-size distribution curve for the soil. This method is generally not as accurate as a direct measurement but may be a reasonable approach depending on the modeling objectives. The procedure involves the use of physico-empirical SWCC models based on the grain-size distribution curve and the capillary tube model. There are a number of models that have been proposed (Fredlund et al. 1997, 2002a). A mathematical equation similar to that used for describing a SWCC can be best-fit to a grain-size distribution curve. The equation for the grain size distribution curve is then used to compute a soil-water characteristic curve (Fredlund et al, 1997).

Figure 7 illustrates the manner in which an equation is fit to grain-size distribution data, which in turn is used to approximate the SWCC (Fredlund et al., 1997). The estimation process does not take soil structure into account but provides an initial estimate that is of value for sands and silts. A series of SWCCs that have been computed from grain-size distribution curves for several soil types using the Fredlund et al. (1997) methodology are shown in Figure 8. The estimation procedure provides an indication of the air entry value and residual conditions for a soil.

Other researchers have proposed alternative methodologies that use grain-size distributions as a basis for estimating the SWCC. The Arya-Paris (AP) model by Arya and Paris (1981) came from an early study on the prediction of the SWCC from grain size distributions. Their physico-empirical approach is based mainly on the similarity between shapes of the cumulative grain-size distribution and soil-water characteristic curves. The AP model was later refined by Arya et al. (1999a) and included a model to compute the hydraulic conductivity function directly from the grain size distribution (Arya et al., 1999b). At least twenty grain-size fractions were necessary to compute a reasonable estimate of the hydraulic properties.

Data Mining and Curve Matching

A compiled database can be of great assistance in selecting the appropriate soil-water characteristic curve (Fredlund et al, 1996). The grain-size distribution curves for a soil can be matched to other grain-size curves in a database to select an approximate soil-water characteristic curve. The estimated SWCC for the grain-size curve that most closely matches the field data can be used for the prediction of unsaturated soil property functions.



a. Grain-size distribution for sand.

b. Comparison between experimental and predicted soil-water characteristic curves for a sand

FIGURE 7: Soil-Water Characteristic Curve computed from a grain-size distribution curve.

Correlation Methods

There are several databases that provide fitted best estimates of the capillary parameters for various SWCC equations (Fredlund et al, 1996). The estimates of the parameters are based on the textural classification of the soil. The soil texture is estimated from grain-size distribution and soil textural triangle. One relatively large database has been compiled by Carsel and Parish (1988), which is based on the US Soil Conservation Service (SCS) soil texture classification system (12 soil textural classifications). The

Carsel and Parish (1988) database is understood to comprise mostly near surface soils used for agricultural purposes. Aqui-Ver, Inc. (2004) includes the "API database" of capillary parameters based for 78 samples of more consolidated earth materials collected near the water table and classified by grain-size analyses and the Folk Classification System. The "API database" is expected to be more representative of subsurface earth materials near the water table while the Carsel and Parish (1988) values may be more representative of capillary parameters of soil near the ground surface.

More recently, Zapata (1999) undertook a correlation study to relate the SWCCs to the textural and plasticity properties of a wide range of soils. A database characterising approximately 190 soils was assembled from the knowledge-database developed by SoilVision Systems. The soils were divided into two categories; namely, soils that have a Plasticity Index (*PI*) greater than zero and soils having a PI equal to zero. Data for approximately 70 soils with PI values greater than zero and 120 soils with PI values equal to zero were collected and the resulting average SWCCs are summarized in Figure 9.

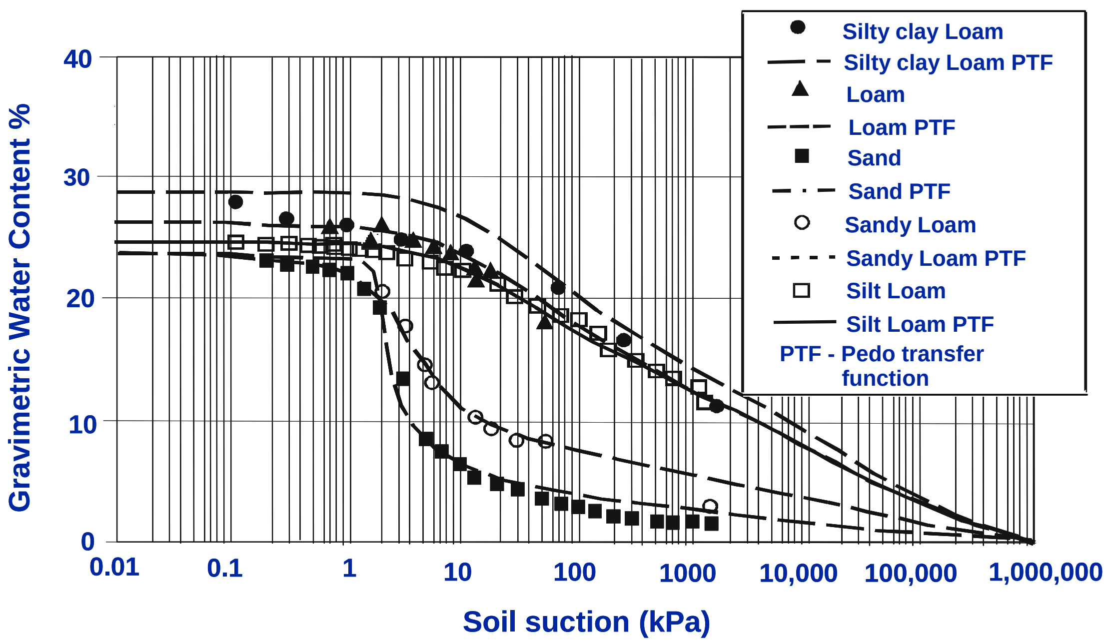


FIGURE 8. Soil-Water Characteristic Curves computed from grain-size distribution data for a variety of soil types.

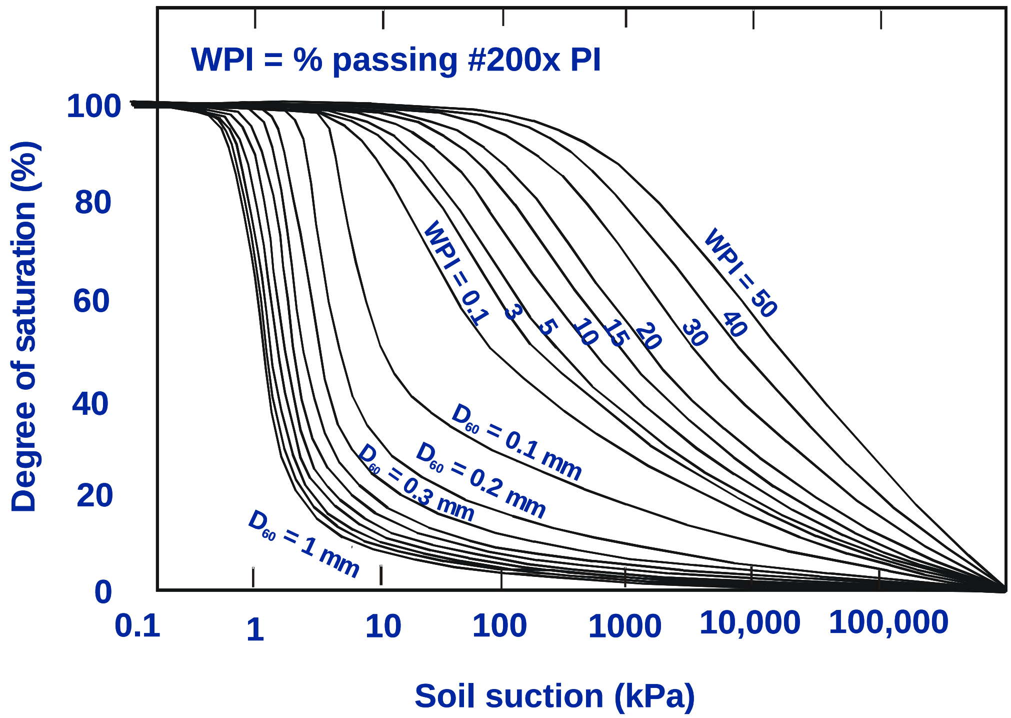


FIGURE 9: Correlation of soil classification properties with previously measured Soil-Water Characteristic Curves (Zapata, 1999; Zapata et al., 2000).

2.3 Unsaturated Soil Hydraulic Conductivity

There are two hydraulic properties required for modeling transient flow processes through an unsaturated soil; namely, the hydraulic conductivity function and the water storage function. The latter function is a direct result of the SWCC (Appendix I). The hydraulic conductivity (or the coefficient of permeability) of a soil refers to the ability of a soil to transmit water. The saturated hydraulic conductivity of a soil, K_s, is a relatively constant value. The unsaturated hydraulic conductivity changes with water content and forms a non-linear function that depends on the water content of the soil. Since the soil water content is also related to soil suction, the hydraulic conductivity is a function of soil suction.

A number of empirical models have been proposed for the estimation of the hydraulic conductivity function for an unsaturated soil. All of the empirical models make use of the soil-water characteristic curve in estimating the permeability function. These functions have proven to be sufficiently accurate for most engineering applications and as a consequence, little attempt is any longer made to directly measure the unsaturated soil permeability function in the laboratory. Table I-2 in Appendix I shows the form of the hydraulic conductivity functions proposed by Brooks and Corey (1964), Campbell (1974) and van Genuchten (1980). The soil parameters used in the hydraulic conductivity function are obtained from the soil-water characteristic curve. A more in-depth discussion of methods and equations for prediction of unsaturated soil hydraulic conductivity is provided in Appendix I.

2.4 Saturated-Unsaturated Seepage Modeling

The movement of pore-water within the unsaturated soil zone can be described in terms of a partial differential equation that satisfies the conservation of mass principle and utilizes constitutive relations for water flow (i.e., Darcy's flow law) and water storage (arithmetic slope of the SWCC). For the case of two-dimensional, saturated-unsaturated water movement through the soil, the general partial differential equation can be written as follows.

$$K_x^w \frac{\partial^2 h}{\partial x^2} + \frac{\partial K_x^w}{\partial x}\frac{\partial h}{\partial x} + K_y^w \frac{\partial^2 h}{\partial y^2} + \frac{\partial K_y^w}{\partial y}\frac{\partial h}{\partial y} = -m_2^w \gamma_w \frac{\partial h}{\partial t} \qquad [2]$$

where: K_i^w = hydraulic conductivity in the i direction, $K^w = f(\Psi)$ (m/s),

h = hydraulic head (m),

Ψ = soil suction (kPa),

γ_w = unit weight of water, approximately 9.81 kN/m^3,

m_2^w = coefficient of water volume change (i.e., water storage) with respect to soil suction,

$m_2^w = \frac{d(\theta_w)}{d(u_a - u_w)}$; the arithmetic slope of the SWCC,

θ_w = Volumetric water content, and

t = time (sec).

The saturated-unsaturated seepage equation has been solved within several software packages and can also be solved using general purpose partial differential equations solvers (i.e., PDE Solver such as FlexPDE, 1999). The highly non-linear nature of unsaturated soil problems provides a challenge to obtain convergence to an accurate solution (Fredlund and Rahardjo, 1993; Gitirana et al, 2005). In this regard, different software packages solve unsaturated soil seepage problems with varying ease and accuracy. Examples of computer software packages that can be used to solve for seepage in saturated-unsaturated soil systems are listed under "Selected Software References" at the end of this report.

When certain simplifying assumptions are made to the partial differential formulation, the movement of water through the unsaturated zone can be described using Richards' Equation, which is derived by combining Darcy's Law for vertical unsaturated flow with conservation of mass. There are three common formulations for Richards' equation, which are head (h) based, water content (θ) based and mixed formula (Celia et al., 1990). The head based equation is subject to poor mass balance results in cases where the soil properties are highly non-linear. In these cases a mixed form of the seepage equation is often used for numerical analysis (Celia et al., 1990). The head based form can be applied to both saturated and unsaturated conditions and heterogeneous soils. The head-based [3a] and mixed [3b] forms of Richard's equation are shown below:

$$\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]=C(h)\frac{\partial h}{\partial t} \quad [3a]$$

$$\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]=\frac{\partial \theta_w}{\partial t} \quad [3b]$$

where,

θ_w = volumetric water content (dimensionless),

$K(h)$ = unsaturated hydraulic conductivity (m/sec),

$C(h)$ = specific moisture capacity function (1/m), $d\theta w/dh$

h = hydraulic head (m), and

t = time (sec).

Due to the non-linear nature of Richards' equation, there is no closed-form analytical solution except for highly simplified conditions.

2.5 Solute Transport in the Unsaturated Zone

The fate and transport of chemicals within the vadose zone is dependent on numerous processes including advection, dispersion, diffusion, sorption, degradation or decay and volatilization. The surface seepage flux boundary condition is a key input to the solute transport equation. Advection is the bulk movement of water under a hydraulic head gradient, whereas, diffusion is the process involving the transfer of chemicals from a higher chemical potential to a lower chemical potential by random molecular motion (Robinson and Stokes, 1959). For non-ionic organic compounds, there are well-established partitioning models based on linear equilibrium partitioning between the contaminant in the aqueous phase and absorbed within organic carbon. For metals, the processes that affect retardation are much more complex and include sorption through ion complexation, surface complexation and precipitation. Further discussion of partitioning goes beyond the scope of this report.

For common organic chemicals such as benzene, toluene, ethylbenzene and xylenes, biodegradation has been demonstrated in groundwater under both aerobic and anaerobic conditions. Similar reaction kinetics would be expected in the unsaturated zone, except possibly for very dry conditions. Volatilization may be an important mechanism for mass loss for volatile chemicals in the vadose zone. Mechanical dispersion in the unsaturated zone appears not to have been as extensively researched as saturated zone dispersion, although there are field scale experiments where a longitudinal dispersivity of greater than 10 cm has been measured (Charbeneau and Daniel, 2000). Conceptually, transverse dispersion within the unsaturated zone could be highly variable depending on the potential for fingering or spreading based on horizontal layering of soil.

Simple relationships for evaluation of unsaturated zone solute transport have been developed for one-dimensional advection, dispersion, sorption and first-order decay for a homogeneous, isotropic soil. For the case of two-dimensional solute transport through porous media, the partial differential equation can be written as follows:

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - \bar{v}_x \frac{\partial C}{\partial x} - \bar{v}_y \frac{\partial C}{\partial y} - \lambda_1 C - \frac{\lambda_2 \rho_d C^*}{\theta} - R = \frac{\partial C}{\partial t} \qquad [4]$$

where:

D_x = hydrodynamic dispersion in x-direction (L^2T),
$\bar{v}_x$ = average linear velocity in x-direction (L^2T^{-1}),
D_y = hydrodynamic dispersion in y-direction (L^2T),
$\bar{v}_y$ = average linear velocity in y-direction (L^2T^{-1}),
λ_1 = dissolved half-life (T^{-1}),
λ_2 = sorbed half-life (T^{-1}),
C = dissolved concentration (ML^{-3}),
C^* = sorbed concentration (ML^{-3}),
ρ_d = bulk density (ML^{-3}),
θ = volumetric water content, and
R = retardation factor of sorption isotherm.

An analytical solution by Kool et al. (1994) for steady state solute transport based on the above processes is provided below. This is the analytical model that was adopted by the B.C. Environment Contaminated Site Soil Taskforce (CSST) (1996) as part of the four-component groundwater model used to derive the BC Contaminated Sites Regulation (CSR) soil standards.

$$\frac{C_Z}{C_L} = exp\left[\frac{b}{2\partial_u} - \frac{b}{2\partial_u}\left(1 + \frac{4\partial_u L_{US}}{v_u}\right)^{1/2}\right] \quad [5]$$

$$v_u = \frac{I}{\theta_w R_u}; R_u = 1 + \frac{\rho_b}{\theta w} K_d \quad [6]$$

$$L_{US} = \frac{0.693}{t_{1/2US}}\left(e^{-0.07d}\right)\left(1 - \frac{D_{1/2US}}{365}\right) \quad [7]$$

where:

C_L	=	Allowable chemical concentration in leachate at the source (mg/L),
C_z	=	Allowable chemical concentration in leachate at the water table (mg/L), calculated below
b	=	Thickness of unsaturated zone below the source (m) = d – Z,
d	=	Depth from surface to groundwater surface (m),
Z	=	Depth to bottom of contaminated soil (m),
∂_u	=	Dispersivity in the unsaturated zone (m) = 0.1b,
L_{US}	=	First-order decay constant for chemical (yr^{-1}) in unsaturated zone,
$T_{1/2US}$	=	Chemical half-life in unsaturated zone (years),
$D_{1/2US}$	=	Days with mean temperature < 0º C,
v_u	=	Average linear leachate velocity (m/y),
I	=	Infiltration rate (m/y) – precipitation minus runoff and evapotranspiration,
θ_w	=	Water-filled porosity (unitless),
R_u	=	Retardation factor in unsaturated zone (unitless),
ρ_b	=	Soil bulk density in unsaturated zone (g/cm^3), and
K_d	=	Distribution coefficient (cm^3/g).

The one-dimensional model includes first-order biodecay. In contrast to common saturated zone models, a modifying factor is applied to the decay rate in the CSST groundwater model. The rate decreases as the thickness of the unsaturated zone increases and as the number of days with mean temperatures less than 0^oC increases. These modifications of the biodecay factor are not presented in Kool et al. (1994), and their technical justification within the BC Contaminated Sites Regulation (CSR) model is not clear.

Further evaluation of unsaturated zone solute transport is presented in Section 4.0 of this report.

3.0 WATER BALANCE CALCULATIONS

A number of different terms are used to describe unsaturated water flow. The terms include infiltration rate (typically limited to processes at the ground surface), percolation rate (typically addressing deeper water movement), recharge (water that reaches the water table) and unsaturated zone Darcy velocity.

The estimation of the rate at which water moves within the unsaturated zone forms an important component of an evaluation of the potential effect of unsaturated zone contamination on groundwater quality. The American Petroleum Institute, API, (1996) describes 13 different models and empirical methods that can be used to estimate recharge for environmental site assessments. Although average recharge rates alone do not yield an estimate of groundwater impacts, they can be used in simple screening models such as the Screening Level Risk Assessment (SLRA) Soil Module, where recharge is one of a handful of parameters used to evaluate the groundwater concentration derived from a soil contaminant source. In arid regions, estimates of average annual recharge may play an important role in determining the applicable standard at a site based on a travel time from the soil source to a down-gradient receptor.

There are two main classes of models that can be used for estimating groundwater recharge: (i) water balance models (e.g., HELP, SESOIL), and (ii) numerical models based on the solution to the saturated-unsaturated partial differential equation [Equation 2] and Richards' equation [Equation 3] (e.g., SVFlux, VS2DT, HYDRUS-2D). There are also physically-based analytical models for infiltration (e.g., Green-Ampt model). In addition, a number of empirical methods have been used to estimate recharge.

The recharge rate can be used for several different purposes including:

1. The recharge rate can be used to adjust the dilution factor for unsaturated zone leachate mixing with groundwater, and thus used to adjust soil standards that are based on a default dilution factor.

2. The recharge rate can used to estimate the seepage velocity for the pore-water. Assuming that compounds leached from a soil contamination zone migrate at the same rate as the pore-water, a conservative travel time for migration of chemicals to the water table can be estimated thus providing a measure to evaluate the possible significance of unsaturated zone contamination.

3. The recharge rate can be input into unsaturated zone solute transport models (e.g., one dimensional analytical model). The recharge rate may also be an input parameter for numerical models of saturated zone solute transport.

Water balance and physically-based models are first described in the section below, followed by two relatively simple applications involving the use of the estimated recharge rate to adjust the dilution factor and estimate the seepage velocity, presented in Section 3.2. Unsaturated zone flow models based on the general unsaturated-saturated partial differential equation [Equation 2] and Richards' equation [Equation 3] are described in Section 4.0, as part of the discussion on solute transport models.

3.1 Methods for Estimation of Recharge

3.1.1 Water Balance Methods

Water balance models couple climatic and hydrological data with a simplified model for unsaturated zone groundwater flow. The simplest model is one where the recharge is assumed to equal the infiltration rate estimated using a simple water balance equation:

$$I = P - ET - R \qquad [8]$$

where P is the precipitation, ET is the evapotranspiration rate and R is the runoff. A slight variation on this model sets the recharge as the minimum of the infiltration rate or saturated hydraulic conductivity (i.e., under a unit gradient assumption), recognizing that in approximate terms, the average annual infiltration rate cannot exceed the saturated hydraulic conductivity of the soil.

Two commonly used water balance models are the HELP: Hydrologic Evaluation of Landfill Performance model and SESOIL: Seasonal Soil compartmental model. The HELP model does not include a solute transport module whereas the SESOIL model includes a solute transport model. The HELP model is described in this section, whereas the SESOIL model is described in Section 4.0.

The HELP model is a layered, water budget (moisture routing) model for hydrologic evaluation of landfill performance, but can be applied more generally to evaluate unsaturated zone recharge at sites. It is essentially a one-dimensional model for the estimation of vertical percolation through a layered soil system. The HELP model also accounts for lateral drainage in coarse layers situated above low permeability layers.

The HELP model provides methods for estimating the infiltration rate based on a water balance approach (i.e., $I = P - ET - R - \Delta S - D$, where ΔS is the change in soil moisture and D is the drainage) along with the following information:

- climatic information (precipitation, temperature, solar radiation);
- evapotranspiration characteristics (site latitude, maximum, leaf area index, length of growing season, evaporative zone depth, average wind speed, average humidity);
- soil properties (porosity, field capacity, wilting point, initial water content, saturated hydraulic conductivity), and;
- information relating to run-off (surface cover vegetation and slope).

The program contains a default soil database with characteristics for 42 types of materials (e.g., soils, waste, and geosynthetics). The precipitation input to the model is partitioned into surface storage, runoff, percolation, evapotranspiration, soil moisture storage, and lateral drainage.

The vertical saturated flow in the HELP model is described by one-dimensional flow using Darcy's law where the pore pressure between soil layers is assumed to be constant. Therefore, the head gradient in the vertical direction is equal to unity. The program developers state that this assumption is reasonable at moisture contents above field capacity, since for higher water contents, flow and pore pressures will be roughly constant (Schroeder et al., 1994). The field capacity is typically defined as the volumetric water content at a soil water suction of 0.33 bars or that remaining after a prolonged (usually several day) period of gravity drainage without additional water supply. The unsaturated hydraulic conductivity is estimated using the Campbell (1974) function shown in Table 1. HELP places low permeability soil layers in a special category of 'barrier soils', which are considered to be saturated at all times. The pore-size distribution index, λ (see Table 1), is obtained from look-up tables for different soil types. An iterative solution is used to determine the percolation rate for a multi-layered system.

The HELP model uses daily precipitation, temperature and solar radiation data. A default climatic database for a number of Canadian cities is now available (i.e., Visual HELP, from Waterloo Hydrogeologic).[3] If detailed daily hydrologic data required by the HELP model are not available, data from the nearest city with default data can be used. As necessary, these data can be scaled according to the available weather data to better represent the site under consideration (e.g., the daily data for the default site can be scaled using ratios for monthly or annual averages). This methodology assumes that the

[3] BC cities with climatic data are Castlegar, Comox, Cranbrook, Kamloops, Penticton, Port Hardy, Sandspit, Prince George, Prince Rupert, Terrace, Smithers, Williams Lake, Vancouver and Victoria.

statistical characteristics of the default station will reasonably match the site under evaluation.

To illustrate how HELP can be used to estimate recharge, the HELP model was run using climatic data for Vancouver and Kamloops for a homogeneous soil column, no runoff or lateral drainage, and two different soil types (loamy sand, loam soil). The predicted average annual percolation rate based on twenty years of simulation time was approximately 43 cm/year for Vancouver and 4.4 cm/year for Kamloops.

3.1.2 Empirical Methods

Recharge can also be estimated from rainfall infiltration measurement data. In the SAM model (GSI, 1996), infiltration data from 101 sandy soil sites in 18 geographic regions in the United States was analyzed and compiled by Stephens & Associates (API, 1996). To obtain a high-range estimate of infiltration, a regression curve was fitted to mean annual precipitation and net infiltration measurements such that 80 percent of the measured infiltration rates would fall below the curve. The "80% regression curve" was considered to provide a reasonably conservative estimate of infiltration rates and leachate impacts in most sandy soil conditions. The equation for the estimation of the infiltration rate is:

$$I = 0.0018P^2 \qquad [9]$$

where I is the mean annual net infiltration (cm/year), P is the mean annual precipitation (cm/year). Equation [9] and the mean precipitation assumed in the CSST protocol results in a net infiltration rate of 18 cm/year (compared to 55 cm/year assumed by CSST). GSI (1996) also provide empirical estimates of the infiltration rate for silt ($I = 0.0009P^2$) and for clay ($I = 0.00018P^2$) soils.

There are a number of other methods for estimating recharge including evaluation of natural tracers (^3H and ^{36}Cl), experimental tracers, correlation of water table elevations to recharge, and monitoring of surface water quality and temperature. There are also methods for assessing the water content distribution in soil, such as time domain reflectrometry (TDR) or neutron probes, and for estimating the infiltration rate (lysimeter, tensiometer, ring infiltrometer). The methods described above may have application for experimental evaluations of infiltration rate and recharge but currently are not commonly used for characterization of sites in BC. Further discussion of field methods goes beyond the scope of this report.

3.2 Application of Recharge Estimates

The section below discusses two practical ways in which estimates of recharge can be used to evaluate the potential significance of unsaturated soil solute transport.

3.2.1 Site Specific Leachate-Groundwater Dilution Factor

Recharge rates estimated using the methods described above can be used to derive a site specific dilution factor, which in turn is used to compute a site-specific soil standard for the protection of groundwater. The BC Contaminated Sites Regulation (CSR) matrix soil standards are based on a model that couples unsaturated leaching, mixing of leachate with groundwater, and saturated zone transport. The Darcy velocity, simplistically referred to as the infiltration rate in the CSR model, is input in the following mass-balance model for dilution of leachate below a contamination source zone:

$$C_W = C_{gW}(1 + Z_d V / I X) \quad [10]$$

$$C_W = C_{gW} DF \quad [11]$$

where C_w is the leachate concentration in the unsaturated zone (mg/L), C_{gw} is the groundwater concentration at the down-gradient boundary of the source zone (mg/L), Z_d is the average thickness of the mixing zone (m), V is the Darcy velocity in groundwater (m/year), I is the infiltration rate (m/year), X in the length of contaminated soil source parallel to groundwater flow (m), and DF is the dilution factor due to mixing of leachate with groundwater (dimensionless).

The default infiltration rate used for the matrix standard development process was 55 cm/year (BCE, 1996). One simple tool that can be considered within the regulatory framework in BC is to allow practitioners to calculate a site specific dilution factor based on the estimated infiltration rate (and perhaps other parameters listed above). A site specific soil standard would, in turn, be then calculated as follows:

$$\mathrm{C_{SS} = DF_{SS} / DF_{CSR} * C_{CSR}} \quad [12]$$

where,

C_{ss} = site-specific soil standard (mg/kg)
DF_{ss} = site-specific dilution factor
DF_{CSR} = CSR dilution factor used to derive matrix soil standards
C_{CSR} = CSR soil standard

3.2.2 Estimation of Travel Time

The seepage velocity and travel time for water percolating downward through the unsaturated zone could potentially provide insight on the significance of contamination within the upper regions of the unsaturated zone. If there is a thick unsaturated zone and calculations indicate relatively long travel times for seepage, there may be limited potential for significant contaminant flux to groundwater. This is particularly true when there are mechanisms that will result in attenuation of contaminants (e.g., biodegradation, sorption). Attenuation may be limited for chemicals with limited sorption or biodegradation properties (e.g., MTBE, salt).

The seepage velocity in the portion of a soil column with constant capillary pressure (i.e., above the capillary fringe under conditions of constant infiltration) can be calculated assuming the infiltration rate is related to the vertical hydraulic gradient and unsaturated hydraulic conductivity at the water content of the vadose zone soil. Unsaturated hydraulic conductivity is commonly expressed as the product of the saturated hydraulic conductivity and the relative permeability, yielding the following vertical flow equation for annual average infiltration:

$$I = K_s \; k_{rw} \; i \quad ; \; K_s < I \qquad [13]$$

where K_s is the saturated hydraulic conductivity (m/year), k_{rw} is the relative permeability of the soil (unitless), i is the hydraulic gradient (m/m), and I is the infiltration rate (m/year). The infiltration rate can be estimated from a simple water balance water (e.g., equation [8] where I = P – ET – R).

By assuming that infiltration occurs under an average unit hydraulic gradient and solving for the relative permeability, the following relationship results:

$$k_{rw} = I \;\; K_s \qquad [14]$$

The relative permeability is a function of the volumetric water content. Using the Brooks and Corey (1964) soil-water characteristic model combined with the Burdine equation (1959) for the relative permeability, the relative permeability function is as follows:

$$k_{rw} = (\theta_w - \theta_r) \,/\, (\theta_S - \theta_w)^{\varepsilon} \qquad [15]$$

where θ_w is the volumetric water content, θ_S is the total (saturated) soil porosity, θ_r is the residual soil water content, $\varepsilon = 3 + 2/\lambda$ and λ = pore size distribution index (unitless) (Brooks and Corey, 1964). Substituting equation [14] into equation [15] yields the following equation for volumetric water content as a function of annual average infiltration:

$$\theta_w = \theta_r + (\theta_S - \theta_r)\,(I / K_s)^{1/\varepsilon} \qquad [16]$$

The average seepage velocity can be estimated through a simplification of Darcy's Law assuming a unit hydraulic gradient, and where below the upper soil zone the capillary pressure is nearly constant. Substituting equation [16] into the Darcy's Law equation results in the following equation for seepage velocity:

$$v = \frac{I}{\theta_{Wr} + (\theta_S - \theta_{Wr})(I/K_S)^{\lambda/(3\lambda+2)}} \qquad [17]$$

The average seepage velocity, which conservatively is equal to the solute velocity, is provided for various US SCS soil textural classifications and average annual recharges shown in Table 2. For example, for loam soil with an average annual recharge of 10 cm, and a 25 m thick unsaturated zone, the travel time for water from ground surface to the water table would be on the order of 50 years based on this simple model.

TABLE 2: Average Seepage Velocities, cm/yr
(from Charbeneau and Daniels, 1993)

Soil Type	**Average annual infiltration, cm**			
	5	**10**	**25**	**50**
Clay	16	31	75	148
Clay loam	19	34	86	164
Loam	26	49	113	211
Loamy sand	53	99	225	416
Silt	21	39	88	164
Silt loam	22	41	93	174
Silty clay	16	30	74	145
Silty clay loam	16	30	72	137
Sand	68	127	286	527
Sandy clay	18	35	82	158
Sandy clay loam	25	48	112	212
Sandy loam	39	73	167	308

Note: The above values represent average seepage velocities for four categories of infiltration rates.

The average seepage velocity and travel time estimated using the above model is approximate and can be considered as an order-of-magnitude screening estimate. This is because the annual seepage velocity in Table 2 is based on a homogeneous soil and an annual infiltration rate. The seepage velocity will vary as a consequence of the seasonal variation in the infiltration rate.

An alternate approach that generally would be considered more accurate than the simple screening model described above is to estimate the average annual seepage velocity using the HELP model. Further accuracy in estimating average annual seepage can be obtained using computer software that couples water balance processes with models for saturated-unsaturated flow of water.

4.0 REVIEW OF SELECTED SOLUTE TRANSPORT MODELS

This section begins with an evaluation of a 1-D analytical model for solute transport (see Section 2.5). Next, five more complex computer models, SESOIL, VLEACH, HYDRUS-2D, VS2DT and SVFlux, are described. The intent of this review was to select a few of the more commonly known solute transport models that are well-documented, have good user interfaces and that provide examples for validation and tutorial purposes.

4.1 Solute Transport Simulations Using 1-D Analytical Model

To gain insight on the 1-D analytical model described in Section 2.6, several simulations were performed to evaluate transport of benzene for different depths from contamination to the water table and infiltration rates (0.55 m (CSST default), 0.3 m, 0.05 m) (Figure 10). A relatively conservative half-life (one year) and fraction organic carbon (0.001) was chosen for the simulations. The predicted concentration of benzene in pore-water at the water table decreases with increasing unsaturated zone thickness, but then increases as a result of the reduction in half life.

Because of the ease of use, this 1-D model for the evaluation of fate and transport of organics in the unsaturated zone is recommended for pathway-based risk assessments, subject to evaluation and modification of the half-life term (Equation 7). This 1-D unsaturated model is not recommended for inorganics. It is recommended that the half-life term be simplified through removal of the terms related to the thickness of the vadose zone and days with temperature less than $0^{o}C$. Instead, a reasonably conservative site specific half-life should be chosen to account for possible reduced biodegradation for thick vadose zone deposits or colder climates.

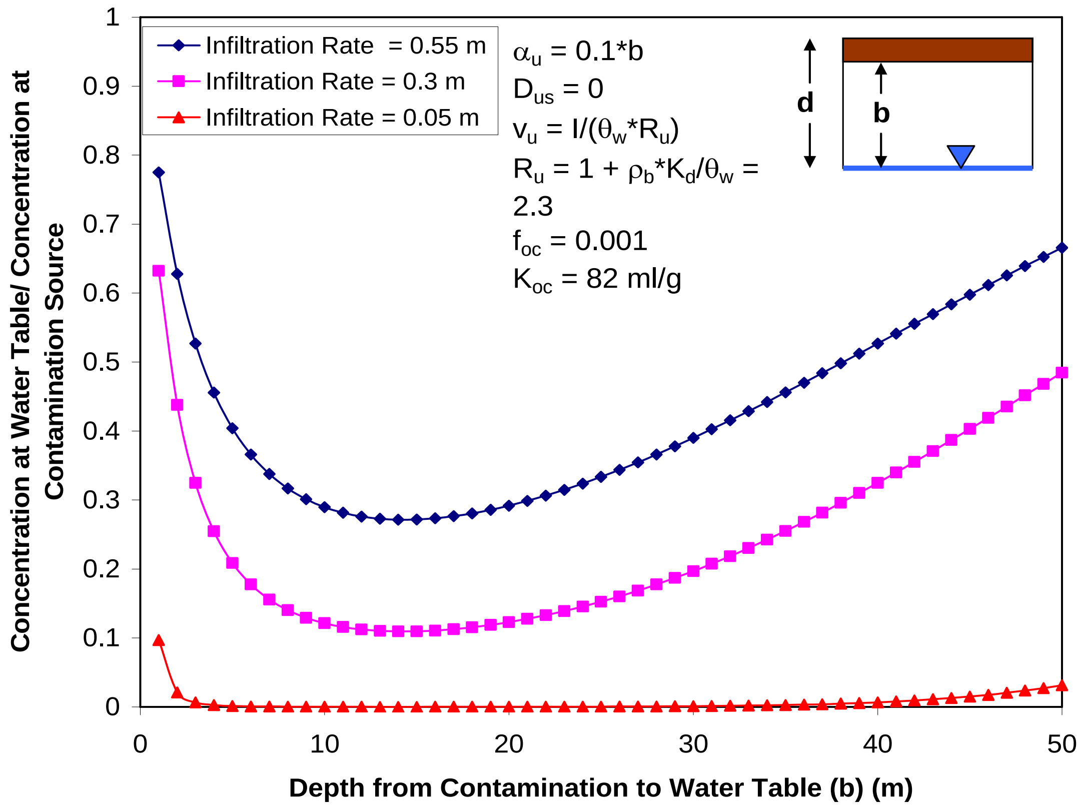


FIGURE 10: Predicted Benzene Concentrations at Water Table Based on 1-D Unsaturated Zone Steady State Model for Advection, Dispersion, Sorption and Decay.

4.2 SESOIL Model

SESOIL was developed for the US Environmental Protection Agency in 1981 by Bonazountas and Wagner (Arthur D. Little Inc.), but has been since updated several times. SESOIL is a seasonal compartment model which simulates long-term contaminant fate and migration in the unsaturated soil zone. SESOIL describes the following components of a user-specified soil column which extends from the ground surface to the ground-water table:

- Hydrologic cycle of the unsaturated soil zone;
- Contaminant concentrations and masses in water, soil, and air phases;
- Contaminant migration to ground water;
- Contaminant volatilization at the ground surface, and
- Contaminant transport in washload due to surface runoff and erosion at the ground surface.

SESOIL estimates all the above components on a monthly basis for up to 999 years of simulation time. The soil column may be composed of up to four different soil layers. In addition, each soil layer may be divided into ten sub-layers to provide for enhanced resolution for contaminant transport modeling. The fate and transport processes that are simulated in the SESOIL model are volatilization, adsorption, cation exchange, biodegradation, hydrolysis and complexation.

The input data required by SESOIL consists of five types: climate, soil, chemical, application and washload. The climatic sub-model is used to estimate the infiltration rate based on a water balance approach similar to, but less complex than the HELP model, in that SESOIL is based on a monthly water budget. Soil data includes bulk density and intrinsic permeability, which are average parameters over the entire soil zone.

A mass balance for contaminant movement between layers is solved for each layer. The pore-water flux is calculated using an iterative solution that considers the infiltration rate from the water balance and unsaturated hydraulic conductivity. The vertically averaged hydraulic conductivity over the unsaturated zone profile is equal to:

$$K_z = d / \Sigma (d_i / K_i) \quad [18]$$

where,

d_i = is the thickness of each layer (m)
d = entire thickness (m)
K_z = vertically averaged hydraulic conductivity (m/s), and
K_i = hydraulic conductivity of individual layers (m/s).

The SESOIL model calculates the unsaturated hydraulic conductivity and seepage velocity for each layer based on the water content. The model calculates the hydraulic conductivity using a soil disconnectedness index, *c*, rather than a SWCC-based equation. The unsaturated hydraulic conductivity function is written as follows:

$$K(S) = K_{sat}\ S^c \quad [19]$$

K(S) = unsaturated hydraulic conductivity (m/s)
K_{sat} = saturated hydraulic conductivity (m/s)
S = degree of saturation, and
c = soil disconnectedness index.

The soil disconnectedness index defaults range between 3.7 for sand to 12 for fine clay.

The contaminant fate and transport model includes retardation through sorption according to the Freundlich isotherm and first-order biodecay.

The SESOIL model is reasonably simple to use. An advantage of the SESOIL model is that it combines a water balance model for infiltration with a contaminant fate and transport model that includes important processes such as sorption and biodecay. A potential disadvantage of SESOIL relative to the HELP model is that it uses monthly water balance information and therefore may yield less accurate estimates of the seepage velocity. According to Ohio EPA (1996), the SESOIL model has been extensively validated. This model was subsequently used to derive the Ohio leach-based soil criteria.

4.3 VLEACH

VLEACH, a One-Dimensional Finite-Difference Vadose Zone Leaching Model, is a U.S. EPA program which describes the movement of an organic contaminant within and between three phases: (1) a solute dissolved in water, (2) a vapour phase, and (3) an adsorbed compound in the solid phase.

These processes are conceptualized as occurring in a number of distinct, user-defined vertical soil columns that are vertically divided into a series of user-defined cells. The columns may differ in soil properties, recharge rate, and depth to water. However, within each soil column, homogeneous conditions are assumed except for contaminant concentration, which can vary between layered cells. During each time step the migration of the contaminant within and between cells is calculated. At the end of the simulation the results from each column are used to estimate an area-weighted ground-water impact for the modeled area.

VLEACH initially calculates the equilibrium distribution of contaminant mass between the liquid, gas, and sorbed phases. Transport processes are then simulated. Liquid advective transport is calculated based on a user-defined infiltration rate. The contaminant in the vapor phase migrates into or out of adjacent cells based on the calculated concentration gradients that exist between adjacent cells. After the mass is exchanged between the cells, the total mass in each cell is recalculated and re-equilibrated between the different phases. The following assumptions were made in the development of VLEACH:

- Linear isotherms and local equilibrium is assumed for partitioning of the contaminant between the liquid, vapor and soil phases.

- The vadose zone is in a steady-state condition with respect to water movement meaning that the water content profile within the vadose zone is constant. This assumption will rarely occur in the field.

- Liquid phase dispersion is neglected. Hence, the migration of the contaminant is simulated as a plug. This assumption causes higher dissolved concentrations and lower travel time predictions than would occur in reality.

- Homogeneous soil conditions are assumed to occur within a particular soil column.

- Volatilization from the soil surface boundary is either completely restricted or completely unimpeded. This assumption may be significant depending upon depth of contamination, soil type and chemical volatility.

- The model does not account for biodegradation of contaminants, which could be significant for certain organic constituents, and does not account for non-aqueous phase liquids.

While the VLEACH model is conceptually simple to understand and relatively easy to use, it does not offer significant advantages relative to 1-D analytical models or other computer models such as SESOIL and HYDRUS-2D. The seepage velocity is based on a user-defined infiltration rate assuming uniform soil water content. The infiltration rate would need to be determined using another model such as HELP. The VLEACH model is also limited in that it does not simulate biodegradation, although it does account for mass loss through volatilization.

4.4 HYDRUS-2D

The HYDRUS-2D program is a finite element model for simulating the movement of water, heat, and multiple solutes in variably saturated media (i.e., fully saturated or unsaturated porous media). The program numerically solves the Richards' equation for saturated-unsaturated water flow and advection-dispersion equations for heat and solute transport. The flow equation also incorporates a sink term to account for water uptake by plant roots. The solute transport equations consider advective-dispersive (mechanical and diffusive) transport of water, and diffusion in the gaseous phase. The transport equations also include provisions for nonlinear and/or nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production (addition) of water. Two first-order degradation reactions can be entered: one which is independent of other solutes, and one which reflects the coupling between solutes involved in sequential first-order decay reactions.

HYDRUS-2D can simulate flow within irregular shaped flow regions. Soils with non-uniform properties may be defined. Two-dimensional flow defined for a vertical-horizontal section may be defined, or within in a three-dimensional region exhibiting radial symmetry about the vertical axis. Constant or time-varying prescribed head and flux boundaries may be defined for the water flow component of the model, as well as boundaries controlled by atmospheric conditions. The code can also handle a seepage face boundary through which water leaves the saturated part of the flow domain, and free drainage boundary conditions. Nodal drains are represented by a relationship derived from analog experiments. For solute transport the code supports both constant and varying prescribed concentration conditions (Dirichlet type) and concentration flux (Cauchy type) boundaries.

The unsaturated soil hydraulic properties are described using van Genuchten (1980), Brooks and Corey (1964) and modified van Genuchten type analytical functions. The modified van Genuchten function is reported in the user manual to allow for better prediction of hydraulic conductivity near saturation. The HYDRUS-2D code incorporates hysteresis by using the empirical model introduced by Scott et al. (1983) and Kool and Parker (1987). This model assumes that drying scanning curves are scaled from the main drying curve, and wetting scanning curves from the main wetting curve. To approximate the hydraulic variability commonly observed in soil, HYDRUS-2D also implements a scaling procedure by means of a set of linear scaling transformations which relate the individual soil hydraulic characteristics to those of a reference soil.

A key potential advantage of the HYDRUS-2D model is that the unsaturated flow is solved using Richards' equation, and flow and transport are appropriately coupled. There is flexibility in defining the model geometry and numerous processes are simulated. However, in practice, model failure or inaccuracies may occur due to solutions that do not converge. Model results may also be difficult to interpret.

Another potential disadvantage is that only a very simple water balance model is incorporated in the HYDRUS-2D model. In many cases, a model such as HELP would be required to adequately define infiltration for input in the HYDRUS-2D model. The HYDRUS-2D model is relatively complex and requires appropriate understanding of flow and solute transport principles prior to use.

4.5 VS2DT

VS2DT ("Variably Saturated 2-Dimensional Transport") is a finite difference model developed by the United States Geological Service (USGS) for flow and solute transport in a porous media with varying degrees of saturation. Flow regions that can be simulated include one-dimensional columns, two-dimensional vertical cross sections, and axially symmetric, three-dimensional cylinders. The VS2DT program simulates advection, dispersion, first-order decay, equilibrium adsorption (Freundlich or Langmuir) isotherms, and ion exchange. The program numerically solves the Richards' equation for saturated-unsaturated water flow and advection-dispersion equations for solute transport. Default moisture characteristic curves include those by the Brooks and Corey (1964), Haverkamp and Parlange (1986) and van Genuchten (1980) models. In addition, user-defined curves can be entered based on user-defined data.

There are a number of available boundary conditions for flow in VS2DT including fixed pressure heads, infiltration with ponding, evaporation from the soil surface, plant transpiration, or seepage faces. A submodule for calculation of infiltration using the Green-Ampt model is included. Compared to HYDRUS-2D, there are greater options in terms of boundary conditions based on water balance considerations.

Boundary conditions for solute transport in VS2DT include fixed solute concentration and fixed mass flux. Solute source/sink terms include first-order decay, equilibrium partitioning to the solid phase (Langmuir or Freundlich isotherms), and ion exchange. There are a number of options for output including mass balances, concentration, chemical flux, seepage rates and soil water content.

The VS2DT model couples water flow and solute transport and includes most of the important processes for solute fate and transport. As for HYDRUS-2D, the VS2DT model is relatively complex and requires an appropriate understanding of flow and solute transport principles prior to use. In addition, there are the same potential disadvantages with VS2DT as the HYDRUS-2D model that are associated with the solution of Richards' equation. For example, Gogolev (2002) presents the results of a modeling study where VS2DT repeatedly failed to simulate the annual seepage rate through a layered soil profile within an acceptable balance error.

4.6 SVFlux Suite of Software Packages

SVFlux is a finite element numerical model that can be used to perform 1-D, 2-D, and 3-D boundary value, seepage problems. The software solves the general partial differential for transient and steady state saturated-unsaturated seepage through a porous medium. The SVFlux software uses a FlexPDE(TM) solver that is automated with adaptive mesh refinement for solving highly nonlinear partial differential equations such as those encountered when solving unsaturated flow problems.

SVFlux can model the infiltration of water at the ground surface and can also compute the actual evaporation of moisture from the ground surface. Climatic data forms the input data for calculating the moisture flux boundary condition at the ground surface. The infiltration of moisture at the ground surface can readily produce an extremely nonlinear condition. The mesh refinement technique automatically refines the mesh as necessary to facilitate convergence to an accurate solution. Actual evaporation is computed in accordance with the Modified Penman procedure described by Wilson (1990). Consequently, SVFlux can be viewed as a soil-atmosphere model that computes water balances at the ground surface based on the input climatic conditions. Application of Lord Kelvin's equation ensures thermodynamic equilibrium between the vapor pressure in the atmosphere and the vapor pressure in the soil at the ground surface. The evapotranspiration associated with vegetation on the ground surface can also be accommodated in the modeling process.

The fully automated mesh design and refinement system changes the mesh as necessary in order to meet the mathematical requirements for convergence. The refinement may occur within a particular time step during a transient analysis or from one time step to the next. There are also automatic time step requirements that must be satisfied during the solution process. The end result for most problems is convergence to an accurate solution.

Groundwater models can be built using a series of surfaces and layers. Borehole or soil survey data can be used to build each groundwater model resulting in the possibility of extremely complex models. Soil properties may be input from laboratory data, approximated from one of several possible estimation techniques or selected from the SoilVision Knowledge-Based database system that contains laboratory data on over 6,000 soils. Soil-water characteristic curves, SWCCs, can be input using a number of well-known equations such as: Brooks and Corey (1964), Campbell (1974), van Guenuchten (1980), and Fredlund and Xing (1994). The water storage function is computed from the selected soil-water characteristic curves. The hydraulic conductivity functions are based on the saturated hydraulic conductivity and the soil-water characteristic curve and can be computed in the SoilVision software and imported to the SVFlux software. Typical hydraulic conductivity function for unsaturated soils are those proposed by Gardner (1954), Brooks and Corey (1964), Campbell (1974), and Fredlund, Xing and Huang (1994).

The output from the SVFlux analysis can be visualized as contour plots of pressure or head on any 2-D slices through the problem. An advanced visualization module allows for viewing pathlines, cut-aways, iso-surfaces, and animation.

4.7 Qualitative Tools

There are several qualitative tools that can be used to assess the potential for groundwater pollution based on comparative rating systems that integrate the major hydrogeologic and physical factors within the unsaturated and saturated zones. Typically, the goal is to evaluate the sensitivity or vulnerability of groundwater to pollution on an areal basis. The DRASTIC model is one example of this approach, and is a model used to describe the sensitivity of groundwater quality to an imposed contaminant load based on the following seven characteristics: (1) **D**epth to groundwater, (2) **R**echarge due to rainfall, (3) **A**quifer media, (4) **S**oil media, (5) **T**opography, (6) **I**mpact of the Vadose zone, and the (7) hydraulic **C**onductivity of vadose zone soils. An overall score, representing vulnerability of groundwater to contamination, is obtained by summing the product of the rating value and weight for the above seven factors. The DRASTIC model is designed to represent areas larger than 0.4 km^2 in size, and is intended primarily as a planning tool.

A similar tool has been recently developed by the API and the California MTBE Research Partnership (API, 2003). This software is designed to evaluate the sensitivity of a groundwater resource to a potential release of compounds of concern at a particular site. The toolkit examines three aspects of sensitivity: Resource Value, Receptor Vulnerability and Natural Sensitivity. The user supplies site-specific information and the toolkit returns a "scorecard" addressing the three aspects of sensitivity. Although this utility was designed with petroleum hydrocarbon releases in mind, it can be used when dissolved chlorinated and inorganic compounds are the chemicals of concern.

There are potentially useful concepts embodied in the above approaches that could be used to evaluate solute transport in the vadose zone; however, these tools are not intended to provide quantitative estimates of parameters that are often required to assess risk at contaminated sites (e.g., concentrations, mass flux).

5.0 CONCLUSIONS AND RECOMMENDATIONS

5.1 General Limitations of Unsaturated Zone Modeling

Limitations and uncertainties in unsaturated zone models must be recognized. While a number of tools have been developed for unsaturated zone solute transport, modeling uncertainty is significant and greater than that associated with saturated groundwater flow modeling. Because of uncertainties in hydraulic conductivity and non-linear relationships between hydraulic conductivity and soil suction, estimates of seepage velocity are highly approximate, particularly when steady state models are used to describe highly transient phenomena. There are also significant uncertainties associated with water balance modeling particularly in arid or semi-arid climates where precipitation can greatly exceed evapotranspiration even on a single day. Water balance models that use daily, as opposed to monthly averaged data will tend to provide more accurate estimates of infiltration.

It is also important that a modeling study be accompanied by a detailed conceptual site model, description of the model characteristics, input parameters, and include a sensitivity analysis for key parameters.

5.2 Recommendations for Simple Pathway Analysis of Vadose Zone Transport

For the purposes of a pathway-based risk assessment, several relatively simple tools are available to evaluate the significance of unsaturated zone contamination and the potential effect of soil contamination on groundwater quality. Three simple modeling approaches are identified:

- The estimated recharge can be used to calculate a site-specific leachate-groundwater dilution factor, which in turn is used to adjust the CSR matrix soil standards. The HELP model is recommended for estimation of the recharge rate.

- A 1-D analytical model for advection, dispersion, sorption and biodecay can be used to estimate the vertical solute transport. The use of the 1-D model for evaluation of fate and transport of degradable organics in the unsaturated zone is recommended, subject to modification of the half-life term for this model. The simple 1-D transport equation is not recommended for inorganics.

- The estimated recharge and pore-water seepage velocity can be used to calculate a site-specific travel time from contamination source to groundwater. Groundwater is unlikely to be impacted by near surface soil contamination if the travel time for pore-water migration is relatively long (i.e., many decades).[4] As an initial screening calculation, the approach and table presented in Section 3.2.2 can be used. This method makes significant simplifying assumptions in terms of the average annual infiltration rate, soil profile water content (constant) and hydraulic conductivity; therefore it is highly approximate (i.e., order-of-magnitude estimate). An alternate approach that generally would be considered more accurate than the simple screening approach is to estimate the average annual seepage velocity using the HELP model.

The above approaches can be relatively easily incorporated into the Screening Level Risk Assessment (SLRA) Level 2 Soil and Groundwater Modules.

The HELP model is a widely used, relatively well-documented and easy to use model for the estimation of infiltration and recharge. It incorporates a well-developed water balance model and climatic database that estimates infiltration and recharge based on daily data. The HELP model may be used to provide a more refined estimate of the recharge for both input into the simple modeling approaches described above and more complex solute transport models described below.

[4] It is recognized that the determination of a sufficiently long travel such that groundwater impacts are unlikely is a subjective evaluation that will depend on a number of factors including size of the contamination source and potential for contaminant attenuation through degradation, volatilization and sorption. While the development of minimum travel times from a soil source to the water table goes beyond the scope of this report (and is in part a policy decision), we suggest that minimum travel times of 50 years for a small contamination source with higher attenuation potential, and 100 years for a larger contamination source with lower attenuation potential may be a reasonable starting point for evaluation purposes.

While the approaches described above represent relatively simple methods for evaluating recharge and solute travel times, more complex projects will often require the use of the numerical solute transport models described in Section 4.0 of this report (SESOIL, VLEACH, HYDRUS-2D, VS2DT, SVFlux). These codes are well documented and may be relatively easy to use, but the underlying equations are relatively complex. Models based on solution to the saturated-unsaturated flow equation (e.g., SVFlux) or Richards' equation (e.g., HYDRUS-2D and VS2DT) can, in some cases, yield inaccurate and/or non-convergent results and the interpretation of model results may not be straightforward. These models should only be used by modelers experienced in the use of numerical models for simulation of unsaturated zone transport. Potential advantages associated with the use of numerical solute transport codes is that complex, time varying boundary conditions and heterogeneous porous media can be simulated. In addition, these codes can not only provide estimates of concentrations, but chemical fluxes, which may be useful for risk assessment purposes.

GOLDER ASSOCIATES LTD.

ORIGINAL SIGNED BY

Michel Mailloux, M.Sc., Eng.
Senior Hydrogeologist

ORIGINAL SIGNED BY

Del Fredlund, Ph.D.,
Senior Geotechnical Specialist

ORIGINAL SIGNED BY

Ian Hers, Ph.D., P.Eng.
Senior Environmental Engineer, Associate

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VS2DT Users Manual,

APPENDIX I
Discussion on the Methodologies and Equations Used for the Prediction of Hydraulic Conductivity in Saturated Soils

The movement of water through an unsaturated soil is driven by the hydraulic head, in accordance with Darcy's Law. In this sense, the physics of flow is the same for saturated and unsaturated water flow. However, the hydraulic conductivity for unsaturated soil is a function of the soil suction. The following equations describe water flow in the Cartesian coordinate directions, in accordance with Darcy's Law.

$$v_{wx} = -K_{wx} \frac{dh}{dx} \quad \text{[I-1]}$$

$$v_{wy} = -K_{wy} \frac{dh}{dy} \quad \text{[I-2]}$$

$$v_{wz} = -K_{wz} \frac{dh}{dz} \quad \text{[I-3]}$$

where: $K_{wx} = K_{wy} = K_{wz}$ are hydraulic conductivities that are a function of soil suction in each of the Cartesian coordinate directions, and v_{wx}, v_{wy}, v_{wz} = velocity of water flow in the x-, y-, and z-directions

The hydraulic conductivity of an unsaturated soil is strongly influenced by the amount of water in the voids of the soil. The total porosity, pore-size and pore continuity are important properties affecting hydraulic conductivity. The nonlinear functional relationship between soil suction and hydraulic conductivity becomes a convenient form for solving unsaturated soils problems. The soil suction versus hydraulic conductivity relationship is also referred to as the permeability function.

To undertake unsaturated soil seepage analyses, it is necessary to be able to estimate the hydraulic conductivity function for an unsaturated soil. All methodologies to date utilize the soil-water characteristic curve for this purpose.

Hydraulic Conductivity Functions

Numerous mathematical procedures have been proposed for the estimation of the water hydraulic conductivity function, $K_w(\psi)$. These models can be categorized as i.) empirical equations and, ii.) theoretical equations derived as macroscopic and microscopic (statistical) models (Mualem, 1986).

Empirical equations describe the variation in the hydraulic conductivity with soil suction, $K_w(\psi)$, (or with volumetric water content, $K^w(\theta)$). The parameters for the equations are generally determined using a curve-fitting procedure. Some of the empirical hydraulic conductivity equations along with an appropriate reference were given in Table 1 of the text. A more detailed summary of hydraulic conductivity equation is given in Table I-1 of Appendix I. The Brooks and Corey (1964) equation is considered to be both an empirical and a macroscopic model because elements of physics are used to relate pore size distribution to the permeability function.

There are two different groups of **theoretical** models, (i.e., macroscopic approaches and microscopic approaches) based on the statistical assumptions regarding pore distributions and the interpretation applied to the soil-water characteristic curve. The macroscopic models provide an analytical, closed-form equation for the unsaturated hydraulic conductivity function. All **macroscopic models** have the following general form:

$$K_r = S_e^{\eta} \qquad S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad \text{[I-4]}$$

where: K_r is the relative permeability (i.e., any coefficient of permeability divided by the saturated coefficient of permeability), S_e is the effective degree of water saturation, (i.e., where, θ_s and θ_r are the volumetric saturated and the residual water content respectively), and η is a fitting constant.

The value of the fitting parameter η depends on the assumptions made in deriving the hydraulic conductivity equation. Numerous researchers have suggested different values for η (e.g., Averjanov, 1950, η= 4; Yuster, 1951, η= 2; Irmay, 1954, η=3; Corey, 1954, η= 4). The effect of pore-size randomness is neglected in macroscopic models. Brooks and Corey (1964) showed that for a soil with a uniform pore-size distribution index, the exponent η can be assumed to be 3, and in general $\eta = \frac{2 + 3\lambda}{\lambda}$, where λ is the (positive) pore-size distribution index. Mualem (1976) suggested using $\eta = 3 - 2m$, where m is a soil parameter that is positive for coarse-grained soils and negative for fine-grained soils.

Several **statistical models** have been proposed with some of the common models referenced to Childs and Collis-George (1950), Burdine (1953), and Mualem (1976a,b). The saturated hydraulic conductivity and the soil-water characteristic curves are used to solve the integral form of the statistical models and thereby compute a hydraulic conductivity function.

Fredlund et al. (1994) used the Fredlund and Xing (1994) SWCC equation and solved the Childs and Collis-George (1950) model to yield a water hydraulic conductivity function. The procedure involves numerical integration of the form shown in Table I-2. The closed- form hydraulic conductivity functions proposed by van Genuchten (1980), Brooks and Corey (1964) and Campbell (1974) are also shown in Table I-2.

Independent hydraulic conductivity functions can be written for the drying and wetting curves of the SWCC. All hydraulic conductivity functions show that as the water content of the soil decreases on an arithmetic scale, the coefficient of permeability decreases on a logarithmic scale. As a result, the hydraulic conductivity can decrease by several orders of magnitude during de-saturation.

All hydraulic conductivity functions appear to provide reasonable approximations of the hydraulic conductivity from saturated conditions, through the air entry value for the soil and well into the transition zone. All equations produce a similar overall form that responds to the air entry value and the rate of de-saturation of the soil. All of the empirical procedures for the prediction of the hydraulic conductivity function involve the usage of the SWCCs. Figure I-1 shows the use of several functions to predict the hydraulic conductivity function for a particular soil (Ebrahimi-B et al., 2004).

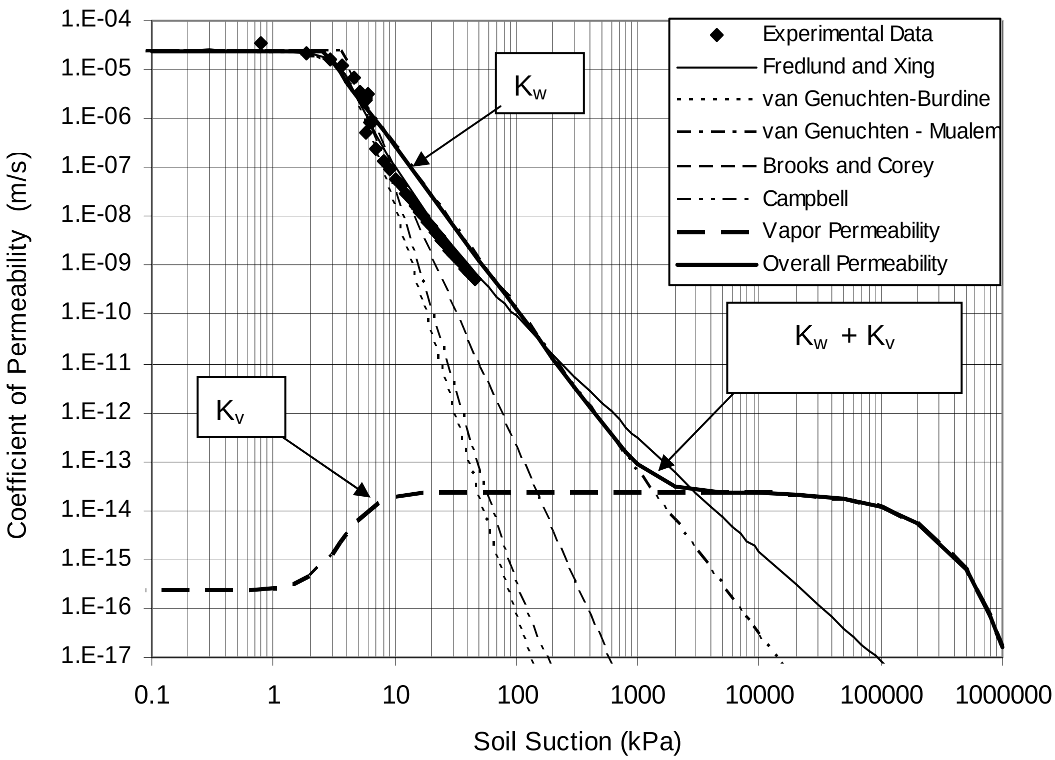

FIGURE I-1: Comparison of several estimated hydraulic conductivity (coefficient of permeability) functions for a particular soil and a suggested lower limit for the permeability function (K_v = vapour conductivity, K_w = water conductivity) (Ebrahimi-B et al., 2004).

Water Storage Functions

The "water storage modulus" is defined as the arithmetic slope, m_2^w, of the (volumetric) water content versus soil suction plot. In other words, the water storage modulus is obtained from the differentiation of the soil-water characteristic curve, SWCC. Even though the SWCC is generally plotted using the logarithm scale for soil suction, it should be noted that the water storage modulus is the slope on an arithmetic scale. The water storage modulus can be obtained through the differentiation of any of the empirical equations that have been proposed for the SWCC. The water storage modulus is required whenever transient or unsteady state seepage processes are being modeled. The differentiation procedure is illustrated in Figure I-2.

1.

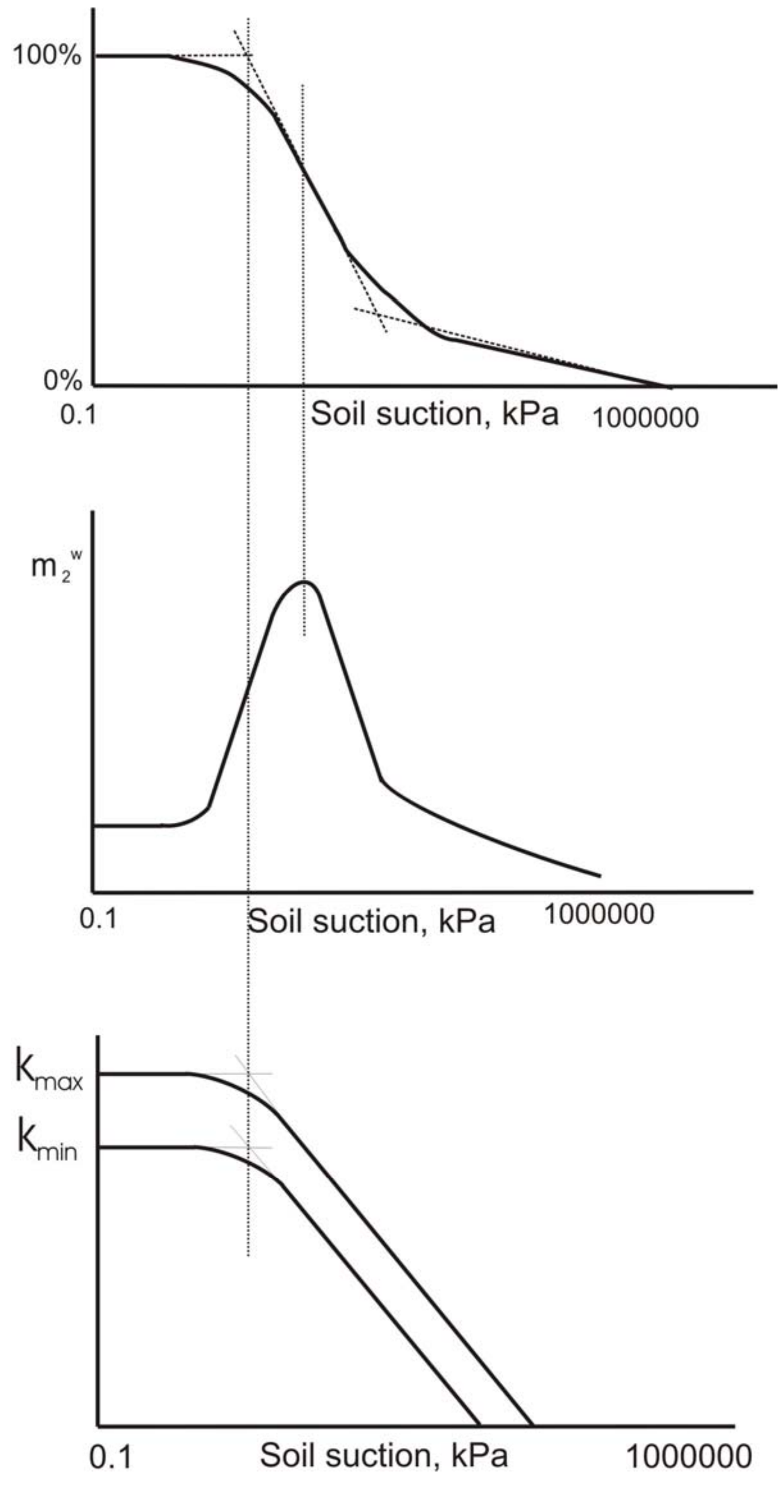

FIGURE 1-2: Example of a hydraulic conductivity functions for an anisotropic soil

TABLE I-1: Some empirical hydraulic conductivity equations

Reference	**Equation**	**Description**
Wind (1955)	$K_w = \alpha\psi^{-n}$	α, and *n* are fitting parameters
Gardner (1958)	$K_w = \dfrac{K_s}{(\alpha\psi^n + 1)}$	α and *n* are fitting parameters
Brooks and Corey (1964)	$K_w = K_s$ for $\psi \le \psi_{aev}$ $K_r = (\dfrac{\psi}{\psi_{aev}})^{-n}$ for $\psi > \psi_{aev}$	
Rijtema (1965)	$K_w = K_s$ for $\psi \ge \psi_{aev}$ $K_r = \exp[-\alpha(\psi - \psi_{aev})]$ for $\psi_1 \le \psi < \psi_{aev}$ $K_w = K_1(\psi/\psi_1)^{-n}$ for $\psi < \psi_1$	ψ_1 = residual soil suction K_1 = hydraulic conductivity at ψ_1

K_w = unsaturated hydraulic conductivity coefficient,

K_s = saturated hydraulic conductivity

$K_r = \dfrac{K_w}{K_s}$ is relative permeability,

ψ = soil suction,

ψ_{aev} = air entry value

w = gravimetric soil water content

TABLE I-2: Some statistical permeability functions based on SWCC and saturated permeability coefficient (Ebrahimi-B. et al., 2004)

	References for the Soil-Water Characteristic Curve			
Permeability Models	van-Genuchten (1980)	Fredlund and Xing (1994)	Brooks & Corey (1964)	Campbell (1974)
Child and Collis- George (1950)	—	$k_r = \dfrac{\int_{\ln(\psi)}^{b} \frac{\theta(e^y)-\theta(\psi)}{e^y}\theta'(e^y)dy}{\int_{\ln(\psi_{aev})}^{b} \frac{\theta(e^y)-\theta_s}{e^y}\theta'(e^y)dy}$	—	$k_r = (\frac{\psi}{\psi_{aev}})^{-2-\frac{2}{b}}$
Burdine (1953)	$k_r(\psi) = \frac{1-(\alpha\psi)^{n-2}[1+(\alpha\psi)^n]^{-m}}{[1+(\alpha\psi)^n]^{2m}}$, $m = 1 - \frac{2}{n}$	—	$k_r(\psi) = (\alpha\psi)^{-2-3\lambda}$	—
Mualem (1976)	$k_r(\psi) = \frac{\{1-(\alpha\psi)^{n-1}[1+(\alpha\psi)^n]^{-m}\}^2}{[1+(\alpha\psi)^n]^{0.5}}$, $m = 1 - \frac{1}{n}$	—	—	—

K_s = saturated hydraulic conductivity

$K_r = \dfrac{K}{K_s}$ is relative permeability,

ψ = soil suction,

ψ_{aev} = air entry value

θ = soil water content,

θ_s = saturated water content

b = Ln (1000000)

y = dummy variable of integration representing the logarithm of integration