PLAXIS LE
Groundwater

1D/2D/3D SATURATED / UNSATURATED
FINITE ELEMENT GROUNDWATER MODELING

Theory Manual

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1 INTRODUCTION

Groundwater flow problems in geotechnical and geo-environmental engineering involve the solution of a partial differential equation referred to as a PDE. The PDE must be solved for all "finite elements" which when combined form a "continuum" (or the geometry of the problem). The theory of groundwater flow expressed in mathematical form embraces the physical behavior of the material (e.g., constitutive laws) and the conservative laws of physics (i.e., conservation of energy). The physical behavior of many materials, (particularly unsaturated soils), is nonlinear and as a consequence, the PDE becomes nonlinear in character. It is well known that the solution of nonlinear PDEs can present a challenge for numerical modeling.

The purpose of the theory manual is to provide the user with details regarding the theoretical formulation of the PDE as well as the numerical method used in the solution. The intent of the theory manual is not to provide an exhaustive summary of all theories associated with groundwater flow. Rather, the intent is to clearly describe details of the theory used in the PLAXIS LE - Groundwater software.

The generic finite element solver solves the partial differential equation for groundwater flow. The solver algorithm has implemented cutting-edge numerical solution techniques that can accommodate linear and highly nonlinear PDEs. The solution technique utilizes adaptive time steps algorithm and automatic mathematically designed mesh generation. The application of these advanced numerical techniques is particularly valuable in solving highly nonlinear and complex problems. Most commonly it is the unsaturated soil portion of the soil continuum that brings in nonlinear soil behavior. The advanced solvers make it possible to obtain converged and accurate solutions for many problems that were previously unsolvable.

The primary attributes of the solution process are as follows:

- Fully automatic mesh generation,
- Integrated climatic calculation of actual evaporation rates
- Handling of seepage face boundary conditions,
- Fully implicit approach in the solver, which provides for a robust solution of difficult models with convergence issues,
- Fluid mass-balance tracking,
- 3-noded triangle and 4-noded quadrilateral elements for 2D analysis and 4-noded tetrahedron elements for 3D analysis,
- Adaptive time stepping
- Automatic generation and control of time steps,
- Newton-Raphson convergence iteration schemes,
- The default preconditioner is the diagonal-block inverse matrix, and

2 FUNDAMENTALS OF SEEPAGE THEORY

The following section presents the fundamentals of the seepage theory implemented in PLAXIS LE - Groundwater. An overview of the PDE's used by the Groundwater module for the analysis of saturated/unsaturated seepage is presented. Several phenomena are considered, including liquid water flow and water vapor flow. The seepage theory is developed based on Darcian flow law, Fick's flow law, and the conservation of mass. The theory presented below is a general outline of the theory needed to solve most seepage problems.

Continuum mechanics principles and partial differential equations (PDEs) have been traditionally used for modeling seepage in saturated/unsaturated soil systems. The partial differential equations governing seepage may involve transient coupled soil-atmosphere processes with nonlinear and heterogeneous soil properties along with nonlinear boundary conditions. Relatively simple steady-state saturated confined flow can also be addressed.

Seepage can be modeled as follows within the context of continuum mechanics principles:

- Identify the physical processes of concern associated with the problem at hand,
- Establish the "continuum variables" acting upon a representative elemental volume (REV) of the medium,
- Develop field equations governing the physical processes of concern by making the assumption that the medium can be considered as a continuum from a macroscopic standpoint (i.e., considering a REV of soil) while using measurable soil properties:
    - Apply conservation laws,
    - Apply verified constitutive laws, and
    - Develop a final system of well-posed determinate partial differential equations.
- Establish initial, internal, and boundary conditions for the problem, and
- Provide a mathematical solution for the PDE or system of PDEs.

A series of assumptions form the backdrop for the derivation of the partial differential equations governing seepage. The following set of assumptions can be considered generally valid:

- Soil phases can be described using a continuum mechanics approach,
- Pore-air and all of its constituents (including water vapor) behave as ideal gases,
- Local thermodynamic equilibrium between the liquid water and water vapor phases exists at all times at any point in the soil, and
- Atmospheric pressure gradients are negligible.

The four assumptions described above may become inadequate under certain situations. For instance, the compressibility of water may have a significant effect in an analysis of regional groundwater systems (i.e., large domains). Therefore, the software provides the capability of taking the compressibility of water into account as part of aquifer storativity (Freeze *et al*. 1979).

2.1 CONSERVATION OF MASS

The conservation of mass of water in a referential element is used to derive the governing equation for saturated/unsaturated seepage. A continuum mechanics framework is used, resulting in the derivation of a differential calculus equation to represent seepage. The assumption is made that the variables involved are continuous and valid from a macroscopic, phenomenological standpoint.

A differential equation for the conservation of mass of water can be derived by considering a REV of soil (Figure 1). The continuity equation can be applied by taking into consideration the flow rates in and out of the REV and equating the difference to the rate of change of mass (or heat) to storage within the REV with time. The following differential equation is obtained by considering three-dimensional flow conditions using the Cartesian coordinate system:

$$-\frac{\partial q_x^w}{\partial x}-\frac{\partial q_y^w}{\partial y}-\frac{\partial q_z^w}{\partial z}=\frac{1}{V_o}\frac{\partial M_w}{\partial t} \qquad \textbf{[1]}$$

where:

q_i^w = total water flow rate in the *i*-direction across a unit area of the soil, *kg/m²-s*; $q_i^w = \rho_w v_i^w$, *kg/m²-s*,

ρ_w = density of water, 1000 *kg/m³*,

v_i^w = water and air flow rate in the *i*-direction across a unit area of the soil, *m/s*,

V_o = referential volume, $V_o = d_x\, d_y\, d_z$, *m³*,

M_w = mass of water within the representative elemental volume, kg, and

t = time, *s*.

The total water flow rate, v^w, also known as specific discharge, is a macroscopic measure of the rate of flow through soils. A measure of the "average actual flow velocity" for a saturated soil can be obtained by dividing v^w by the soil porosity ($n = V_v/V$). The total water flow rate, v^w, can occur as liquid water and/or water vapor flow.

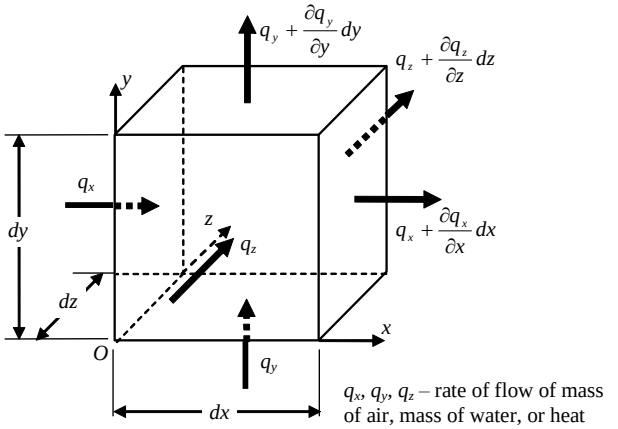

Figure 1 Soil representative elemental volume and fluxes at the element faces

2.1.1 Changes in Volume of Stored Water

The constitutive relationship for the amount of water stored in the soil pores is usually written in terms of the volume of water referenced to the overall total volume. The change in volume of water stored in the soil pores can be expressed as a coefficient of water storage, m_2^w, as follows:

$$\frac{dV_w}{V_o}=m_2^w d\left(u_a-u_w\right) \qquad \textbf{[2]}$$

where:

m_2^w = $\frac{d(V_w/V_o)}{d(u_a-u_w)}=\frac{e}{1+e}\frac{dS}{d(u_a-u_w)}$

V_w/V_o = volumetric water content,

e = void ratio,

S = degree of saturation, and

$(u_a - u_w)$ = matric suction.

The above equation is based on the assumption that changes in the volume of pore-water stored in the soil are a function of soil suction and are independent of changes in total stress. The soil property, m_2^w, is obtained by taking the derivative of the soil-water characteristic curve, swcc, (i.e., the slope), as shown in Figure 2.

Using the derivative of the SWCC provides a smooth transition between saturated and unsaturated conditions, provided that appropriate coefficients of water storage are used. As the soil saturates, the effects of changes in soil suction and changes in effective stresses (in a saturated soil) become equal (i.e., $m_2^w = m_v$). Consequently, for saturated conditions, changes in water volume can be referenced to changes in void ratio. Usually, the value of m_v is considerably lower than the maximum value of m_2^w, which occurs as the soil desaturates.

Numerical difficulties can arise from the use of extremely low values of m_2^w. This is a possible source of convergence problems when modeling ground surface infiltration problems. In order to alleviate convergent difficulties, the value of m_v must be slightly (but not excessively) raised as illustrated in Figure 2.

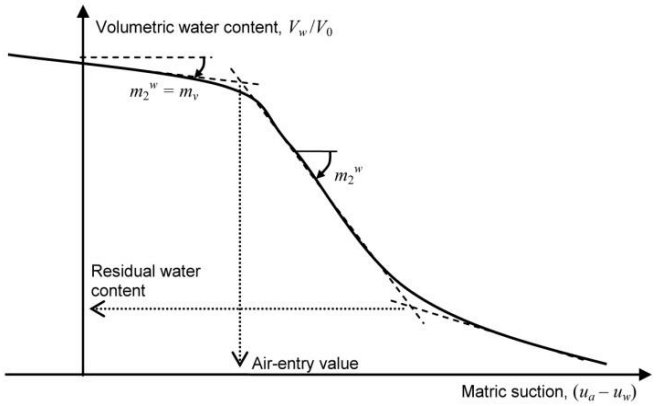

Figure 2 Soil-water characteristic curve showing the water storage characterization at low suction values.

2.2 FLOW LAWS

Table 1 presents an overview of flow laws traditionally used for modeling saturated/unsaturated soil flow. The flow laws establish relationships between measures of flow and driving potentials. Driving potentials can be established based on spatial gradients of the energy stored per unit volume (Bear, 1972). There are several flow equations that have a similar form, but have distinct potentials and different material properties. The flow laws presented in Table **1** have well established equations that have been experimentally verified.

Table 1 **Overview of types of flow within an unsaturated soil and the corresponding mechanisms, driving potentials, and flow laws**

Flow mechanism (1)	Driving Potential (2)	Flow Law (3)
Liquid water	Hydraulic head, h (m)	Darcy's law
Water vapor diffusion	Mass concentration of vapor per unit volume of soil, C_v (kg/m^3)	Modified Fick's law

Pore-air and pore-water have both miscible and immiscible mixture characteristics. Water can flow as liquid water or as water vapor diffusing through the free air-phase. PLAXIS LE - Groundwater takes into account both liquid and vapor flow. Both flow mechanisms are essential in the modeling of certain water flow conditions. For instance, evaporation requires the consideration of the phase change from liquid to vapor water and the flow of water vapor (Wilson et al., 1994).

2.2.1 Flow of Liquid Water

The rate of flow of liquid water in a saturated/unsaturated soil can be described using a generalization of Darcy's Law (Bear, 1972), where the driving mechanism is the total hydraulic head gradient. The hydraulic conductivity is assumed to mainly vary with matric suction in the soil. The generalized Darcy's law can be written as follows:

$$v_{wx} = -k_{wx}(\psi)\frac{\partial h}{\partial x}; \quad v_{wy} = -k_{wy}(\psi)\frac{\partial h}{\partial y}; \quad v_{wz} = -k_{wz}(\psi)\frac{\partial h}{\partial z} \qquad \textbf{[3]}$$

where:

v_{wi} = liquid pore-water flow rate in the *i*-direction across a unit area of the soil due to hydraulic head gradients, *m/s*,

$k_{wi}(\psi)$ = hydraulic conductivity in the *i*-direction, *m/s*. For unsaturated soil, it is the function of soil suction.

ψ = soil suction, *kPa*, which is equal to matric suction, $u_a - u_w$, plus osmotic suction, π,

h = hydraulic head, *m*, which is equal to $\frac{u_w}{\gamma_w} + y$

u_w = pore-water pressure, *kPa*,

u_a = pore-air (gauge) pressure, *kPa*,

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

y = elevation, *m*.

The hydraulic conductivity function, $k_w(\psi)$ provides the relationship between the hydraulic conductivity and the soil suction. The hydraulic conductivity function can also be written in terms of volumetric water content. As a soil dries, there is less and less water present in the soil. Since water will flow only where there is water present, the hydraulic conductivity decreases accordingly as the volumetric water content decreases. This behavior is represented in PLAXIS LE - Groundwater by entering a hydraulic conductivity function for each soil. In the following context, the $k_{wi}(\psi)$ is simplified as k_w.

The use of a continuous k_w function provides a smooth transition between saturated and unsaturated soil conditions. For saturated conditions, k_{wsat} is generally considered a constant and equal to the saturated hydraulic conductivity.

The hydraulic conductivity function can be obtained experimentally using laboratory tests or field tests. The hydraulic conductivity function can also be estimated using the saturated hydraulic conductivity and the soil-water characteristic curve (Fredlund and Xing, 1994). PLAXIS LE - Groundwater provides several options for estimating the hydraulic conductivity function.

2.2.2 Anisotropic Flow of Liquid Water

Natural deposition of soil layers often results in angled layering. The angled layering results in dominant water flow in a direction parallel to the direction of the layering. This observed phenomenon can be simulated in PLAXIS LE - Groundwater by specifying anisotropic angled behavior in either 2D or 3D.

Figure 3 illustrates how angled anisotropy is considered. The angle origin, reference orientation, is in the horizontal direction and the angle increases counter-clockwise.

A mathematical transformation must be performed to translate rotated anisotropic permeability parameters on to the coordinate system used to solve the problem. The general form of the conductivity matrix in two-dimensional problems is as follows (Bear, 1972):

$$\begin{Bmatrix} v_{wx} \\ v_{wy} \end{Bmatrix} = \begin{bmatrix} -k_{wxx} & -k_{wxy} \\ -k_{wyx} & -k_{wyy} \end{bmatrix} \begin{Bmatrix} \frac{\partial h}{\partial x} \\ \frac{\partial h}{\partial y} \end{Bmatrix} \quad \textbf{[4]}$$

where:

$k_{wxx} = \frac{k_{w1} + k_{w2}}{2} + \frac{k_{w1} - k_{w2}}{2} \cos 2\alpha$

$k_{wyy} = \frac{k_{w1} + k_{w2}}{2} + \frac{k_{w1} - k_{w2}}{2} \cos 2\alpha$

$k_{wxy} = \frac{k_{w1} - k_{w2}}{2} \sin 2\alpha$

k_{w1} and k_{w2} are the values of hydraulic conductivity at the principal directions of anisotropy. These values can have constant values for saturated conditions or can vary according to water content in unsaturated soil conditions. The angle α defines the principal directions of anisotropy (Figure 3).

The transformation in 3D is slightly more complex than in 2D. Three angles are required to describe the hydraulic conductivity transformation. The theory for the hydraulic conductivity transformations is not presented in this manual.

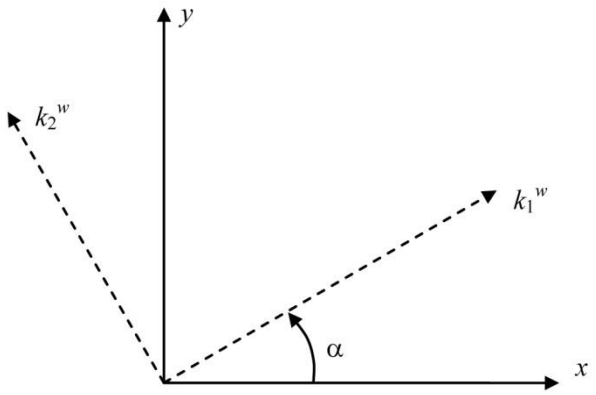

Figure 3 Principal directions of anisotropy in two-dimensions

3 PDE'S FOR SEEPAGE ANALYSIS

The flow law equations (Darcy law and Fick's law), and a water volume change constitutive equation must be combined with the continuity of water mass equation to obtain the partial differential equation that governs the conservation of water mass (i.e., both liquid and vapor). The next sections present the partial differential equations used by PLAXIS LE - Groundwater for the analysis of saturated-unsaturated soil seepage problems.

3.1 ONE-DIMENSIONAL SEEPAGE

One-dimensional seepage analysis is often used for modeling large planar areas. Cover system design is one of many typical applications. The number of nodes normally used in one-dimensional analyses is relatively low when compared to the number of nodes used in two-dimensional analyses. Therefore, computation times are dramatically reduced when adopting a one-dimensional model.

3.1.1 1D Seepage

Considering the reference volume, V_o, and assuming that water is incompressible, the following equation is obtained for one-dimensional transient saturated/unsaturated seepage:

$$\frac{\partial}{\partial y}\left[k_{wy} \frac{\partial h}{\partial y} + k_{vd} \frac{\partial u_w}{\partial y} \right] = -\gamma_w m_2^w \frac{\partial h}{\partial t} \qquad \textbf{[5]}$$

where:

y = coordinate in vertical direction, (corresponding to elevation).

The PDE governing the flow and storage of water within a saturated/unsaturated soil is presented using total head, h, as the primary variable. However, pore-water pressure, u_w, can also be used producing identical results provided the geometry dimension in the y-coordinate is small. It is also possible to use pore-water pressure as the primary variable when studying the dissipation of excess pore-water pressures.

Three soil property functions can be identified for the transient seepage PDE; namely:

- hydraulic conductivity function, k_w,
- vapor conductivity function, k_{vd}, and
- soil-water characteristic curve, whose derivative with respect to soil suction is represented by m_2^w.

The above-mentioned soil properties functions vary with soil suction. Therefore, the PDE is physically nonlinear.

The partial differential equation for water flow is based on the assumption that the rate of water mass flow across a REV is continuously distributed in space. Therefore, the spatial distribution of water flow rate can be described using the partial derivative of water flow in a particular direction. These comments apply to the all the seepage PDEs presented in the next sections.

For steady-state conditions, the PDE for liquid and vapor water flow reduces to the following equation:

$$\frac{\partial}{\partial y}\left[k_{wy} \frac{\partial h}{\partial y} + k_{vd} \frac{\partial u_w}{\partial y} \right] = 0 \qquad \textbf{[6]}$$

The hydraulic conductivity can be considered as being constant when solving saturated seepage problems. Therefore, the PDE for saturated and unsaturated water seepage has the same form.

3.2 TWO-DIMENSIONAL SEEPAGE

Two-dimensional seepage analysis is used for modeling cross-sections passed through elongated geometries, such as an earth dam.

3.2.1 2D Seepage

Assuming the reference volume, V_o, remains constant and the water is incompressible, the following equation can be written for transient saturated/unsaturated seepage:

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}+k_{vd}\frac{\partial u_w}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}+k_{vd}\frac{\partial u_w}{\partial y}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \quad \textbf{[7]}$$

where:

x = horizontal direction, and

y = vertical direction, (corresponding to elevation).

The partial differential equation, PDE, is presented for anisotropic properties with the principal direction of anisotropy corresponding to the x- and y-directions. Anisotropic material properties that do not coincide with the Cartesian coordinate axis can be considered as presented in the previous chapter.

For steady-state conditions, the water storage portion of the equation is set to zero and the PDE reduces to the following equation:

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}+k_{vd}\frac{\partial u_w}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}+k_{vd}\frac{\partial u_w}{\partial y}\right]=0 \quad \textbf{[8]}$$

The governing PDE for steady state seepage can be further reduced by assuming vapor flow is negligible and soil is saturated. The resulting PDE can be considered to be in its simplest form for two-dimensional seepage.

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}\right]=0 \quad \textbf{[9]}$$

3.3 THREE-DIMENSIONAL SEEPAGE

Three-dimensional seepage analysis is often used when the problem geometry cannot be adequately represented by a one-dimensional column, a two-dimensional, a plan, or an axisymmetric model.

3.3.1 3D Seepage

The PDE used in PLAXIS LE - Groundwater for the solution of three-dimensional transient saturated/unsaturated seepage problems is as follows:

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}+k_{vd}\frac{\partial u_w}{\partial x}\right]+\frac{\partial}{\partial z}\left[k_{wz}\frac{\partial h}{\partial z}+k_{vd}\frac{\partial u_w}{\partial z}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}+k_{vd}\frac{\partial u_w}{\partial y}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \quad \textbf{[10]}$$

where:

x = first horizontal direction,

z = second horizontal direction, orthogonal to the *x*-direction, and

y = vertical direction, corresponding to elevation

The partial differential equation for flow in the three main orthogonal directions is equal to the flow along each direction, (i.e., the *x*, *y*, and *z*-directions). For steady-state conditions, the PDE for seepage reduces to the following equation:

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}+k_{vd}\frac{\partial u_w}{\partial x}\right]+\frac{\partial}{\partial z}\left[k_{wz}\frac{\partial h}{\partial z}+k_{vd}\frac{\partial u_w}{\partial z}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}+k_{vd}\frac{\partial u_w}{\partial y}\right]=0 \quad \textbf{[11]}$$

Neglecting vapor flow and assuming the soil is saturated, the PDE governing steady state seepage reduces to:

$$\frac{\partial}{\partial x}\left[k_{wx}\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial z}\left[k_{wz}\frac{\partial h}{\partial z}\right]+\frac{\partial}{\partial y}\left[k_{wy}\frac{\partial h}{\partial y}\right]=0 \quad \textbf{[12]}$$

3.4 UNSATURATED FLOW EQUATION

A transient-state seepage problem in which the permeability and volumetric water content variables change in accordance with soil suction is common to geotechnical engineering. The fluid motion in unsaturated soils is generally assumed to obey the partial differential equations presented in the previous chapter. These equations are similar to the classical Richards equation (Hillel, 1980). The PDEs for water seepage in unsaturated soils can be written in several forms. The three most common formulations of the unsaturated flow equation are identified as the "*h*-based" form, the "*q*-based" form, and the "mixed form". There are advantages and disadvantages associated with each of the formulations. The advantages and disadvantages become apparent when solving particular unsaturated seepage problems.

There are several advantages associated with the *q*-based form. One advantage is that it can be formulated to be perfectly water mass conservative. It is not commonly used, however, because this form degenerates in fully saturated systems and material discontinuities produce discontinuous *q* profiles.

The *h*-based form of the PDE seepage equation is the most commonly implemented form. Its primary drawback is that it can suffer from poor water mass balance when solving transient seepage problems. The poor water mass balance problem is exacerbated in situations where the soil-water characteristic curve for the material is highly nonlinear.

Celia (1990) proposed a "mixed form" of the Richards equation. The "mixed form" was designed to improve the water mass-balance of the "*h*-based" formulation.

3.4.1 H-Based Formulation

The most commonly implemented form of the governing partial differential equation for transient seepage is shown below. The PLAXIS LE - Groundwater formulation is presented here and is based on total head:

$$\frac{\partial}{\partial x}\left[\left(k_{wx}+k_{vd}\right)\frac{\partial h}{\partial x}\right]+\frac{\partial}{\partial y}\left[\left(k_{wy}+k_{vd}\right)\frac{\partial h}{\partial y}-k_{vd}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \qquad \textbf{[13]}$$

The partial differential equation governing water flow and the storage of water within a saturated/unsaturated soil is formulated using total head, *h*, as the primary variable. However, pore-water pressure, u_w, (written as a water head, u_w/γ_w), can be used when solving certain seepage problems.

The formulations presented above satisfy the condition that the difference between the water flow entering or leaving a unit volume is equal to the change in volumetric water content. Under steady-state conditions, the water flux entering and leaving a unit volume is the same and as a consequence, the storage term (i.e., right-hand side of the equation) becomes zero.

The above formulation makes the assumptions that there is no loading or unloading of the soil mass during the transient process. Pore-air pressures are assumed to remain constant and at atmospheric pressure. Changes in volumetric water content are assumed to be strictly dependent on changes in the soil suction state variable.

4 BOUNDARY CONDITIONS IN SEEPAGE

Several types of boundary conditions can be applied when solving seepage problems. The boundary conditions associated with seepage are as follows:

- Natural (or Neumann) boundary condition: flux,
- Essential (or Dirichlet) boundary conditions: imposed value, and
- Special boundary conditions: combinations of the above conditions.

The two basic boundary conditions intrinsically related to the formulations normally used in the finite element solutions are: Essential (or Value) boundary condition and Natural boundary conditions. Essential boundary conditions are assigned to nodes as fixed values. Natural boundary conditions are assigned to the sides of elements (and are defined by a surface integral). Natural boundary conditions correspond to the surface integral of the term inside the outer derivative of second order partial differential equations.

4.1 NATURAL BOUNDARY CONDITION

Natural (or Neumann) boundary conditions arise from the integration by parts of second order derivatives. The integration results in a surface integral that corresponds to a flux quantity. Therefore, natural boundary condition associated with the seepage PDE corresponds to the total amount of water flow normal to the surface (m^3/s).

$$\text{Natural boundary condition} = \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) dS \qquad \textbf{[14]}$$

where:

Γ = boundary area,

v = total flux vector,

n = outward surface-normal vector, and

dS = an infinitesimal element at the boundary.

Natural boundary conditions are called "flux boundary conditions" in PLAXIS LE - Groundwater.

Natural boundary conditions are appropriate choices for the representation of situations such as simple soil-atmosphere fluxes, the water uptake inside a well, and the groundwater flow taking place at the bottom of a domain. The absence of a boundary condition corresponds to a zero flux natural boundary condition.

Natural boundary conditions can be applied as constant values). An expression can be a function of time, space, or any other meaningful variable. Flux expressions can be used to represent several hypothetical and real world scenarios such as the increase in water uptake in a well during the course of a day or the increase in groundwater flow with depth.

The natural boundary conditions associated with the seepage PDEs do not make a distinction between the types of flow (i.e., whether it is liquid or vapor flow). The determination of the amount of flow taking place in the form of a liquid or a vapor is not required for the application of a natural boundary condition.

For instance, the imposition of a negative flux at a soil surface can result in both liquid and vapor fluxes at the surface. The partitioning of the imposed total flux into vapor and liquid flux will depend on the soil properties and pore-water pressures. Nevertheless, the total amount of flux at the surface will always correspond to the applied boundary conditions. The fractions of liquid and vapor flow can be determined from the resulting pore-water pressure gradients, temperature gradients and the soil property functions.

4.1.1 Differences Between Actual and Applied Boundary Flux

It is possible that a natural boundary condition might apply more fluid at the boundary than the model can reasonably accept. This is particularly true when running numerical models which are saturated. The mass-balance of the modeling domain must be of primary consideration. Therefore, if the user applies a large boundary flux which cannot be accepted by the modeling domain, then the natural boundary condition will need to be reduced to represent the flux which can be applied while maintaining an appropriate mass balance over the modeling domain. The excess flux which is not applied is conceptually similar to "runoff" but this type of runoff may be present even if the "runoff" specifier in the software is not specified.

4.2 ESSENTIAL BOUNDARY CONDITION

Essential (or Dirichlet) boundary conditions correspond to predetermined hydraulic head values.

$$\text{Essential Boundary Condition} = h \qquad \textbf{[15]}$$

where:

h = specified hydraulic (total) head value = $\frac{u_w}{\gamma_w} + y$

u_w = pore-water pressure,
γ_w = unit weight of water,
y = elevation (y in a model).

This type of boundary condition is called "head" or "hydraulic head" in PLAXIS LE - Groundwater. Essential boundary conditions can be used to represent numerous situations such as the head imposed by a water reservoir (Figure 4) or the head at the bottom of a domain where the water table is relatively constant. Essential boundary conditions are always required in steady-state problems. Transient problem may or may not present an essential boundary condition.

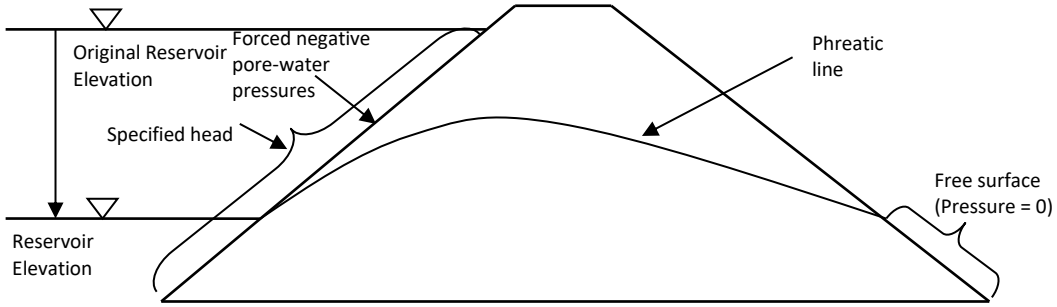

Figure 4 Head upstream boundary conditions in the case of rapid drawdown simulation

Essential boundary conditions can be applied as constant values.Similar to the natural boundary condition, an expression can be a function of time, space, or any other meaningful variable. Head expressions can be used to represent several hypothetical and real world scenarios such as the increase in the filling of a reservoir or transient heads imposed by tides.

Essential boundary conditions must be consistent with the initial conditions of a problem. Discontinuity not only misrepresents the actual problem, but also results in numerical oscillations. For instance, the simulation of a sudden reduction in pore-water pressure at a surface should always be done using the ramping of head over time, starting with an initial head equal to initial conditions. An appropriate ramping time interval that represents the actual rate of change should be selected.

The user must be careful when applying a head boundary condition to the upstream side of an earth levee or dam during a rapid drawdown scenario. The head boundary condition may be inappropriate for some situations as it inherently forces unsaturated soil conditions above the water table. Professional judgment is needed to determine whether or not the "forcing" of negative pore-water pressures is appropriate within the context of the problem under consideration.

4.2.1 Review Boundary Condition (Drain)

More complex boundary conditions are required in order to model certain seepage problems. An example is the situation of a free drainage surfaces with an unknown seepage exit point. This situation commonly occurs on the downstream slope of an earth fill dam (Figure 5). The downstream face of the dam can be represented as a modification of the natural and essential boundary conditions.

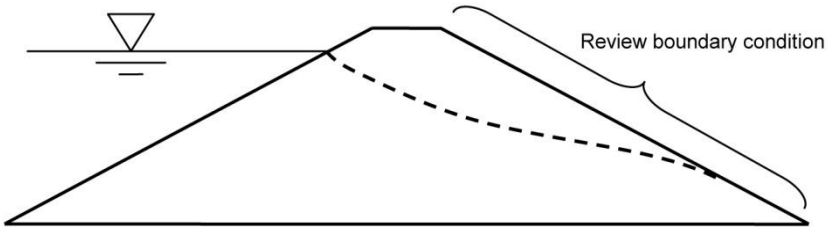

Figure 5 "Review boundary" condition for a free flow surface

The boundary condition used to represent the free flow condition is shown in Figure 5. The boundary is called a "Review boundary condition" in PLAXIS LE - Groundwater. The terminology "drain boundary condition" is sometimes used to refer to this type of boundary condition.

A review boundary condition is applied as follows:

- If pore-water pressures are negative, then the boundary condition has zero flux,

- If pore-water pressure is positive, then the boundary condition is equal to a negative (outward) flux that brings pore-water pressures on the surface to zero.

If the amount of negative flux is large, changes at the boundary will take place nearly instantaneously. A large negative flux is equivalent to setting the essential boundary condition equal to the elevation relative to the datum:

$$h = y \qquad \textbf{[16]}$$

The essential boundary condition creates another degree of nonlinearity in the system that must be solved through the use of an iterative process. Another type of special boundary condition available in PLAXIS LE - Groundwater is called the "climate boundary condition".

Climate boundary conditions are used to model complex soil-atmosphere fluxes. Additional input data is required in order to use climatic boundary conditions. The following chapter presents the theory for this type of boundary condition.

4.3 GRADIENT OR UNIT GRADIENT BOUNDARY CONDITION

The gradient or unit gradient boundary condition may be applicable in certain cirmustances, where the user wants to control the flow out of the model by controlling of hydraulic head gradient. The rate of water flow can be described using Darcy's law (see section 2.2.1). The rate of water flow can be written as:

$$q = -kA\frac{dh}{dl} \qquad \textbf{[17]}$$

where:

q	= rate of water flow (volume per unit time)
k	= hydraulic conductivity of the medium,
A	= cross-sectional area of the column through which the water flows through,
dh/dl	= hydraulic gradient, that is, the change in head over the length of interest.

For a unit gradient boundary condition, $dh/dl = 1$. This type of boundary condition is typically applied to the bottom of a 1D numerical model when performing cover design as there is reasonable precedence for the unit gradient boundary condition in the cover design application. The solver implicitly applies $dh/dl = 1$ and no value is required to input from the user. For a gradient boundary condition, a value other than 1 can be entered by the user. Since the gradient boundary conditions assume the flow is always outward of the model, the entered gradient value should not be negative. The recommended value should be in the range of $0 < dh/dl <= 1$.

The current implementation allows control of the gradient in one direction only, i.e., the flow to move outward in the vertical direction only. Hence, the recommended use of a gradient or unit gradient boundary condition is at the bottom of the model only.

4.4 INITIAL WATER TABLE

Initial pore-water pressure conditions can be calculated assuming hydrostatic conditions and the following equation:

$$u_w = \gamma_w \left(h - y\right) \qquad \textbf{[18]}$$

where:

u_w	= pressure, *kPa*,
γ_w	= unit weight of water, kN/m^3,
h	= total water head, *m*, and
y	= elevation, *m*.

Therefore,

when	$h = y$	$u_w = 0$; represents the phreatic surface
when	$h > y$	$u_w > 0$; represents the saturated region
when	$h < y$	$u_w < 0$; represents the unsaturated region

Defining a water table as initial conditions is well-suited for some situations requiring a quick solution. For more complex situations, using hydrostatic conditions may not be realistic and may cause convergence problems. To overcome convergence problems with complex models it is best to import the initial head conditions from a steady-state run of the model.

5 FLUX SECTIONS

In PLAXIS LE - Groundwater, the flux of water across a user-defined section can be determined in either steady state or transient analysis. This flux section tool is used to calculate water fluxes into or out of a specific line segment, region segment or other places of interest. Some common applications are to determine the amount of seepage on the downstream face of a dam or below cut-off walls.

5.1 FLUX SECTION THEORY CALCULATION

The theoretical calculation of flux section is illustrated in this section. Refer to Figure 6 for a diagram illustrating the theory. A 3-noded linear triangular element is used to demonstrate the theory and the flux of water across section A-A is calculated. The line section A-A crosses the element at points *a* and *b* with Cartesian (global) coordinates, (x_a, y_a) and (x_b, y_b), respectively. Point *C* (*x, y*) is at the center of the flux section, and water flux passing this point is defined as (Bathe, 1982):

$$\mathbf{q} = \begin{Bmatrix} q_x \\ q_y \end{Bmatrix} = -\mathbf{DB}(x,y)\mathbf{H} \qquad \textbf{[19]}$$

where:

q_x = flux in *x*-direction

q_y = flux in *y*-direction

D = material property matrix

B = matrix for head gradient interpolation, and

H = vector of of total head at the element nodes

The **D** matrix for an isotropic material is defined as:

$$\mathbf{D} = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix} \qquad \textbf{[20]}$$

The **B** matrix is defined as:

$$\mathbf{B} = \begin{bmatrix} \dfrac{\partial N_1}{\partial x} & \dfrac{\partial N_2}{\partial x} & \dfrac{\partial N_3}{\partial x} \\ \dfrac{\partial N_1}{\partial y} & \dfrac{\partial N_2}{\partial y} & \dfrac{\partial N_3}{\partial y} \end{bmatrix} \qquad \textbf{[21]}$$

where:

N_1, N_2, N_3 = shape functions at nodes 1, 2 and 3, respectively

The **H** is the total head vector of the element nodes:

$$\mathbf{H} = \begin{bmatrix} H_1 \\ H_2 \\ H_3 \end{bmatrix} \qquad \textbf{[22]}$$

where:

H_1, H_2, H_3 = the total head at nodes 1, 2 and 3, respectively

The total head at a point (*x, y*) within the element can be defined using the shape functions and head values at the nodes as:

$$H(x,y) = \sum_{i=1}^{3} N_i H_i \qquad \textbf{[23]}$$

The above shape functions are usually expressed in local (natural) coordinates and for triangular elements (shown in Figure 7) they are defined as:

$$\begin{aligned} N_1 &= 1-\alpha-\beta \\ N_2 &= \alpha \\ N_3 &= \beta \end{aligned} \qquad \textbf{[24]}$$

The **B** matrix can be rewritten as:

$$\mathbf{B} = \begin{bmatrix} \frac{\partial x}{\partial \alpha} & \frac{\partial y}{\partial \alpha} \\ \frac{\partial x}{\partial \beta} & \frac{\partial x}{\partial \beta} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial N_1}{\partial \alpha} & \frac{\partial N_2}{\partial \alpha} & \frac{\partial N_3}{\partial \alpha} \\ \frac{\partial N_1}{\partial \beta} & \frac{\partial N_1}{\partial \beta} & \frac{\partial N_1}{\partial \beta} \end{bmatrix} = \mathbf{J}^{-1} \begin{bmatrix} \frac{\partial N_1}{\partial \alpha} & \frac{\partial N_2}{\partial \alpha} & \frac{\partial N_3}{\partial \alpha} \\ \frac{\partial N_1}{\partial \beta} & \frac{\partial N_1}{\partial \beta} & \frac{\partial N_1}{\partial \beta} \end{bmatrix} \quad \textbf{[25]}$$

The matrix $\mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \alpha} & \frac{\partial y}{\partial \alpha} \\ \frac{\partial x}{\partial \beta} & \frac{\partial x}{\partial \beta} \end{bmatrix}$ is called Jacobian matrix and $\mathbf{J}^{-1}$ is the inverse of **J**.

For iso-parameter elements, the same shape functions are used to determine coordinates of a point (*x, y*) within the element in global coordinates.

$$x = \sum_{i=1}^{3} N_i x_i$$
$$y = \sum_{i=1}^{3} N_i y_i \quad \textbf{[26]}$$

Combining the equations **[19]**, **[20]**, **[22]** and **[25]**, the flux vector $q(q_x, q_y)$ at the centre point of the flux section is determined. The flux crossing the flux section is determined as:

$$\|q\| = \sqrt{q_x^2 + q_y^2}$$
$$l = \sqrt{(x_a - x_b)^2 + (y_a - y_b)^2}$$
$$\begin{Bmatrix} Q_x \\ Q_y \end{Bmatrix} = \begin{Bmatrix} q_x & 0 \\ 0 & q_y \end{Bmatrix} \begin{Bmatrix} \|x_a - x_b\| \\ \|y_a - y_b\| \end{Bmatrix} \quad \textbf{[27]}$$

The normal flux across the flux section is determined as:

$$Q_n = (\mathbf{q} \cdot \mathbf{n}) \times l \quad \textbf{[28]}$$

where:

n	= unit normal vector to the flux section shown in Figure 6
l	= length of the flux section
Q_x, Q_y, Q_n	= fluxes in *x*-, *y*-directions and normal flux across the flux section, respectively

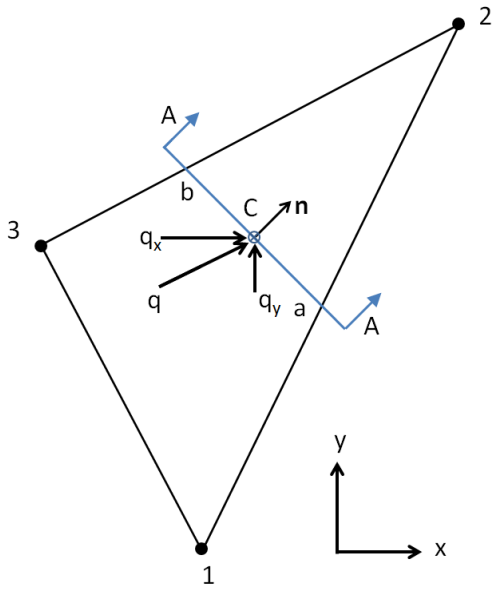

Figure 6. Flux section calculation for a 3-noded element

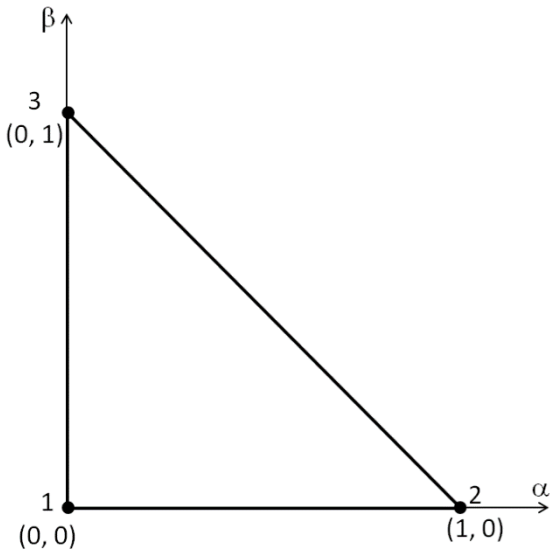

Figure 7. 3-noded element in local (natural) coordinates

6 MATERIAL PROPERTIES

This section will present the theory behind material properties used in the PLAXIS LE - Groundwater modeling software.

6.1 SOIL-WATER CHARACTERISTIC CURVE

The *soil-water characteristic curve* is central to the application of unsaturated soil mechanics. It defines the nonlinear relationship between the amount of water in the soil (i.e., water content) and soil suction. Historically, the amount of water in the soil has been represented using the volumetric water content variable. However, other designations such as the degree of saturation of the soil prove to be superior designations of the amount of water in the soil when the soil undergoes volume change as soil suction is increased. Representation of the soil-water characteristic curve is accomplished either through fitting existing data or estimating the curve from grain-size information.

6.1.1 Fredlund and Xing (1994) Equation

Fredlund and Xing (1994) presented a three-parameter equation with the flexibility to fit a wide range of materials. The equation also contained a correction variable that provided increased accuracy in the high suction range. The parameters of the equation were typically found using a least-squares algorithm. The original form of the equation was as follows.

$$\theta_w = \theta_s \left[1 - \frac{In\left(1+\frac{\psi}{h_r}\right)}{In\left(1+\frac{10^6}{h_r}\right)} \right] \left[\frac{1}{\left[In\left[\exp(1) + \left(\frac{\psi}{a_f}\right)^{nf} \right] \right]^{mf}} \right] \quad \textbf{[29]}$$

where:

ψ = soil suction value (*kPa*).

θ_w = volumetric water content at soil suction, ψ,

θ_s = saturated volumetric water content,

a_f = material parameter which is primarily related to the air-entry value of the soil in *kPa*,

n_f = material parameter which is primarily a function of the rate of water extraction from the soil once the air-entry value has been exceeded,

m_f = material parameter which is primarily a function of the residual water content,

h_r = suction at residual water content (*kPa*), and

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of volumetric water content versus soil suction.
Applicable material types: All soils

6.1.2 Fredlund (2000) Bimodal Equation

The bimodal equation can be viewed as two superimposed unimodal SWCC curves. The fitting algorithm fits the bimodal equation by subdividing the overall curve into an upper and lower portion. Each of the two portions is then fit with a nonlinear least squares regression algorithm and the results are then combined through the use of superposition. The breaking point between the two curves is designated using the *w* parameter which must be selected by the analyst.

$$w = w_s \left\{ s \left[\frac{1}{\ln\left(\exp(1) + \left(\frac{a_{fb}}{\psi} \right)^{n_{fb}} \right)^{m_{fb}}} \right] + (1-s) \left[\frac{1}{\ln\left(\exp(1) + \left(\frac{j_{fb}}{\psi} \right)^{k_{fb}} \right)^{l_{fb}}} \right] \right\} \left[1 - \left(\frac{\ln\left(1+\frac{\psi}{3000}\right)}{\ln\left(1+\frac{1000000}{3000}\right)} \right) \right] \quad \textbf{[30]}$$

where:

w = gravimetric water content at any soil suction,

w_s = gravimetric water content at any soil suction,

ψ = soil suction, *kPa*,

a_{fb} = fitting parameter,

n_{fb} = fitting parameter,

m_{fb} = fitting parameter,

j_{fb} = fitting parameter, *kPa,*

k_{fb} = fitting parameter,

l_{fb} = fitting parameter, and

s = Fredlund bimodal split

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of volumetric water content versus soil suction.
Applicable material types: All soils

6.1.3 Van Genuchten (1980) Equation

Van Genuchten (1980) presented a three-parameter equation with the flexibility to fit a wide range of materials. The parameters of the equation could be found using a least-squares algorithm.

$$w_w = w_{rvg} + \left(w_s - w_{rvg}\right)\left[\frac{1}{\left[1+\left(a_{vg}\psi\right)^{n_{vg}}\right]^{m_{vg}}}\right] \quad \textbf{[31]}$$

where:

w_w = gravimetric water content at any soil suction,

w_{rvg} = residual gravimetric water content,

w_s = saturated gravimetric water content,

a_{vg} = material parameter which is primarily a function of the air-entry value of the soil in *kPa*,

n_{vg} = material parameter which is primarily a function of the rate of water extraction from the soil once the air-entry value has been exceeded, and

m_{vg} = fitting parameter, and

ψ = soil suction (*kPa*).

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of gravimetric water content versus soil suction. It should be noted that data points well beyond residual suction conditions may distort the best-fit analysis.
Applicable material types: All soils

6.1.4 Van Genuchten (1980) and Mualem (1976) Equation

Van Genuchten (1980) proposed a closed form simplification for solving the Mualem (1976) integral equation. The relationship between the *m* and *n* parameters of the van Genuchten (1980) equation was first prescribed in order to reduce the number of fitting parameters from three to two. The simplification proposed by Mualem (1976) is shown below.

$$w_w = w_{rm} + \left(w_s - w_{rm}\right)\left[\frac{1}{\left[1+\left(a_m\psi\right)^{n_m}\right]^{\left(1-\frac{1}{n_m}\right)}}\right] \quad \textbf{[32]}$$

where:

w_w = gravimetric water content at any soil suction,

w_{rm} = residual gravimetric water content,

w_s = saturated gravimetric water content,

a_m = material parameter which is primarily a function of the air-entry value of the soil in *kPa*,

n_m = material parameter which is primarily a function of the rate of water extraction from the soil once the air-entry value has been exceeded, and

ψ = soil suction (*kPa*).

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of gravimetric water content versus soil suction.
Applicable material types: All soils

6.1.5 Gardner (1958) Equation

Gardner (1958) presented a continuous equation for the first coefficient of permeability function. The form of the equation has subsequently been the basis for the soil-water characteristic curve as well as many other equations proposed in subsequent literature. However, it should be noted that the equation was originally proposed as an equation to best-fit measured permeability data.

$$w_w = w_{rg} + \left(w_s - w_{rg}\right)\left[\frac{1}{\left[1 + a_g \psi^{n_g}\right]}\right] \quad \textbf{[33]}$$

where:

w_w = gravimetric water content at any soil suction,

w_{rg} = residual gravimetric water content,

w_s = saturated gravimetric water content,

a_g = material parameter which is primarily a function of the air-entry value of the soil in *kPa*,

n_g = material parameter which is primarily a function of the rate of water extraction from the soil once the air entry value has been exceeded, and

ψ = soil suction (*kPa*).

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of gravimetric water content versus soil suction.
Applicable material types: All soils

6.1.6 Brooks and Corey (1964) Equation

Brooks and Corey (1964) proposed a power-law relationship for the SWCC. The model represented an attempt to use an equation to describe the soil-water characteristic curve. The equation can be written as follows:

$$w_w = w_r + \left(w_s - w_r\right)\left[\frac{a_c}{\psi}\right]^{n_c} \quad \textbf{[34]}$$

where:

w_w = gravimetric water content at any soil suction,

w_r = residual gravimetric water content,

w_s = saturated gravimetric water content,

a_c = bubbling pressure (*kPa*),

n_c = pore size distribution index (dimensionless), and

ψ = soil suction (*kPa*).

Fitting method: Least squares nonlinear regression
Required input: Drying laboratory data consisting of points on the curve of gravimetric water content versus soil suction.
Applicable material types: All soils

6.1.7 Zapata Estimation (2000)

Zapata (2000) performed a statistical regression analysis on a sampling of soils from 50 states in the USA. The regression led to "average" recommended curves based on categorization groupings as fine or coarse-grained soils. The average values for the SWCCs were further grouped according to plasticity index (PI). This estimation method provides a simple approximate method for the user to enter simple information about the SWCC for a soil and can be best-fit with the Fredlund and Xing (1994) fitting parameters.

6.2 HYDRAULIC CONDUCTIVITY FIT METHODS

The PLAXIS LE - Groundwater software implements Gardner's equation for fitting unsaturated permeability data.

6.2.1 Gardner's (1958) Equation

Gardner (1958) permeability function for unsaturated soils is expressed as a function of suction:

$$k_w = \frac{k_s}{1 + a\left\{\frac{\psi}{\rho_w g}\right\}^n} \qquad \textbf{[35]}$$

where:

k_w = hydraulic conductivity or permeability of the water phase,

k_s = saturated hydraulic conductivity of the water,

ρ_w = density of water,

a = fitting parameter,

n = fitting parameter,

g = acceleration of gravity, and

ψ = soil suction (*kPa*).

Fitting method: Least squares nonlinear regression
Required input: Laboratory data consisting of at least three points.
Applicable material types: All soils.

The Gardner (1958) equation provides a flexible permeability function that is defined using two parameters, *a* and *n.* The parameter, *n* defines the slope of the function, and *a* is a parameter related to the breaking point of the function. The Gardner (1958) equation is meant to be obtained from laboratory data.

Figure 8 shows the sensitivity of the parameters, *a* and *n*. The permeability function has been quite often used in saturated-unsaturated flow modeling. The Gardner (1958) equation is sensitive to the air-entry value of the soil and the rate of desaturation. These features are modeled in a continuous manner.

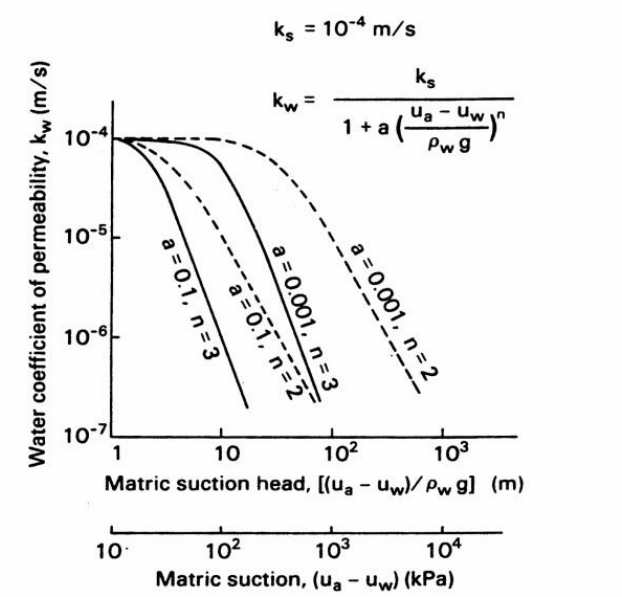

Figure 8 Sensitivity of Gardner's (1958) equation for the coefficient of permeability as a function of the matric suction (from Fredlund and Rahardjo, 1993)

A set of data is presented in Figure 9 to demonstrate the ability of the Gardner (1958) equation to fit laboratory data of the coefficient of permeability for various soils. The equation is easy to apply for saturated-unsaturated flow modeling.

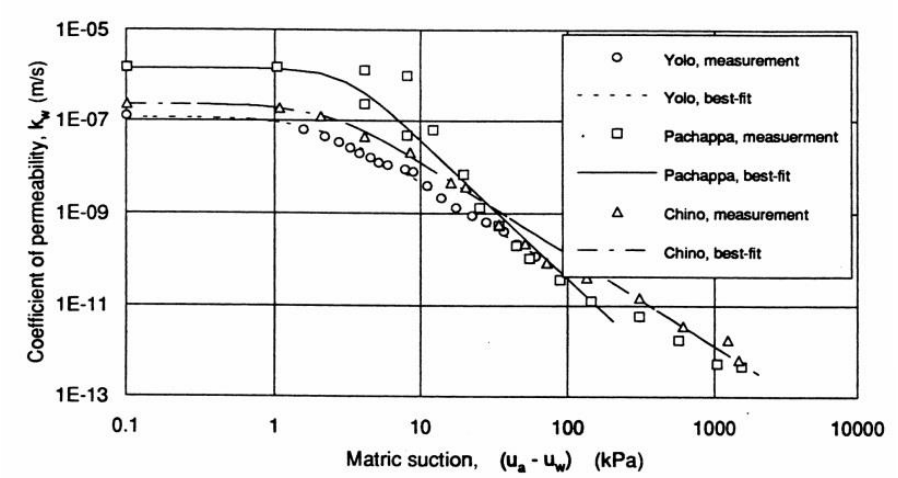

Figure 9 Comparison between the measured and the predicted coefficient of permeability values for different materials using the Gardner (1958) equation (from Huang et al., 1994)

6.3 HYDRAULIC CONDUCTIVITY ESTIMATION

Estimation methods (also known as pedo-transfer functions) are provided in the PLAXIS LE - Groundwater software in order to facilitate the estimation of the unsaturated portion of the hydraulic conductivity curve. Most estimation methods are based on a description of the soil-water characteristic curve and therefore require a specific fit to be present in the software. Commonly used estimation methods are provided in the following sections.

6.3.1 Brooks and Corey Estimation

Estimation methods (also known as pedo-transfer functions) are provided in the PLAXIS LE - Groundwater software in order to facilitate the estimation of the unsaturated portion of the hydraulic conductivity curve. Most estimation methods are based on a description of the soil-water characteristic curve and the saturated coefficient of permeability. Specific fits for the hydraulic conductivity are present in the PLAXIS LE - Groundwater software. Commonly used estimation methods are provided in the following sections.

$$k = k_{sat}\left(\frac{\psi_b}{\psi}\right)^{2+3\lambda} \quad \text{for suction, } \psi > \psi_b$$
$$k = k_{sat} \quad \text{for suction, } \psi \leq \psi_b \qquad \textbf{[36]}$$

where:

k = hydraulic conductivity (or coefficient of permeability) with respect to the water phase, *m/s*

k_{sat} = saturated hydraulic conductivity with respect to the water, *m/s*

ψ_b = Brooks and Corey (1964) soil-water characteristic curve fitting parameter,

λ = Brooks and Corey (1964) soil-water characteristic curve fitting parameter,

ψ = soil suction, *kPa*.

Required input: Saturated hydraulic conductivity and a fit of the soil-water characteristic curve using the Brooks and Corey (1964) equation.

Applicable material types: All soils

The Brooks and Corey (1964) equation that fits some soil-water characteristic curve data can be written in the form of a power-law relationship.

$$\Theta = \left(\frac{\psi_b}{\psi}\right)^{\lambda} \quad \text{for suction, } \psi \geq \psi_b \qquad \textbf{[37]}$$

where:

Θ = normalized water content (defined in Equation **[38]**),

ψ_b = air-entry value,

ψ = any suction, and

λ = pore-size distribution index.

The normalized volumetric water content, Θ, is defined as follows:

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad \textbf{[38]}$$

where:

θ_s = saturated volumetric water content, and

θ_r = residual volumetric water content.

Equation **[40]** is suitable for fitting laboratory SWCC data for coarse materials that have a low air-entry value.

Brooks and Corey (1964) also suggested a procedure for estimating the residual water content. The Brooks and Corey (1964) permeability function is based on the model of a porous media developed by Burdine (1953), Kozeny (1927), and Wyllie and Gardner (1958). The recommended function is shown below:

$$k_w = k_s \text{ for } \psi \geq \psi_b \qquad \textbf{[39]}$$

$$k_w = k_s \Theta^{\delta} \text{ for } \psi < \psi_b \qquad \textbf{[40]}$$

where:

k_w = coefficient of permeability with respect to the water phase for the soil saturation (i.e., S = 100%),

δ = empirical constant.

The empirical constant, δ in turn is related to the pore-size distribution index.

The Brooks and Corey (1964) model is simple to use and appears to be quite reasonable for coarse-grained soils such as sands and gravels.

6.3.2 Modified Campbell (1996) Estimation

The Modified Campbell (1996) equation is implemented into PLAXIS LE - Groundwater to provide a hydraulic conductivity equation that levels off at high soil suctions. The shape of the function is consistent with theoretical considerations for hydraulic conductivity of an unsaturated soil when water flow transitions to the vapor phase. The point of residual suction can be assumed to be the point at which water movement becomes discontinuous or transitions to vapor flow. The Campbell (1973) equation was modified to produce an equation that tends to level off at approximately the residual suction for the soil. The modified equation as implemented into the PLAXIS LE - Groundwater software is presented below (Fredlund, 1996).

$$k(\psi) = (k_s - k_{\min}) \left[\left[1 - \frac{\ln\left(1 + \frac{\psi}{h_r}\right)}{\ln\left(1 + \frac{10^6}{h_r}\right)} \right] \left[\frac{1}{\left[\ln\left[\exp(1) + \left(\frac{\psi}{a_f} \right)^{nf} \right] \right]^{mf}} \right] \right]^p + k_{\min} \qquad \textbf{[41]}$$

where:

k = hydraulic conductivity or permeability of the water phase, *m/s*

k_s = saturated hydraulic conductivity of the water phase, *m/s*

k_{min} = calculated minimum hydraulic conductivity, *m/s*

p = parameter used to control the modified Campbell (1973) estimation of hydraulic conductivity,

a_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter,

n_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter,

m_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter,

h_r = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter, and

ψ = soil suction.

Required input: Saturated hydraulic conductivity and a fit of the soil-water characteristic curve by the Fredlund and Xing (1994) equation.

Applicable material types: All soils

As a material dries, there is less and less water present in the soil matrix. The hydraulic conductivity then decreases accordingly as the volumetric water content decreases. The modified Campbell equation reflects this behavior by using the following equation.

$$k = k_s \Theta^p(\psi) \qquad \textbf{[42]}$$

where:

k = hydraulic conductivity at any level of suction, *m/s*

k_s = saturated hydraulic conductivity, *m/s*,

Ψ = soil suction, *kPa*,

Θ = normalized volumetric water content or θ_w/θ_s represented with any equation (i.e., van Genuchten, 1980; Fredlund and Xing, 1994), and

p = power factor to adjust the prediction (same as in Equation **[41]**).

A modification was made to Campbell's (1973) equation before it was implemented into the PLAXIS LE - Groundwater software. The modification adjusts the Campbell equation such that the function flattens once a minimum permeability has been reached.

The hydraulic conductivity remains relatively constant once the water phase in the soil becomes discontinuous. Water flow in the soil is then primarily the result of vapor diffusion through air. The vapor phase flow can be accommodated through use of the Campbell (1973) equation as shown below:

$$k(\psi) = (k_s - k_{\min})\Theta^p(\psi) + k_{\min} \qquad \textbf{[43]}$$

where:

k_{min} = minimum permeability.

The above equation allows the hydraulic conductivity versus soil suction function to level off after a particular soil suction has been reached. Initially, it was suggested that the equation could be set to level off once the residual water content conditions had been reached. However, it was observed for some laboratory data that the permeability function tended to flatten at about one log cycle of suction higher than the suction corresponding to the residual water content.

The method proposed by Campbell (1973) is implemented in PLAXIS LE - Groundwater. The implemented algorithm uses the soil-water characteristic curve and the saturated hydraulic conductivity to estimate the hydraulic conductivity of a soil at all levels of suction.

6.3.3 Fredlund, Xing and Huang (1994) Estimation

Fredlund et al., (1994) presented a modification of the Mualem (1976) integration method for estimating the hydraulic conductivity of a material as a function of soil suction. The integration procedure is complex and a closed-form solution is not available. PLAXIS LE - Groundwater performs the integration and computes a series of data points that can be written onto a graph as *x-y* data.

Solution method: Integration by Simpsons rule
Required input: Saturated hydraulic conductivity and Fredlund and Xing (1994) fit of soil-water characteristic curve
Applicable material types: All soils

Equations available in the literature for predicting the coefficient of permeability use the soil-water characteristic curve data only for a limited range of suction values (e.g., Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980). These equations require knowledge of the residual water content. The residual water content θ_r is the water content below which a large increase in suction is required to remove additional water. Kunze et al., (1968) investigated the effect of using a partial soil-water characteristic curve for the prediction of coefficient of permeability and concluded that the accuracy of prediction significantly improved when the complete soil-water characteristic curve was used.

Fredlund et al., (1994) proposed an equation to estimate the coefficient of permeability of a soil over an extended range of soil suction values. The estimation procedure makes use of the soil-water characteristic curve data for the entire suction range of 0 to 1,000,000 kPa. This equation tends to be more practical for the estimation of the coefficient of permeability over a large range of suction values. The coefficient of permeability function is of interest at large suction values particularly for structures such as soil covers, as well as other near-ground-surface structures.

The equation suggested by Fredlund et al., (1994) for predicting the coefficient of permeability is given below:

$$k_r(\psi) = \frac{\int_{\ln(\psi)}^{b} \frac{\theta(e^y) - \theta(\psi)}{e^y}\theta'(e^y)\,dy}{\int_{\ln(\psi_{aev})}^{b} \frac{\theta(e^y) - \theta(\psi_{aev})}{e^y}\theta'(e^y)\,dy} \qquad \textbf{[44]}$$

where:

b = ln(1,000,000),

y = dummy variable of integration representing the logarithm of suction, and

Ψ = soil suction, given a function of volumetric water content, and

Ψ_{aev} = air entry value of the soil under consideration.

The Fredlund et al., (1994) permeability equation makes use of the Fredlund and Xing (1994) equation (i.e., equation for fitting the soil-water characteristic curve data for the entire range of suctions). The Fredlund and Xing (1994) equation has been found to fit the soil-water characteristic data for essentially all type of soils and over all suction ranges (Benson et al., 1997; Leong and Rahardjo, 1997). More details are available in Fredlund et al., (1994).

6.3.4 Van Genuchten (1980) and Mualem (1976) Estimation

The equation for calculating the permeability function by the van Genuchten (1980) and Mualem (1976) estimation method is based on Equation **[32]**. The van Genuchten and Mualem SWCC fitting equation is as follows.

$$k(\psi) = k_s \left[\frac{\left\{ 1 - (a\psi)^{n\left(1-\frac{1}{n}\right)} \left[1 + (a\psi)^n \right]^{-\left(1-\frac{1}{n}\right)} \right\}^2}{\left[1 + (a\psi) n \right]^{\left(1-\frac{1}{n}\right)/2}} \right] \qquad \textbf{[45]}$$

where:

k = hydraulic conductivity or permeability of the water phase, *m/s*,

k_S = saturated hydraulic conductivity of the water phase, *m/s*,

a = van Genuchten and Mualem soil-water characteristic curve fitting parameter,

n = van Genuchten and Mualem soil-water characteristic curve fitting parameter, and

ψ = soil suction, *kPa*.

Required input: Saturated hydraulic conductivity and van Genuchten and Mualem fit of the soil-water characteristic curve

Applicable material types: All soils

6.3.5 Van Genuchten (1980) Estimation

Several investigators such as Brooks and Corey (1964) and Mualem (1976) have proposed closed-form equations for estimating the coefficient of permeability of unsaturated soils based on Burdine's theory (1953). Brooks and Corey (1964) equation may not converge rapidly when used in numerical simulations of seepage in saturated-unsaturated soils. The Mualem (1976) equation is in an integral form. However, it is possible to derive a closed-form analytical equation provided there is a fixed relationship between two of the fitting parameters.

The equation proposed for fitting the soil-water characteristic curve by *van Genuchten (1980)* is flexible, continuous and has a continuous slope. The closed-form equation proposed for estimating the coefficient of permeability function has been extensively used for saturated-unsaturated soils flow modeling.

$$k(\psi) = k_s \left[\frac{\left\{ 1 - (a\psi)^{nm} \left[1 + (a\psi)^n \right]^{-m} \right\}^2}{\left[1 + (a\psi) n \right]^{m/2}} \right] \qquad \textbf{[46]}$$

where:

k = hydraulic conductivity or permeability of the water phase, *m/s*,

k_S = saturated hydraulic conductivity of the water phase, *m/s*,

a = van Genuchten soil-water characteristic curve fitting parameter, *kPa*,

n = van Genuchten soil-water characteristic curve fitting parameter,

m = van Genuchten soil-water characteristic curve fitting parameter, and

ψ = soil suction, *kPa*.

Required input: Saturated hydraulic conductivity and van Genuchten fit of the soil-water characteristic curve

Applicable material types: All soils

The van-Genuchten's equation (1980) for fitting the soil-water characteristic curve data is given below:

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{\left[1 + (a\psi^n) \right]^m} \qquad \textbf{[47]}$$

where:

θ = volumetric water content,

θ_s = saturated volumetric water content,

θ_r = residual volumetric water content, and

a, n, m = material constants.

van Genuchten (1980) suggests the use of 1,500 kPa to represent residual conditions for a soil. For many soils, a volumetric water content corresponding to a residual suction of 1,500 kPa is a reasonable approximation. An analytical procedure has also been suggested for estimating the residual water content.

Figure 10 provides the comparison between the predicted and measured values of the soil-water characteristic curve along the drying and wetting paths with respect to suction for Guelph loam (van Genuchten, 1980). Also shown is the variation in the coefficient of permeability. The equations proposed by van Genuchten (1980) provide excellent fits for many soil types.

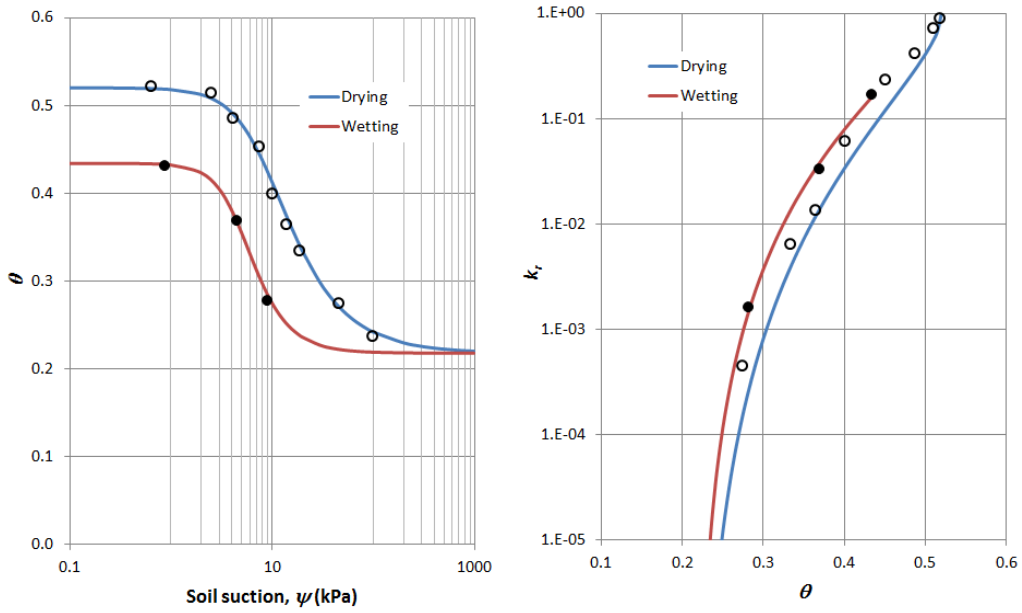

Figure 10 Comparison between the predicted (continuous solid lines) and measured values (circles) of the soil-water characteristic curve along drying and wetting paths and the variation of coefficient of permeability with respect to suction (from van Genuchten, 1980)

6.3.6 Leong and Rahardjo (1997) Estimation

Leong and Rahardjo (1997) proposed a permeability function for predicting the unsaturated coefficient of permeability. The estimation is based on a fit of the soil-water characteristic curve with the Fredlund and Xing (1994) equation. The equation for estimation of the unsaturated soil permeability function can be written as follows:

$$k(\psi) = k_s \left[\frac{1}{\left[\ln\left[\exp(1) + \left(\frac{\psi}{a_f} \right)^{n_f} \right] \right]^{m_f}} \right]^{p} \quad \textbf{[48]}$$

where:

k = hydraulic conductivity or permeability of the water phase, *m/s*,

k_s = saturated hydraulic conductivity of the water, *m/s*,

p = parameter used to control the Leong and Rahardjo (1997) estimation of hydraulic conductivity,

a_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter, *kPa,*

n_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter,

m_f = Fredlund and Xing (1994) soil-water characteristic curve fitting parameter,

ψ = soil suction, *kPa*.

In Leong and Rahardjo (1997), the best fitted permeability function was used when comparing the predicted and measured coefficient of permeability for several soil types. The results were tested for both the wetting and drying curves. A good fit was obtained for a wide range of experimental data. It was found that if the exponent *p* was known for a given soil, the coefficient of permeability could be obtained indirectly from the soil-water characteristic curve. Otherwise, *p* needed to be determined using a curve fitting process with permeability data. The value of *p* varied from 4.3 to 52.1 for the soils studied.

7 SOIL ATMOSPHERE MODELING

Soil-atmosphere moisture fluxes can be modeled by using "Climate boundary conditions". Soil-atmosphere moisture fluxes are influenced by the following types of processes:

- Infiltration fluxes,
- Runoff, and
- Evaporative fluxes.

Moisture infiltration and runoff can be modeled by considering the amount of precipitation and the infiltration capacity of the soil. The infiltration capacity is determined by applying a modified version of the "Review boundary condition".

Evaporative fluxes are modeled by using an appropriate negative flow boundary condition and by considering moisture movement through vapor flow. Consideration of vapor flow becomes important when modeling soil-atmosphere fluxes. Liquid flow alone cannot represent the entire moisture migration associated with evaporation at the soil surface. Eventually there will essentially be a shut-off of both liquid and vapor moisture movement near the ground surface. The vapor flux component theory has been presented in the previous chapters.

The following section presents a detailed description of the theory of soil-atmosphere modeling.

7.1 ATMOSPHERIC FLUX BALANCE

There is an atmospheric moisture flux balance and a thermal flux balance that must be satisfied at the ground surface when calculating *Actual Evaporation, AE*. Basically, water falling on the ground surface either infiltrates the soil (or runs off) or else rises to the sky through the process called "*Actual Evaporation*, *AE*". The ground surface moisture and thermal flux equation can be written as follows.

$$P = AE + NP + R_{off} \quad \textbf{[49]}$$

$$Q_n = Q_h + Q_l + Q_g \quad \textbf{[50]}$$

where:

P	= precipitation, $m^3/m^2/day$, or m/day
AE	= actual evaporation from ground surface, $m^3/m^2/day$ or m/day
NP	= net Percolation or infiltration, $m^3/m^2/day$ or m/day
R_{off}	= runoff, $m^3/m^2/day$ or m/day
Q_n	= net radiation, $kJ/m^2/day$, or equivalently converted into m/day,
Q_h	= sensible heat transferring from ground surface to air, kJ/m^2/day, or equivalently converted into m/day,
Q_l	= latent heat associated with the water phase change including evaporation or freezing, $kJ/m^2/day$, or equivalently converted into m/day, and
Q_g	= ground heat flux, $kJ/m^2/day$, or equivalently converted into m/day.

Precipitation information can be obtained from weather station records and is usually provided on a daily basis. Preferably precipitation data should be collected on an hourly basis when modeling near-ground-surface phenomena. The mechanics of net infiltration, *NP*, can be described by Darcy law. Net radiation, Q_n, can also be obtained from weather station records or it can be approximated using an equation suggested by Penman in (1948). The latent heat component, Q_l, can be estimated using actual evaporation, *AE*, or the formation of ice near the ground surface during freezing. The sensible heat component, Q_h, reflected from the ground surface to the air is described as follows (Penman, 1948; Gray, 1970; Wilson 1990):

$$Q_h = C_f \eta f(u)(T_s - T_a) \quad \textbf{[51]}$$

where:

Q_h	= sensible heat, m/day,
C_f	= conversion factor, (i.e., 1 kPa = 0.0075 mHg),
η	= psychometric constant, 0.06733 $kPa/^oC$ at 20 ^oC,
$f(u)$	= function depending on wind speed, $f(u)$ = 0.35(1+ 0.146 W_w), and
W_w	= wind speed, km/hr.

Actual Evaporation, *AE*, is difficult to measure directly but can be calculated from fundamental thermodynamic considerations.

Equations **[49]** and **[50]** are fundamental to describing the coupling of moisture and heat flow processes. Actual evaporation, *AE,* depends on the water content and temperature of the soil at ground surface. In addition, the rate of evaporation also depends on the air temperature and air relative humidity. The air temperature and soil temperature at the ground surface are generally not the same but are inter-related through net radiation, Q_n, latent heat, Q_l, and sensible heat, Q_h. The available surface water is controlled by total precipitation, actual evaporation, and runoff. These variables play an important role in partitioning convective heat flux into sensible heat and latent heat (Wetzel and Boone, 1995).

7.2 INFILTRATION AND RUNOFF WITHOUT CONSIDERATION OF EVAPORATION

Infiltration, evaporation and runoff are determined simultaneously. If the moisture evaporation can be neglected, the moisture flux balance at the soil surface is rewritten:

$$P = NP + R_{off} \qquad \textbf{[52]}$$

The amount of precipitation and the hydraulic properties of the soil are the main variables required when calculating net infiltration. Runoff is computed in an iterative manner and the amount of infiltration can be determined by consideration of previous conditions.

Normal flux boundary conditions can be set to include the effects of runoff.

Depending on the amount of moisture flux applied to the uppermost boundary, the pore-water pressure, u_w, may tend to become higher than zero. The higher the influx, the higher the pore-water pressure, u_w becomes. If u_w becomes higher than zero, a condition occurs that corresponds to ponding.

However, if the ground surface is assumed to be well-drained with no ponding, a mechanism must be implemented in order to limit the amount of infiltration to a lowest possible value. The low value would keep the u_w value at the surface equal to zero. One common way of applying this limiting condition is to switch the boundary condition to an essential boundary condition equal to zero. This would occur when the pore-water pressure, u_w, becomes equal to zero. Another option, switches the boundary condition to a different natural boundary condition that is equivalent to the essential boundary condition (Gitirana Jr., 2004).

The natural boundary condition is similar to the "Review Boundary Condition" presented in the previous chapter.

The ponding height for a model is by default set to zero. This means that when water is applied to the boundary of a model, the maximum pore-water pressure will be restricted to a maximum of 0 kPa. Any additional water applied which causes the upper boundary to exceed 0 kPa and will be re-classified as runoff. If a value greater than zero is specified for ponding then the maximum pressure allowed at the ground surface is increased to the pond height times γ_w. Runoff conditions will not occur until the increased maximum pressure is encountered.

The calculation of runoff adds significant complexity to the calculations in a numerical model. It is possible that adding a runoff calculation might double or triple computational times. A simple model should be set up and solved prior to the addition of a model implementing a runoff calculation.

7.2.1 Pressure Head Calculated Runoff Correction

This runoff correction option is similar to the equation presented by Gitirana (Gitirana Jr., 2004), but uses the pressure head variable instead of the hydraulic conductivities and the FAC. This equation, developed by SoilVision Systems Ltd., is able to achieve the same goal as the Estimated Runoff Correction option, while offering increased stability. It also removes the need for a user-defined FACTOR input.

$$\text{Natural BC} = \begin{cases} \text{if } u_{ws} \geq 0 \text{ then } \left(pond - h_{ps} \right) \\ \text{if } u_{ws} < 0 \text{ then } n_p \cos\alpha \end{cases} \qquad \textbf{[53]}$$

where:

u_{ws} = pore-water pressure at the surface, *kPa*,

h_{ps} = pressure head at the surface, *m*,

pond = the height of the pond, being 0 if no pond is allowed,

n_p = is the net precipitation available at the ground surface, and

α = slope of the ground surface with the horizontal direction.

This is the runoff correction option implemented in PLAXIS LE - Groundwater.

7.3 EVAPORATION

The effects of evaporation on a soil near the ground surface depend on the vapor pressure gradient between the soil surface and the atmosphere. Atmospheric coupling is achieved in PLAXIS LE - Groundwater in the form of an evaporative flux boundary condition. PLAXIS LE - Groundwater provides a number of methods for defining the evaporative flux in terms of potential evaporation (PE) or actual evaporation (AE).

When an evaporative boundary condition is being considered in PLAXIS LE - Groundwater, the governing equations must include vapor pressure gradients.

7.3.1 Potential Evaporation

Potential evaporation, *PE,* is the amount of evaporation that would occur from a saturated soil surface. The potential evaporation can be entered: i.) as measured data (i.e., Pan evaporation), ii.) as a constantor iii.) it can be calculated using different formulations (Gitirana, 2005; Fredlund et al., 2012), such as:

a) Penman (1948) equation,
b) Thornwaite (1948) equation, or
c) Priestley-Taylor (1972) equation.

7.3.1.1 Penman (1948) Equation

The original Penman method is used for the calculation of potential evaporation (PE). The Penman equation uses the routine weather data as input, namely, relative humidity, air temperature, wind speed, and net radiation.

The potential evaporation at a material-atmosphere boundary can be calculated using the following formulation (Penman, 1948):

$$PE = \frac{\Gamma Q_n + \eta E_a}{\Gamma + \eta} \qquad \textbf{[54]}$$

where:

PE	= potential evaporation, *m/day*,
E_a	= flux associated with "mixing"; $f(u)\ C_f\ u_{v0}^{air}\ (1 - h_r)$, *m/day*,
$f(u)$	= 0.35 (1. + 0.146 W_w),
W_w	wind speed, *km/hr*,
C_f	conversion factor, (i.e., 1 *kPa* = 0.00750 *mHg*),
h_r	= relative humidity in the air above the ground (i.e., $h_r = u_v^{air}/u_{vo}^{air}$), obtained from weather station record,
u_v^{air}	= water vapor pressure in the air above ground surface, *kPa*,
u_{vo}^{air}	= saturated vapor pressure at the mean air temperature, *kPa*,
Γ	= slope of saturation vapor pressure versus temperature curve, *kPa/°C*,
Q_n	= net radiation at the water surface, *m/day*,
η	= psychrometric constant, (*kPa/°C*), η = 0.06733 *kPa/°C*.

The u_v^{air} , u_{vo}^{air} and Γ can be calculated from temperature as proposed by Lowe (1977).

The net radiation can be calculated (as suggested by Penman) in the following manner:

$$Q_n = (1-r)R_c - \sigma(273.15+T_a)^4\left(0.56 - 0.92\left(p_{vsat}{}^{air}\right)^{0.5}\right)(0.10 + 0.90n/N) \qquad \textbf{[55]}$$

where:

Q_n	= net radiation, *m/day*,
r	= reflection coefficient,
R_c	= 0.95 R_a(0.18 + 0.55n/N) = shortwave radiation , *m/day*,

0.95	= coefficient suggested by Penman for evaporation from a wet and bare soil as compared to evaporation from an open water surface,
R_a	= solar radiation, $MJ/m^2/day$,
σ	= Stefan Bolzman's constant, $W/m^2/K^4$,
T_a	= air temperature, ^oC,
P_{vsat}^{air}	= vapor pressure of the air above the surface, *mmHg*, and
n/N	= sunshine ratio (actual/possible hours of bright sunshine).

Note: *The vapor pressure, P_{vsat}^{air} in Equation **[55]** must be in mmHg.*

In addition to the above equation suggested by Penman (1948), the net radiation data can be measured in the field, and is a typical weather station reading. The net radiation is usually measured in units of $MJ/day\text{-}m^2$. Entry of the measured net radiation is also in units of $MJ/day\text{-}m^2$. The software will automatically convert the net radiation from units of $MJ/day\text{-}m^2$ into the units of *m/day* used in the evaporation calculations in the following expression:

$$Q_n = 10^6 Q_{mn} / (L_v) \qquad \textbf{[56]}$$

where:

Q_{mn}	= measured net radiation , $MJ/day\text{-}m^2$,
L_v	= latent heat of evaporation, $L_v = 4.187\times10^6\ (591 - 0.51T_a),\ J/m^3$.

7.3.1.2 Thornthwaite (1948) Equation

Thornthwaite incorporated the variables of length of daylight hours, mean monthly temperature, and an empirical constant into the calculation of potential evaporation (Fredlund et al., 2012). The daily potential evaporation can be calculated as follows:

$$PE = 0.0005333\left(\frac{L_d}{12}\right)\left(\frac{N}{30}\right)\left(\frac{10T_a}{I}\right)^{a_t} \qquad \textbf{[57]}$$

where:

PE	= potential evaporation, *m/day*,
L_d	= length of daylight, *hr*,
N	= number of days in the month,
T_a	= mean monthly air tempterature, ^oC,
I	= summation for 12 months of the function $(T_a/5)^{1.514}$; i.e., $I = \sum_{month=1}^{12}\left[T_a/5\right]^{1.514}$,
a_t	= complex function of the variable *I* (i.e., $a_t = (6.75\times10^{-7})\,I^3 - (7.71\times10^{-5})\,I^2 + (1.79\times10^{-2})\,I + 0.492$.

The Thornthwaite (1948) equation is commonly used to assess the climatic conditions of aridity and humidity based on the calculation of a moisture index I_m. The moisture index I_m can be calculated following the modification of the moisture index equation by Thornthwaite and Mather (1955), and Thornthwaite and Hare (1955):

$$I_m = 100\left(\frac{P}{PE} - 1\right) \qquad \textbf{[58]}$$

where:

I_m	= 1955 Thornthwaite moisture index,
P	= Total annual precipitation,
PE	= total annual potential evapotranspiration calculated as the summation of the Thornthwaite (1948) monthly potential evaporations.

The climate classification criteria are as shown in Table 2. The moisture index I_m is as defined in Equation **[58]**.

Table 2. Criteria for climate classification

I_m	Category of Climate

> 100	Perhumid
20 – 100	Humid
0 – 20	Moist humid
-33 – 0	Dry subhumid
-67 to -33	Semiarid
-100 to -67	Arid

7.3.2 Actual Evaporation

Actual Evaporation, *AE*, is difficult to measure directly but it can be calculated from fundamental thermodynamic considerations. There are several procedures that have emerged for the calculation of the actual evaporative flux. However, there have been few studies that assess the relationship between each of the suggested solution procedures. As well, the reliability of the proposed procedures seems to not have been completely verified.

In 1994 Wilson proposed a modification to the well-known Penman (1948) equation for the calculation of Potential Evaporation, *PE*. The modified equation has become known as the Wilson-Penman (1994) equation to calculate the actual evaporation. The Wilson-Penman equation took into consideration the difference in temperature and relative humidity (and therefore vapor pressure) between the soil surface and the overlying air. The difference in conditions between the air and the water at ground surface has formed the basis for the Soil-Atmospheric Model which was subsequently implemented into the *SoilCover*, version 1.0, computer code (1994).

In 1997 a "Limiting Function" type relationship was proposed by Wilson, Fredlund and Barbour. The "Limiting Function" related Actual Evaporation and Potential Evaporation by scaling the vapor pressures associated with the relative humidity at ground surface and the relative humidity in the air above ground surface. Inherent in the derivation was the assumption that the air and soil temperatures were the same.

Wilson (1994) also presented experimental results that showed a unique relationship between total suction at any soil surface and the ratio of Actual Evaporation to Potential Evaporation, *AE/PE*. Wilson et al., (1997) presented a unique equation that passed through the experimental data. As a consequence, there was now another way to empirically relate Actual Evaporation and Potential Evaporation fluxes.

The above-mentioned relationships give rise to different possibilities for the calculation of Actual Evaporation from the ground surface. The major difference in the methodologies is related to the assumption regarding the air and soil temperatures. For example, the soil temperature can be assumed to be equal to the air temperature. This is known to not be the case but there does not appear to have been a thorough study performed that quantifies the magnitude of the error in calculating *AE* based on this assumption.

The ***Case 1 Solution*** presented below for Actual Evaporation considers the isothermal case (i.e., no ground thermal flux, Q_g = 0). This assumption greatly simplifies the solution for *AE* since all temperature values are taken as equal to the air temperature recorded above ground surface. The "Limiting Function" proposed by Wilson et al., (1997) was used to relate Actual Evaporation and Potential Evaporation. The procedure for solving this case is referred to as the ***Case 1 Solution***.

The second solution procedure considered for calculating Actual Evaporative, *AE*, utilizes the Wilson-Penman (1994) equation for the case where ground thermal flux, Q_g, is equal to zero beneath the soil surface. *However, the soil temperature at ground surface can be different from the air temperature above ground surface*. The solution procedure is referred to as the ***Case 2 Solution***.

The third solution procedure is quite similar to the ***Case 1 Solution***, except that the Actual Evaporative, *AE*, is approximated using an empirical expression that is best-fit with Wilson's 1994 experimental results. This solution procedure is referred to as the ***Case 3 Solution***.

7.3.3 Case 1 Solution: "Limiting-Function" for AE/PE Model

The following assumptions are made in the isothermal, "*Limiting-Function*" model.

- There can be liquid and vapor flow through the soil, (i.e., liquid and vapor flow is in response to a hydraulic head gradient and a vapor pressure gradient, respectively).
- The soil temperature in the entire domain is assumed to be the same, and equal to the air temperature above the soil surface. (i.e., ground thermal flux is neglected, Q_g = 0).
- The ground surface temperature is assumed to be equal to the air temperature.
- Actual evaporation is calculated using the "Limiting Function" proposed by Wilson et al., (1997).

7.3.3.1 Mass Flow Governing Equation

Moisture flow in one-dimension beneath the soil surface is described using the following partial differential equation,

$$\frac{\partial}{\partial y}\left[\left(k_{wy}+k_{vh}\right)\frac{\partial h}{\partial y}-k_{vh}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \quad \textbf{[59]}$$

$$k_{vh}=\frac{\beta\theta_a g D_v \omega_v \rho_{sv0} h_r}{\rho_w R(273.15+T)} \quad \textbf{[60]}$$

$$D_v=2.29\times10^{-5}\left(1+\frac{T}{273.15}\right)^{1.75} \quad \textbf{[61]}$$

$$\beta=(\theta_a)^{2/3}=(n-\theta_L)^{2/3} \quad \textbf{[62]}$$

$$h_r=e^{\frac{-g\omega_v\Psi}{\gamma_w R(273.15+T)}} \quad \textbf{[63]}$$

$$\psi=(u_a-u_w)+\pi \quad \textbf{[64]}$$

where:

h = water head, *m*,

γ_w = unit weight of water, *kN/m³*,

k_w = hydraulic conductivity, *m/s*,

k_{vh} = water vapor conductivity by diffusion within the air phase, *m/s*,

β = soil tortuosity of a dimensionless factor,

θ_a = volumetric air content, $\theta_a = n - \theta$, *m³/ m³*,

θ = volumetric water content, *m³/ m³*,

n = porosity,

D_v = molecular diffusivity of vapor through soil, *m²/s*,

ω_v = molecular weight of water vapor, 0.018016 *kg/mol,*

ρ_{sv0} = saturation vapor density that is dependent of temperature, *kg/m³*,

h_r = relative humidity,

ρ_w = water density, *kg/m³*,

R = universal gas constant, 8.314 *J/(mol-K),*

T = temperature, °*C*, and

Ψ = total suction, *kPa*,

u_a = pore-air pressure, *kPa*,

u_w = pore-water pressure, *kPa*,

π = osmotic suction, *kPa*, and

y = elevation, *m*.

The osmotic suction in a soil is related to the salt content in the soil. For typical field water content conditions, osmotic suction may range from 100 *kPa* to 1000 *kPa* or more. As the soil dries, the salt contents increase, and the osmotic component increases (Fredlund, 1991).

It should be noted that PLAXIS LE - Groundwater supports one-dimensional, two-dimensitonal, and three-dimensional formulations for moisture flow; however, only the one-dimensional partial differential equation is shown (i.e., Equation **[59]**).

7.3.3.2 Initial soil water contents

The soil moisture can be initialized using an initial set of values for pore-water pressure, water head. It is also possible to designate the location of the water table (i.e., phreatic line) and assume that hydrostatic conditions exist above and below the phreatic line.

7.3.3.3 Boundary condition for moisture flow

Using Equation **[49]** infiltration to the ground surface (i.e., the boundary condition for moisture flow) can be defined as.

$$q_y\big|_{surface} = P - AE - R_{off} \quad \textbf{[65]}$$

where:

q_y = moisture flow rate at soil surface, *m/day*,
P = precipitation flux, *m/day*,
R_{off} = water runoff, *m/day*,
AE = actual evaporation, *m/day*

7.3.3.4 Actual Evaporation

The "limiting function" proposed by Wilson et al., (1997) is written as follows.

$$AE = PE\left[\frac{u_v^{soil} - u_v^{air}}{u_{vo}^{soil} - u_v^{air}}\right] \quad \textbf{[66]}$$

where:

AE = actual evaporation, m/day,
PE = potential evaporation, m/day,
u_v^{soil} = actual vapor pressure at the soil surface, kPa,
u_{vo}^{soil} = saturated vapor pressure in the soil at the ground surface, kPa, and
u_v^{air} = vapor pressure in the air above the soil surface, kPa.

For the ***Case 1 Solution***, it is assumed that $\boldsymbol{T_s = T_a}$, and this leads to the vapor pressure in the air being equal to the saturated vapor pressure in the soil (i.e., $u_{v0}^{air} = u_{v0}^{soil}$). Equation **[66]** can also be written in term of relative humidity as follows (Wilson et al., 1997):

$$AE = PE\left[\frac{h_s - h_r}{1 - h_r}\right] \quad \textbf{[67]}$$

where:

h_r = relative humidity of the air above the ground surface, and
h_s = relative humidity at the soil surface.

Equations **[59]**, **[65]**, and **[66]** or **[67]** together with the initial water content conditions are the equations required to solve for Actual Evaporation, AE.

7.3.3.5 Determining vapor pressure values throughout each day

The daily air temperature, T_a, and daily relative humidity, h_r, of the air above the ground surface are usually measured at a weather station. Minimum and maximum daily temperature and relative humidity values are generally recorded for each day. However, usually the hourly values of these variables are also recorded. The amount of data becomes quite excessive when hourly values are obtained. When minimum and maximum values are given for temperature and relative humidity, then an assumption can be made regarding their distributions throughout each day.

Figure 11 and Figure 12 shows two options of several possible methods implemented in PLAXIS LE - Groundwater to describe the daily changing pattern of air temperature and relative humidity based on the daily minimum and maximum value. Figure 11 indicates that the relative humidity has a maximum value at about 6:00 a.m. and a minimum value at about 1:00 p.m. The time at minimum and maximum value can be specified with other value. In Figure 12, the maximum value of relative humidity is assumed at the midnight (24:00 a.m.), and minimum value is at noon (12:00 p.m.). The daily changing pattern of air temperature is in general, opposite to the pattern for relative humidity.

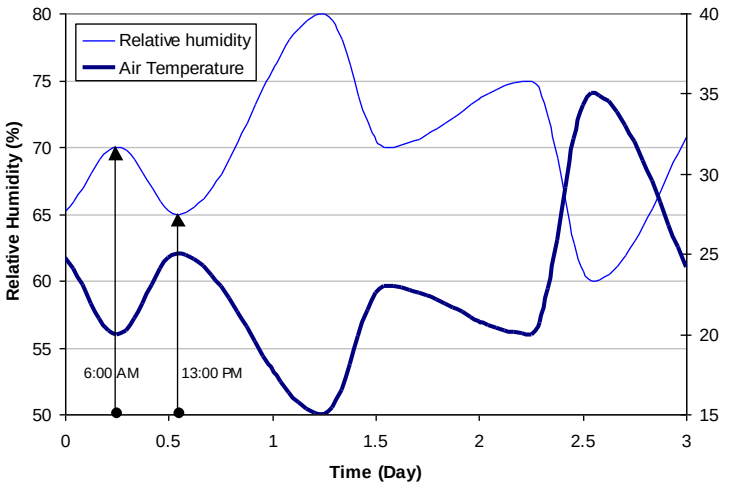

Figure 11 Daily changing pattern of air temperature and relative humidity of overlying air

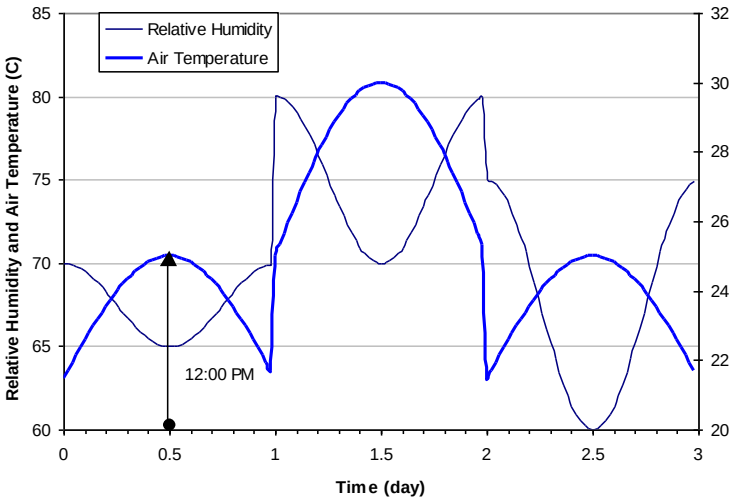

Figure 12 Symmetric distributions of daily changing of air temperature and relative humidity

The calculated relative humidity at the unsaturated soil surface based on Edlefsen and Anderson (1943) equation may be larger than the actual value particularly for an unsaturated sand. It can be seen from Figure 13 that when the total suction in soil is less than about 3000 *kPa*, the relative humidity at the soil surface approaches 100% (i.e., $h_s \rightarrow 1$). Consequently, *AE* = *PE*, which is not valid for sand soil since the sand may have desaturated at a suction considerably below 100 kPa.

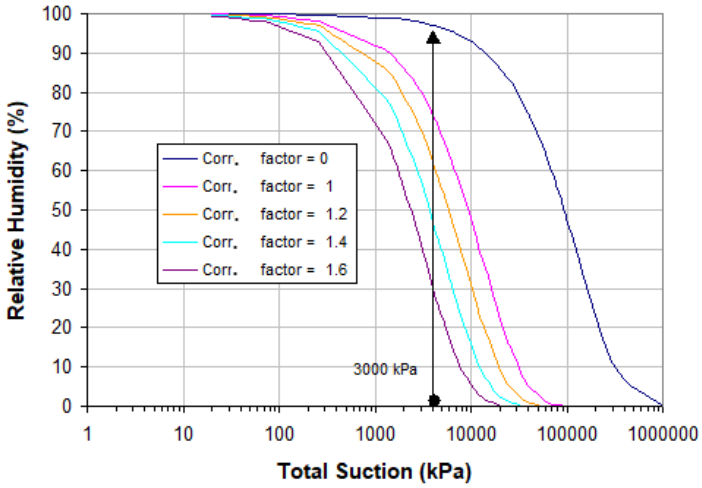

Figure 13 Relationship between relative humidity and total suction using Edlefsen and Anderson (1943) equation

PLAXIS LE - Groundwater provides options to improve the accuracy and stability of evaporative and atmospheric modeling.

Apply Surface Suction Correction

When the Surface Suction Correction option is selected, the total suction that is used to calculate the relative humidity at the soil surface is adjusted based on an empirical correction factor (Alvenas and Jansson, 1997). In other words, the relative humidity at soil surface is modified in accordance with the following expression:

$$h_s = \frac{u_v^{soil}}{u_{vo}^{soil}} = \exp\left(\frac{-g\omega_v \psi \delta_{corr}}{\gamma_w R(273.15 + T_s)} \right) \quad \textbf{[68]}$$

$$\psi = (u_a - u_w) + \pi \quad \textbf{[69]}$$

$$\delta_{corr} = 10^{f_{corr}} \quad \textbf{[70]}$$

where:

Ψ = total suction, *kPa*,

ω_v = molecular weight of water, 0.018 *kg/mol*,

γ_w = unit weight of water, 9.807 *kN/m*^{3},

g = gravity acceleration, *m/s*^{2},

R = universal gas constant, 8.314 *J/(mol-K),*

T_s = soil surface temperature, *°C*,

T_a = air temperature obtained from weather station, *°C*

u_a = pore-air pressure, *kPa*,

u_w = pore-water pressure, *kPa*,

π = osmotic suction, *kPa*.

δ_{corr} = correction factor of soil surface suction ranging between 1 to $10^{3.48}$, and

f_{corr} = empirical number changing from 0 to 3.48. By default, f_{corr} = 1.2, which corresponds to δ_{corr} = 15.8.

Figure 13 illustrates the correction factor effect on the relative humidity.

There are two ways the surface suction adjustment factor can be applied: a) Manual input of f_{corr} value at Evaporation Properties dialog, or b) estimation of the f_{corr} value based on soil suction relationship proposed by Fredlund et al. (2016). In the case of manual input of f_{corr} value, the same suction correction factor will be applied to all the surface materials whereas the latter option will calculate different f_{corr} values for each surface material based on its residual suction.

Fredlund et al., (2016) used the residual suction of the drying SWCC as a reference point to calculate the correction factor, δ_{corr}. This correction factor translates the SWCC to a suction value of 3000 kPa on the Lord Kelvin's curve (Fredlund et al., 2016). Equation **[71]** shows the relationship between the residual suction and the empirical number, f_{corr} and the equation is plotted in Figure 14 The f_{corr} adjustment factors for various residual suction values. For coarse-grained soils, the maximum correction factor, f_{corr}, is 3.48 and there is no correction factor required for fine-grained soils with a high air-entry value (Fredlund et al., 2016).

$$f_{corr} = 3.48 - log\, \psi_{residual} \quad \textbf{[71]}$$

where:

$\psi_{residual}$ = residual soil suction on the drying SWCC, *kPa*.

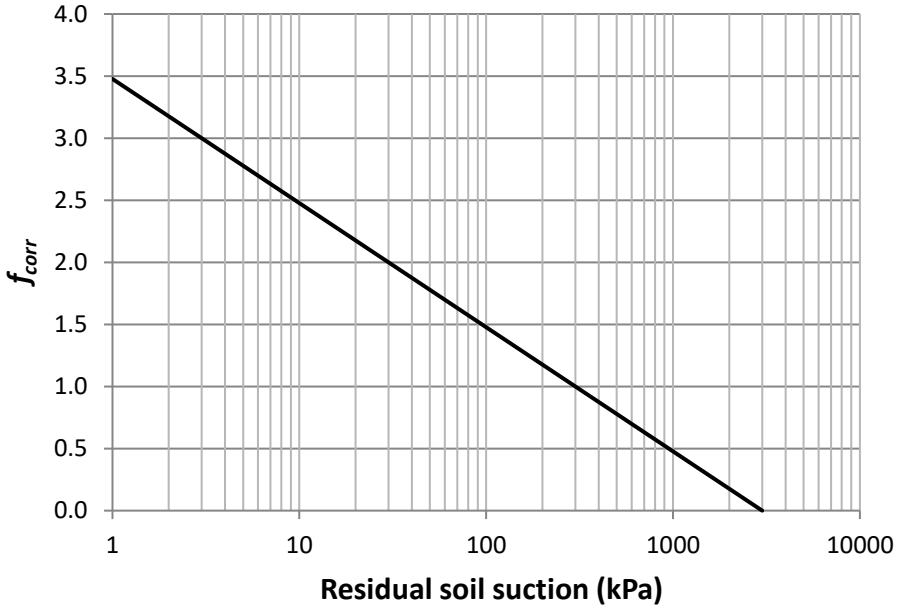

Figure 14 The f_{corr} adjustment factors for various residual suction values

Apply Maximum Gradient Limit at Evaporation Boundaries

When the Apply Maximum Gradient Limit option is selected, it is possible for extremely high gradients to develop at the upper boundary during evaporative conditions when using the Wilson-Penman climate boundary condition. Extremely high surface gradients can lead to unreasonable numerical instability. Limiting the gradient to a reasonable maximum value can improve convergence of climate-based numerical models. A reasonable Gradient Limit might be between 50 to 1000; however, it could go as high as 10,000.

The vapor pressure of u_v^{soil} used in diffusive flow Equation **[66]** can be calculated using the following equation.

$$u_v^{soil} = u_{vo}^{soil} h_s = u_{vo}^{soil} \exp\left(\frac{g \omega_v \psi \delta_{corr}}{\gamma_w R(273.15 + T_s)} \right) \qquad \textbf{[72]}$$

The saturated vapor pressure is a function of soil surface temperature as given by the following expression (Lowe, 1977; Gitirana, 2004):

$$u_{v0}^{soil} = a_0 + a_1 T_s + a_2 T_s^2 + a_3 T_s^3 + a_4 T_s^4 + a_5 T_s^5 \qquad \textbf{[73]}$$

where:

a_0 = 0.6183580754
a_1 = 0.0411427320
a_2 = 0.0017217473
a_3 = 0.0000174108
a_4 = 0.0000003985
a_5 = 0.0000000022

Note : *$T_s = T_a$ in this case.*

7.3.4 Case 2 Solution: Wilson-Penman (1994) Model

In Case2, the PLAXIS LE - Groundwater model assumes that

- Moisture and vapor flow occurs through the soil.

- Soil temperatures in the entire domain are the same. In other words, the ground thermal flux is neglected (i.e., $Q_g = 0$).
- The soil temperature at soil surface can be different from the air temperature. The heat exchanged between air and soil surface follows the convection law as given the closed-form Equations **[50]** or **[51]**. However, the surface temperature is not imposed as a boundary condition for distribution through the underlying soil.
- Actual Evaporation, *AE*, is calculated using Wilson-Penman (1994) equation.

7.3.4.1 Governing Equations

Moisture flow in one-dimension is defined by equation **[74]**, (note: same as Equation **[59]**)**:**

$$\frac{\partial}{\partial y}\left[\left(k_{wy}+k_{vh}\right)\frac{\partial h}{\partial y}-k_{vh}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \qquad \textbf{[74]}$$

Since the soil temperature is different from the air temperature, it is necessary to use another equation to determine the soil temperature. Because this is an isothermal model (i.e., $Q_g = 0$), controlled by Equations **[50]** and **[51]**, a closed-form for the soil temperature can be written (Wilson, 1994):

$$T_s = T_a + \frac{1}{C_f \eta f(u)}(Q_n - AE) \qquad \textbf{[75]}$$

where:

T_s = soil temperature at soil surface, *°C*,
T_a = air temperature, *°C*,
C_f = conversion factor (i.e., 1 *kPa* = 0.00750 *mHg*),
η = psychometric constant , 0.06733 *kPa/°C*,
f(u) = function depending speed, *f(u)* = 0.35 (1. + 0.146 W_w),
W_w = wind speed, *km/hr*,
Q_n = net radiation, *m/day*, and
AE = actual evaporation, *m/day*.

7.3.4.2 Initial soil water content profile

The water content in the soil can be initialized using an initial set of values for pore-water pressure or water pressure head. It is also possible to designate the location of the water table (i.e., the phreatic line) and assume that hydrostatic conditions exist below and above the water table.

7.3.4.3 Initial soil surface temperature

Temperature can be initialized to the air temperature. The initialized air temperature is:

$$T_s = T_a \qquad \textbf{[76]}$$

7.3.4.4 Boundary condition for moisture flow

The boundary condition for moisture flow at the ground surface is defined using equation **[77]**.

$$q_y\big|_{surface} = P - AE - R_{off} \qquad \textbf{[77]}$$

where:

q_y = moisture flow rate at soil surface, *m/day*,
P = precipitation flux. *m/day*,
R_{off} = water runoff, *m/day*, and
AE = actual evaporation, *m/day*

7.3.4.5 Actual Evaporation

The Wilson-Penman (1994) equation for actual evaporation, *AE*, can be re-written as follows:

$$AE = \frac{\Gamma Q_n + \eta E_a}{\Gamma + \eta / h_s} \qquad \textbf{[78]}$$

where:

AE	= actual evaporation, *m/day*,
PE	= potential evaporation, m/day
E_a	= flux associated with "mixing"; $f(u)\ C_f\ u_v^{air}\ (1/h_r - 1/h_s)$, *m/day*,
f(u)	= 0.35 (1. + 0.146 W_w),
W_w	wind speed, *km/hr*,
C_f	conversion factor, (i.e., 1 *kPa* = 0.00750 *mHg*),
h_r	= relative humidity in the air above the ground (i.e., $h_r = u_v^{air}/u_{vo}^{air}$),
h_s	= relative humidity at the soil surface (i.e., $h_s = u_v^{soil}/u_{vo}^{soil}$),
u_v^{air}	= water vapor pressure in the air above ground surface, *kPa*,
u_{vo}^{air}	= saturated vapor pressure at the mean air temperature, *kPa*,
u_v^{soil}	= vapor pressure in the soil at ground surface, *kPa*,
u_{vo}^{soil}	= saturated vapor pressure in the soil at ground surface, *kPa*,
Γ	= slope of saturation vapor pressure vs. soil temperature curve (*kPa/°C*),
Q_n	= net radiation at the water surface, *m/day*, and
η	= psychrometric constant, *kPa/°C*, η = 0.06733 *kPa/°C*.

The governing Equations **[74]** and **[75]**, initial condition Equation **[76]**, boundary condition Equations **[77]** and **[78]** are essential for solving the isothermal model with atmospheric coupling.

Note: To calculate Actual Evaporation, *AE*, using Equation **[78]**, the soil temperature at the ground surface must be known. But when using Equation **[75]** to calculate the soil temperature, the Actual Evaporation, *AE*, must be known. In other word, the Equations **[75]** and **[78]** are coupled to each other (i.e., must be solved simultaneously). The coupling Equation **[75]** is one of governing equations. Therefore, it must be initialized to a specific value. The Actual Evaporation can be calculated initially using Equation **[78]**.

7.3.4.6 Determining Vapor Pressure Values throughout each Day

The saturated vapor pressure, u_{v0}^{air} in Equation **[78]**, is calculated based on air mean temperature.

$$u_{v0}^{air} = a_0 + a_1 T_a + a_2 T_a^2 + a_3 T_a^3 + a_4 T_a^4 + a_5 T_a^5 \qquad \textbf{[79]}$$

where:

T_a	= air mean temperature, measured at a weather station.

The parameters of a_0, a_1, a_2, a_3, a_4 and a_5 are previously given in Equation **[73]**. The water vapor pressure in the air, u_v^{air}, is defined as follows:

$$u_v^{air} = u_{v0}^{air} h_r \qquad \textbf{[80]}$$

where:

h_r	= relative humidity of the air above the soil surface.

The relative humidity, h_r, of the air above the soil surface is measured at a weather station. The relative humidity, h_s, and water vapor pressure, u_v^{soil}, at the soil surface are calculated using Equations **[68]** and **[72]**. It should be noted that soil surface temperature, T_s, in Equations **[68]**, **[72]**, or **[73]** are calculated using Equation **[75]**.

7.3.5 Case 3 Solution: "Experimental-Based" for AE/PE Model

For case 3, it is assumed that

- Moisture flow and vapor flow beneath the soil surface are driven by the hydraulic head gradient and the vapor pressure gradient, respectively.
- Soil temperatures in the model domain are the same, and assumed to be equal to the air temperature above the soil surface. In other words, the ground thermal flux can be neglected (i.e., $Q_g = 0$).
- The soil surface temperature is assumed to be equal to the air temperature.
- The actual evaporation is calculated using an empirical "experimental-based" equation proposed by Wilson et al., (1997).

7.3.5.1 Governing Equation

The partial differential equation for the one-dimensional flow of water through a saturated –unsaturated soil is defined as follows:

$$\frac{\partial}{\partial y}\left[\left(k_{wy}+k_{vh}\right)\frac{\partial h}{\partial y}-k_{vh}\right]=-\gamma_w m_2^w\frac{\partial h}{\partial t} \qquad \textbf{[81]}$$

7.3.5.2 Initial water content conditions

The water contents of the soil can be initialized using an initial set of values for pore-water pressure or water pressure head. It is also possible to designate the location of the water table (i.e., the phreatic line) and assume that hydrostatic conditions exist below and above the phreatic line.

7.3.5.3 Boundary condition for moisture flow

Using the water balance Equation **[49]**, the boundary condition for moisture flow at the ground surface is defined as:

$$q_y\big|_{surface}=P-AE-R_{off} \qquad \textbf{[82]}$$

where

q_y = moisture flow rate at soil surface, *m/day*,
P = precipitation flux. *m/day*,
R_{off} = water runoff, *m/day*, and
AE = actual evaporation, *m/day*.

7.3.5.4 Determine an empirical expression for the ratio of actual evaporation, AE, to potential evaporation, PE

If the soil suction is known at the ground surface, then the rate of evaporation from the ground surface can be estimated from the empirical "experimental-based" relationship shown in Figure 15.

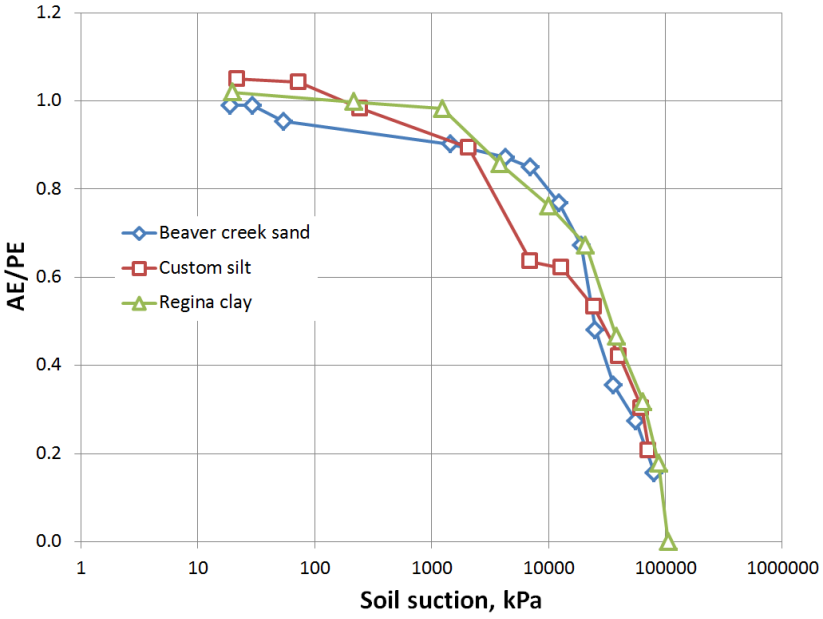

Figure 15 Relationship between radio of *AE/PE* and total suction

The ratio of actual evaporation to potential evaporation, *AE/PE,* can be approximated using the form of the thermodynamic equilibrium relationship between relative humidity and total suction (Edlefsen and Anderson, 1943). However, a correction factor, δ_{corr}, must be applied to the calculation of AE and the magnitude of the correction is dependent upon the type of soil near the ground surface. The ratio of *AE/PE* has a format similar to that used for Equation **[68]**.
The ratio of *AE/PE* has a format similar to that used for Equation **[68]**.

$$AE / PE = \exp\left(\frac{-g\omega_v\psi\delta_{corr}}{\gamma_w R(273.15+T_s)}\right) \quad \textbf{[83]}$$

$$\delta_{corr} = 10^{f_{corr}} \quad \textbf{[84]}$$

where:

AE	= Actual evaporation, *m/day*,
PE	= Potential evaporation, *m/day*,
ψ	= total suction (i.e., matric suction plus osmotic suction), *kPa*,
ω_v	= molecular weight of water, 0.018 *kg/mol*,
γ_w	= unit weight of water, 9.807 *kN/m³*,
g	= gravity acceleration, *m/s²*,
R	= universal gas constant, 8.314 *J/(mol-K)*,
T_s	= soil surface temperature, *°C*, and
f_{corr}	= correction variable, and
δ_{corr}	= correction factor by which total suction must be multiplied.

The correction factor, δ_{corr}, is computed based on the difference between the residual suction of the soil and a total suction of 3000 *kPa*. The variable f_{corr}, is determined based on the shift of the SWCC of the soil and Lord Kelvin's thermodynamic equilibrium equation. The f_{corr}, variable is typically about 1.8 for a coarse sand soil.

To include the relative humidity of the overlying air in equation **[83]**, the equation can be modified to the following format:

$$AE / PE = \exp\left(\frac{-g\omega_v\psi\delta_{corr}}{\zeta(1-h_a)\gamma_w R(T_s+273.15)}\right) \quad \textbf{[85]}$$

where:

ζ	= a dimensionless empirical parameter with a suggested value of 0.7, and
h_a	= relative humidity overlying air.

Figure 16 shows the predicted values for the ratio of *AE* to *PE* when using Equation **[67]**, equation **[83]**, and Equation **[85]**. In Figure 16, the data for the "Limiting Function (1997)" is calculated using Equation **[67]**. The data for the Wilson-Penman (1994) ratio of *AE* to *PE* is calculated using Equation **[83]**. The data for the empirical "experimental-based" ratio of *AE* to *PE* is calculated using Equation **[85]**.

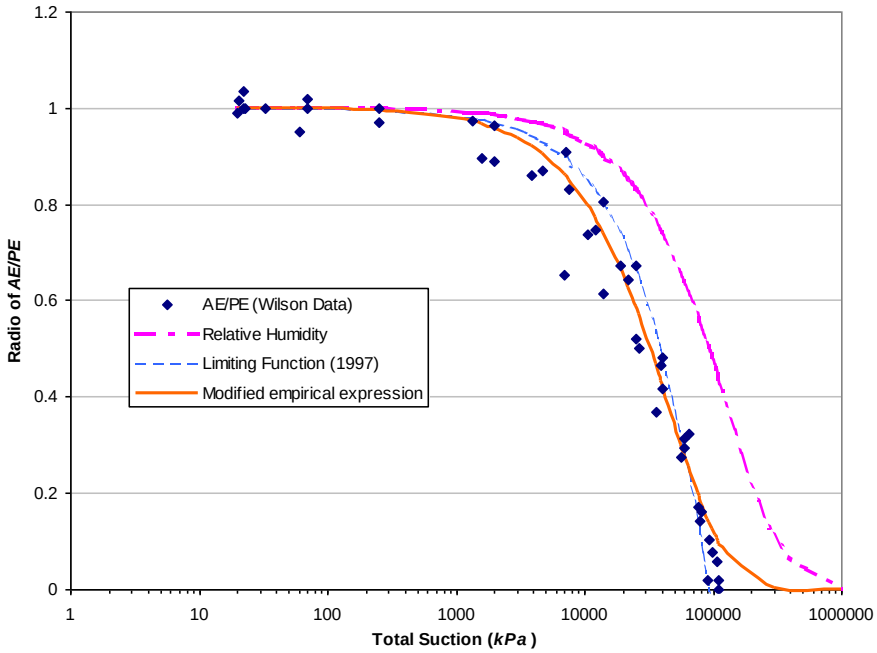

Figure 16 Comparison of predicted values of AE/PE using different suggested equations

Note: *Equation* ***[85]*** *is currently utilized in PLAXIS LE - Groundwater for obtaining the* ***Case 3 Solution***.

8 STREAM TRACES

For seepage models, the underground water flow velocity can be expressed using the following formulas. With v_x and v_y, the direction of the stream trace can be determined at a specific point.

$$V_x = k_x \frac{\partial h}{\partial x} = flux\_x$$
$$V_y = k_y \frac{\partial h}{\partial y} = flux\_y \quad \textbf{[86]}$$

where:

k_X = hydraulic conductivity in the *x*-direction,

k_Y = hydraulic conductivity in the *y*-direction,

h = total head,

flux_x = the flow in the *x* direction,

flux_y = the flow in the *y* direction.

9 PARTICLE TRACKING

The Particle Tracking feature allows the user to track the advective movement of contaminant particles in a solution. Clicking a location in the mesh will initiate the plotting of a path of a particle moving from the clicked location. The calculations assume zero diffusion.

The particle tracking feature is only for transient models. The theory behind the particle tracking is defined as follows:

$$x_1 = x_0 + \theta_w k_x \frac{\partial h}{\partial x} \Delta t$$
$$y_1 = y_0 + \theta_w k_y \frac{\partial h}{\partial y} \Delta t \qquad \textbf{[87]}$$

10 NUMERICAL IMPLEMENTATION

The PLAXIS LE - Groundwater module makes use of a finite element solver. The following sections provide a brief overview of some of the more significant numerical methods used in the software.

Primary advantages of this finite element solver are as follows:

- Fully implicit approach in the solver, which provides for a robust solution of difficult models with convergence issues,
- 2-noded line elements for 1D analysis, 3-noded triangle and 4-noded quadrilateral as elements for 2D analysis and 4-noded tetrahedron elements for 3D analysis,
- Automatic generation and control of time steps,
- The implicit integration scheme using the Weighted Residual Method,
- Newton-Raphson convergence iteration schemes, and
- Uses a high performance linear solver engine allowing solution of large models with more than million nodes.

10.1 INTERPOLATION ORDER

Finite element basis is linear. The selected interpolation equation will have an impact on the number of nodes on the resulting elements.

10.2 TIME STEPPING

Implicit method has been presented in literature as viable methods of solving for nodes while moving forward in time. Explicit methods use known data to "explicitly" define each nodal value at an advanced time. Such explicit methods usually suffer in accuracy and stability unless the time step is small. Implicit methods solve "implicitly" for self-consistent values at the advanced time (i.e., the simultaneous finite element spatial equations are solved at the advanced time). This improves the stability and accuracy for large time steps, at the cost of a simultaneous solution for all nodes in the mesh.

The implicit method has been selected in the software as the most robust method for general application. The research literature supports this decision.

10.2.1 Time Integration

The transient equations mentioned above can be spatially discretized and the Galerkin's principle of weighted residual method can be applied for the finite element formualations. The numerical integration of the partial differential equations results in a simpler expression of the equation:

$$\mathbf{M}\dot{\mathbf{h}} + \mathbf{K}\mathbf{h} = \mathbf{q} \qquad \textbf{[88]}$$

where :

M = mass matrix,

K = stiffness matrix,

q = flux vector reflecting the boundary conditions,

h = unknown hydraulic head vector, and

$\dot{\mathbf{h}}$ = time derivative of hydraulic heads at the nodal points = $\partial \mathbf{h} / \partial t$

The time derivative of Equation **[88]** can be approximated using a finite difference technique. The relationship between the nodal heads of an element at two successive time steps can be expressed using the backward difference approximation (implicit method):

$$\left(\mathbf{K} + \frac{\mathbf{M}}{\Delta t} \right) \mathbf{h}_{t+\Delta t} = \frac{\mathbf{M}}{\Delta t} \mathbf{h}_t + \mathbf{q} \qquad \textbf{[89]}$$

The finite element flow equation (i.e., Equation **[88]**) can be written for each element and assembled to form a set of global flow equations. The set of global flow equations for the whole system is then solved using the sparse linear solver for the hydraulic heads at the nodal points, **h**. However, Equation **[88]** is nonlinear because the coefficients of permeability are a function of matric suction in unsaturated seepage analysis, which is related to the hydraulic head at the nodal points.

The hydraulic heads are the unknown variables in Equation **[88]** or **[89]**. Therefore, Equation **[89]** must be solved using an iterative procedure that involves a series of successive approximations. In the first iteration, the coefficients of permeability are

estimated based on the initial conditions of the hydraulic head or water table in order to calculate the fist set of hydraulic heads at the nodal points. The computed hydraulic heads are used to calculate the average matric suction in the element. The coefficient of permeability is adjusted in the subsequent iteration with the new set of matrix suctions. The adjusted set of coefficients of permeability is then used in the finite element formulations to calculate the new set of hydraulic heads. The above procedure is repeated until the difference in hydraulic heads at two successive iterations are smaller than a user specified tolerance.

10.2.2 Convergence Criteria

The convergence criterion used is known as relative residual norm criterion. The solution is deemed to have converged when the following criterion is satisfied:

$$\frac{\left\|\mathbf{h}_{k+1}-\mathbf{h}_{k}\right\|}{\left\|\mathbf{h}_{k}\right\|} \leq tol \qquad \textbf{[90]}$$

where $\mathbf{h}_{k+1}$ is the solution of Equation **[89]** at $(k+1)_{th}$ iteration for a particular time step and $\mathbf{h}_{k}$ is the solution at k_{th} iteration.

The tolerance (*tol*) is a user specified parameter. Once a solution for a particular time step satisfies the criterion **[90]**, the calculation for the time step concludes and moves forward for the next time step.

The convergence rate is highly dependent on the degree on nonlinearity of the permeability function of the materials and spatial discretization of the problem. A steep permeability function requires more iterations and a larger convergency tolerance. A finer discretization in both element size and time step will assist in obtaining convergence faster with a smaller tolerance (Fredlund and Rahardjo, 1993).

10.2.3 Time-Step Control

Staged analysis is obtained by discretizing a stage into several small time-steps and using an incremental analysis. The time-step for each sub-step is controlled by the following:

- The time discretization set by the user
- The time discretization set by the user for the outputs such as Contour plots and Graph plots or for any other printed output of the simulations results
- The time discretization of the applied boundary conditions
- The time discretization based on automatic adjustment of the time-step based on the global error in solution in each subsequent iteration

The adaptive time steps algorithm implemented is based on a slightly modified form of the error control algorithm proposed by Söderlind (2002). The solver adopts the next time-step considering above controls. If the solution failed to converge within the maximum iteration set by the user, the time-step is reduced based on the global error in the solution and re-try using a smaller time step. The above procedure repeats until the solution converges. If the time increment reaches to the "minimum" time cincrement set by the user in the Stage Settings dialog, the solution is deemed to have failed to converge. If such situation occurs, the user is advised to review the material properties if there are any materials with a sharp changes in coefficients of permeability. Similarly, the initial conditions, boundary conditions, and the mesh density can also be reviewed for problems with convergence issues.

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