

Unsaturated Soil Mechanics as a Series of Partial Differential Equations

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Abstract

Unsaturated soils theory can be laid out as a series of governing partial differential equations (PDEs), allowing for the solution of complex problems, including the analysis of volume change of expansive and collapsible soils, the design of soil cover systems, the analysis of transient slope stability, to name only a few problems. The practical relevance of design approaches based on PDEs has increased as a result of recent advances in computer geotechnics and the rise of *problem solving environments*. This paper presents an overview of PDEs governing the behaviour of unsaturated soils. Numerous phenomena were considered, including air flow, liquid water and vapour water flow, static equilibrium, total volume change, yield, heat transfer, and freeze-thawing processes. The PDEs describing unsaturated soil behaviour may also be simplified and de-coupled, in order to neglect processes that are unimportant in certain situations. Several degrees of de-coupling traditionally adopted in commercially available software packages are described and the consequences of such simplifications are explored. Finally, the use of general PDE systems along with general purpose partial differential equations solvers is shown as the way forward. It is envisaged that state-of-the-art *problem solving environments* can be used as the ultimate tool in unsaturated soil mechanics practice.

Keywords: unsaturated soils, continuum mechanics, partial differential equation, numerical modelling, soil-water characteristic curve.

1 Relevance of partial differential equations to unsaturated soil mechanics

Continuum mechanics and differential calculus have been traditionally used for modelling geotechnical engineering problems. Continuum mechanics theories are often expressed in the form of partial differential equations (PDEs) that govern the distribution of soil state variables in space and time.

The partial differential equations governing unsaturated soil behaviour involve numerous coupled processes with nonlinear and heterogeneous soil properties and nonlinear boundary conditions. PDEs have been applied for the analysis of several unsaturated soil problems,

such as volume change of expansive and collapsible soils, the design of soil cover systems, and the transient slope stability, to name only a few problems.

The practical relevance of analyses based on PDEs has increased as a result of recent advances in computer geotechnics and the rise of *problem solving environments*, PSEs. In depth knowledge of finite element theory and other numerical formulations becomes unnecessary when reliable PSEs are available.

In order to use a PSE effectively the analyst must understand the physics and soil properties involved and be able to select appropriate boundary and initial conditions that reproduce field conditions. It becomes advantageous to be able to “read” and formulate PDEs for a problem in hand.

Figure 1 presents the elements required in order to model an unsaturated soil problem, considering as an example a three-dimensional slope. According to the continuum mechanics approach, unsaturated soil phenomena can be modelled as follows:

1. Identify the physical processes of concern associated with the problem in hand;
2. Establish the “continuous variables” acting upon a representative elemental volume (REV) of soil;
3. Develop field equations governing the physical processes of concern by making the assumption that the media can be considered a continuum from a macroscopic standpoint (i.e., considering a REV of soil) and using measurable soil properties:
 - a. Develop conservation laws;
 - b. Develop constitutive laws;
 - c. Develop a final system of well-posed determinate partial differential equations.
4. Establish initial, internal, and boundary conditions for the problem;
5. Provide a mathematical solution of the system of PDEs.

The objective of this paper is to show how unsaturated soils theory can be laid out based on the continuum mechanics approach described above and as a series of PDEs. An overview of PDE's governing the behaviour of unsaturated soils is presented along with a detailed description of how the PDE's can be derived. Several phenomena are considered herein, including liquid water flow, water vapour flow, air flow, static equilibrium, total volume change, and heat flow.

The coupling between several unsaturated soil phenomena are described in terms of the coefficients and variables of the PDEs. The PDEs describing unsaturated soil behaviour may also be simplified and de-coupled, in order to neglect processes that are unimportant in certain situations. Several degrees of de-coupling traditionally adopted in commercially available software packages are described and the consequences of such simplifications are explored. The Cartesian coordinate system was adopted throughout the paper and all equations were written for a general three-dimensional case. Two-dimensional conditions can be easily obtained, as a simplification of the equations presented herein. The equations presented can also be converted to axis-symmetric conditions by using a cylindrical coordinate system. Though tensor notation offers an elegant and general way of presenting the differential equations governing unsaturated soil behaviour, engineering notation was adopted. Engineers in general are more prepared to understand the physics of soil behaviour, but may not grasp tensor notation promptly.

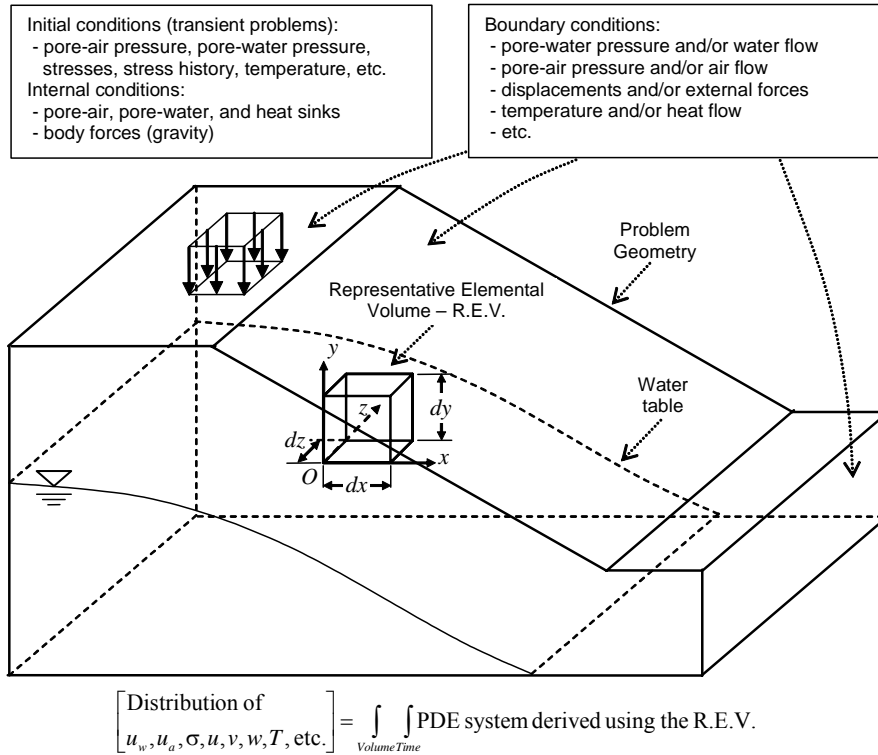


Figure 1 Continuum mechanics approach for solving unsaturated soil problems: problem domain subjected to initial and boundary conditions and governed by a system of PDE's (variables defined later in the text).

2 Assumptions traditionally adopted in the derivation of partial differential equations governing unsaturated soil behaviour

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

1. soil phases can be described using a continuum mechanics approach;
2. pore-air and all of its constituents (including water vapour) behave as ideal gases;
3. local thermodynamic equilibrium between the liquid water and water vapour phases exists at all times at any point in the soil; and
4. atmospheric pressure gradients are negligible.

In addition to the above general assumption, a number of specific simplifications can be adopted. The following simplification limit the generality of the PDE's presented herein, but are valid for most conditions found in the practice of geotechnical engineering:

1. liquid water and soil particles are assumed incompressible;
2. small strain theory is valid;
3. thermal strains are negligible;

4. osmotic pressure gradients become negligible at total suctions less than 1500 kPa;
5. temperature within the soil remains below the boiling point and above the freezing point of water at all times;
6. hysteretic behaviour of the soil-water characteristic curve can be neglected or approximated by taking the logarithmic average between the main drying and main wetting curves.

The six assumptions described above may become inadequate under certain situations. For instance, small strain theory may result in high inaccuracies for highly compressible media, such as certain landfills and mine tailings. Water compressibility has an important impact on the analysis of regional groundwater systems (i.e., large domains). Water flow analysis may require the consideration of freeze and thawing for cold regions. Also, thermal strains may be of interest in specific design conditions, such as confined clay buffers used for underground radioactive waste disposal.

Other simplifying assumptions are acceptable for numerous practical problems but are not adopted herein. Some of these assumptions are as follows:

1. the air phase may be assumed as in permanent contact with the atmosphere (i.e., pore-air pressure gradients are negligible);
2. dissolution of air into the liquid water phase may be neglected;
3. overall volume change may be neglected in air and water flow analyses;

The description of typical assumptions presented in this section is not exhaustive. Additional assumptions associated with the development of constitutive relationships will be described along this paper.

3 Stress state variables

Appropriate stress state variables must be used, that are able to accommodate the characteristics of a multi-phased continuum, such as an unsaturated soil. Fredlund and Morgenstern (1977) presented a theoretical justification for the use of two independent stress state variables.

The stress state variables for an unsaturated soil are made of possible combinations of the total stress, σ , the pore-air pressure, u_a , and the pore-water pressure, u_w . The net stress, $(\sigma - u_a)$, and matric suction, $(u_a - u_w)$, are normally used. Tensors for the two independent stress variables can be written as follows:

$$\begin{bmatrix} \sigma_x - u_a & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y - u_a & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z - u_a \end{bmatrix} \text{ and } \begin{bmatrix} u_a - u_w & 0 & 0 \\ 0 & u_a - u_w & 0 \\ 0 & 0 & u_a - u_w \end{bmatrix} \quad (1)$$

where:

- σ_i = normal stress acting on the i plane, on the i direction;
- τ_{ij} = shear stress acting on the i plane, on the j direction.

The net stress and matric suction tensors reduces to a single stress variable (i.e., effective stress) for saturated conditions, providing an approach consistent with that traditionally used in saturated soil mechanics (Terzaghi, 1943). The two stress state variables above are used throughout this paper.

4 Differential conservation equations for unsaturated soils

Three fundamental conservation laws are generally required in order to establish governing equation for unsaturated soils; namely, conservation of momentum; conservation of mass; and conservation of heat. A continuum mechanics framework is employed herein, resulting in the use of differential calculus to represent these fundamental conservation laws. The assumption that the variables involved are continuous is assumed valid from a macroscopic, phenomenological standpoint.

4.1 Conservation of linear and angular momentum

The distribution of total stresses within an unsaturated soil is governed by the static equilibrium of forces. Stresses acting in each face of a REV can be decomposed as the normal and shear components in the x , y , and z -directions, as shown in Fig. 2. According to the convention adopted herein, the stresses shown in Fig. 2 are all positive. The balance of angular momentum, taken with respect to any axis, shows that the Cauchy tensor (Eq. 1) must be symmetric (i.e., $\tau_{ij} = \tau_{ji}$). The balance of linear momentum (i.e., the equilibrium of forces) results in the PDE's governing static equilibrium of forces (Chou and Pagano, 1992). The equilibrium equations, in Cartesian coordinates, are as follows:

$$\begin{aligned} \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + F_x &= 0 \\ \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + F_y &= 0 \\ \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \sigma_z}{\partial z} + F_z &= 0 \end{aligned} \quad (2)$$

where:

$$F_i = \text{body force acting on the } i \text{ direction.}$$

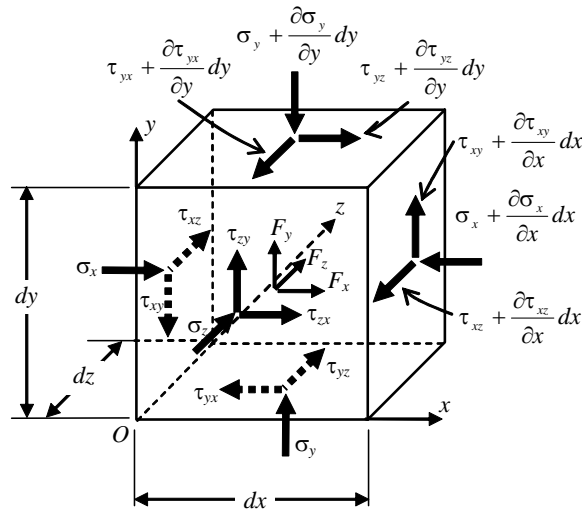


Figure 2 Soil representative elemental volume and stresses acting on the REV faces (stresses at the negative z -face are not shown for clarity).

The same equations above can be obtained by defining an arbitrary finite body and utilizing the divergence (or Gauss) theorem. It is important to point out that pore-water and pore-air pressures have no direct role in the equilibrium of forces acting upon the faces of an unsaturated soil REV. However, the partitioning of total forces into total stresses, pore-water, and pore-air pressures will depend on the relative compressibility of each soil phase.

4.2 Conservation of mass and heat energy

Differential equations for the conservation of mass of water, mass of air, and heat can be developed by considering a REV of soil (Fig. 3). The equations of conservation can be derived by taking the flow rates in and out of the REV and equating the difference to the rate of change of mass or heat stored in the REV with time. The following differential equations are obtained by considering three-dimensional flow conditions:

$$-\frac{\partial q_x^w}{\partial x} - \frac{\partial q_y^w}{\partial y} - \frac{\partial q_z^w}{\partial z} = \frac{1}{V_0} \frac{\partial M_w}{\partial t} \quad (\text{conservation of mass of pore-water}) \quad (3)$$

$$-\frac{\partial q_x^a}{\partial x} - \frac{\partial q_y^a}{\partial y} - \frac{\partial q_z^a}{\partial z} = \frac{1}{V_0} \frac{\partial M_a}{\partial t} \quad (\text{conservation of mass of pore-air}) \quad (4)$$

$$-\frac{\partial q_x^h}{\partial x} - \frac{\partial q_y^h}{\partial y} - \frac{\partial q_z^h}{\partial z} = \frac{1}{V_0} \frac{\partial Q_h}{\partial t} \quad (\text{conservation of heat}) \quad (5)$$

where:

- $q_i^{w,a}$ = total water and air flow rate in the i -direction across a unit area of the soil, $\text{kg/m}^2 \text{ s}$;
- q_i^w = $\rho_w v_i^w$, $\text{kg/m}^2 \text{ s}$;
- q_i^a = $\rho_a v_i^a$, $\text{kg/m}^2 \text{ s}$;
- ρ_w = density of water, $\approx 1000.0 \text{ kg/m}^3$;
- ρ_a = density of air, kg/m^3 ;
- $v_i^{w,a}$ = water and air flow rate in the i direction across a unit area of the soil, m/s ;
- V_0 = referential volume, $V_0 = dx dy dz$, m^3 ;

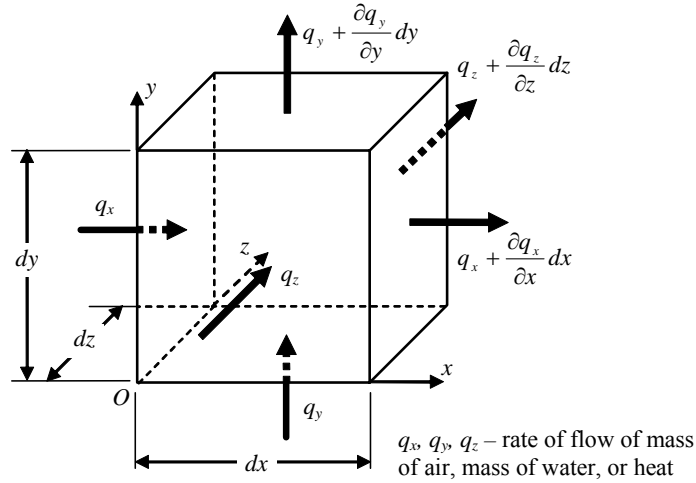


Figure 3 Soil representative elemental volume and fluxes q at the REV faces.

$M_{w,a}$	=	mass of water and air within the representative elemental volume, kg;
t	=	time, s;
q_i^h	=	heat flow rate in the i direction per unit of total area, J/(m ² s);
Q_h	=	heat within the representative elemental volume, J.

The total water flow rate, v^w , also known as specific discharge, is a macroscopic measure of flow rate 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 flow rate, v^w , may take place as liquid water and/or water vapour flow, as will be explained in the next sections. The average actual air flow velocity for a completely dry soil can be obtained by dividing v^a by the porosity. The total air flow rate, v^a , may take place as free air and/or air dissolved in liquid water, as will be explained in the next sections. Heat flow may take place by conduction, convection, or latent heat consumption. The mechanisms of air, water, and heat flow within unsaturated soils will be described in details later in this paper.

5 Strain-displacement relationships and compatibility equations

The classical definition of strain can be applied to an unsaturated soil body. The normal strain in a given direction, ϵ , is defined as the unit change in length (change in length per unit length) of a line which was originally oriented in the given direction. Shear strain, γ , is defined as the change in the right angle between reference axes, measured in radians (Chou and Pagano, 1992). The relationships between the normal and shear strains and the displacement in the x -, y -, and z -direction are as follows:

$$\epsilon_x = \frac{\partial u}{\partial x}, \quad \epsilon_y = \frac{\partial v}{\partial y}, \quad \epsilon_z = \frac{\partial w}{\partial z} \quad (6)$$

$$\gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}, \quad \gamma_{xz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}, \quad \gamma_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \quad (7)$$

where:

ϵ_i	=	normal strain in the i -direction;
γ_{ij}	=	shear strain with respect to the i and j reference axes;
u, v, w	=	displacement in the x -, y -, and z -direction, respectively.

The relationships above are obtained by making the assumption of small strains (i.e., neglecting the product of two or more derivatives of displacement). The assumption of small strains adopted herein applies to most engineering problems. Small strain formulations may be applied to large strain problems if geometry updating is performed along with an incremental analysis (Cook, 1981).

In addition to the strain-displacement relationships, strain compatibility equations can be derived (Chou and Pagano, 1992). The geometric significance of the strain compatibility equations rests in the fact that a strain field that does not satisfy the compatibility equations may result in “gaps” in the continuum. Nevertheless, compatibility equations are irrelevant because the continuous displacement functions generally used automatically satisfy the compatibility equations.

6 Constitutive laws for unsaturated soils

The modelling of unsaturated soil behaviour requires constitutive laws for stress-strain

behaviour, volume change of the pore-air and pore-water phases, and flow of pore-water, pore-air, and heat. Constitutive laws must be combined with the conservation laws in order to render the governing equations determinate.

Constitutive laws are generally established based on the phenomenological observation of the relationships between the state variables. Most constitutive laws for unsaturated soil are defined based on nonlinear soil properties (i.e., stress state dependent). The term *unsaturated soil property function* is used herein to refer to the function describing the relationship between a soil property and the stress state variables $(\sigma - u_a)$ and $(u_a - u_w)$.

6.1 Stress-strain relationship

Numerous stress-strain relationships have been proposed for unsaturated soils, mostly as extensions of existing models for saturated soils. Figure 4 presents an overview of some types of stress-strain relationships available in the literature. The most popular stress-strain models available can be classified as either elastic or elastoplastic models. Visco-elastoplastic and other types of models that have not received much attention in unsaturated soils modelling have not been included in Fig. 4.

Regardless of the model adopted, most elastic and elastoplastic stress-strain relationships for unsaturated soils can be written in the following generic format:

$$d\boldsymbol{\varepsilon} = \mathbf{D}^{-1}d(\boldsymbol{\sigma} - u_a\boldsymbol{\delta}) + \mathbf{H}d(u_a - u_w) \tag{8}$$

$$d(\boldsymbol{\sigma} - u_a\boldsymbol{\delta}) = \mathbf{D}d\boldsymbol{\varepsilon} - \mathbf{h}d(u_a - u_w) \tag{9}$$

where:

$$d = \text{indicates increment};$$

$$\boldsymbol{\varepsilon}^T = [\varepsilon_x \ \varepsilon_y \ \varepsilon_z \ \gamma_{xy} \ \gamma_{xz} \ \gamma_{yz}] ;$$

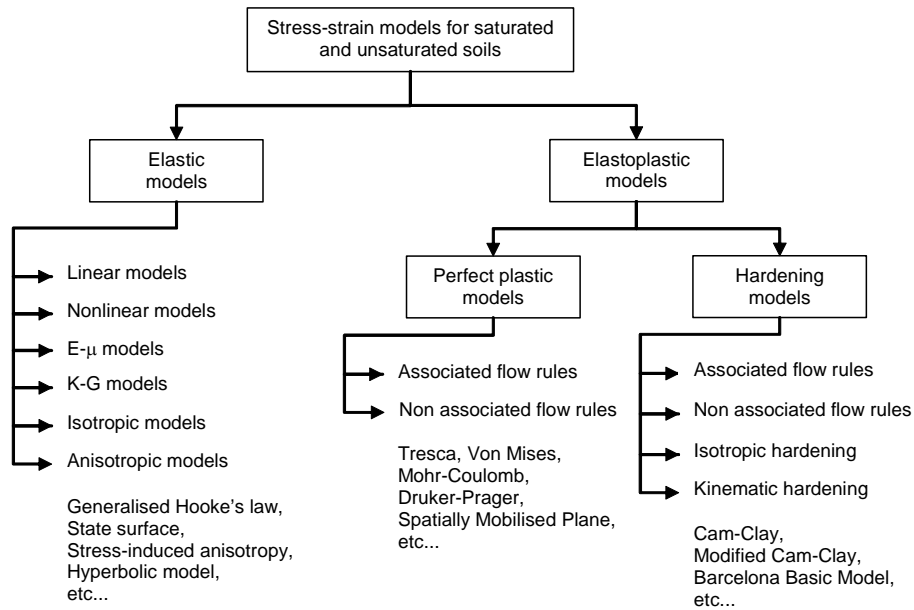


Figure 4 Stress-strain constitutive models for saturated and unsaturated soils.

$$\begin{aligned}
\mathbf{D}, \mathbf{H} &= \text{constitutive matrices;} \\
\mathbf{D} &= \begin{bmatrix} D_{11} & D_{21} & D_{31} & D_{41} & D_{51} & D_{61} \\ D_{12} & D_{22} & D_{32} & D_{42} & D_{52} & D_{62} \\ D_{13} & D_{23} & D_{33} & D_{43} & D_{53} & D_{63} \\ D_{14} & D_{24} & D_{34} & D_{44} & D_{54} & D_{64} \\ D_{15} & D_{25} & D_{35} & D_{45} & D_{55} & D_{65} \\ D_{16} & D_{26} & D_{36} & D_{46} & D_{56} & D_{66} \end{bmatrix}; \\
\mathbf{H}^T &= [H_1 \ H_2 \ H_3 \ H_4 \ H_5 \ H_6]; \\
\mathbf{h} &= \mathbf{DH}; \\
\mathbf{h}^T &= [h_1 \ h_2 \ h_3 \ h_4 \ h_5 \ h_6]; \\
\boldsymbol{\sigma}^T &= [\sigma_x \ \sigma_y \ \sigma_z \ \tau_{xy} \ \tau_{xz} \ \tau_{yz}]; \\
\boldsymbol{\delta}^T &= [1 \ 1 \ 1 \ 0 \ 0 \ 0].
\end{aligned}$$

The **bold** characters indicate matrices and vectors. The superscript (T) designates a transposed matrix. Some matrices were written in the transposed form for convenience.

6.1.1 Elastic models

Elastic models for unsaturated soils (left branch in Fig. 4) are usually based on extensions of Hooke's law (Fredlund and Morgenstern, 1976), using the two stress state variables, $(\sigma - u_a)$ and $(u_a - u_w)$:

$$\begin{aligned}
d\varepsilon_x &= \frac{1}{E} d(\sigma_x - u_a) - \frac{\mu}{E} d(\sigma_y + \sigma_z - 2u_a) + \frac{1}{H} d(u_a - u_w) \\
d\varepsilon_y &= \frac{1}{E} d(\sigma_y - u_a) - \frac{\mu}{E} d(\sigma_x + \sigma_z - 2u_a) + \frac{1}{H} d(u_a - u_w) \\
d\varepsilon_z &= \frac{1}{E} d(\sigma_z - u_a) - \frac{\mu}{E} d(\sigma_x + \sigma_y - 2u_a) + \frac{1}{H} d(u_a - u_w) \\
d\gamma_{xy} &= \frac{1}{G} d\tau_{xy}, \quad d\gamma_{xz} = \frac{1}{G} d\tau_{xz}, \quad \text{and} \quad d\gamma_{yz} = \frac{1}{G} d\tau_{yz}
\end{aligned} \tag{10}$$

where:

$$\begin{aligned}
E &= \text{Young modulus;} \\
\mu &= \text{Poisson's ratio;} \\
H &= \text{elastic modulus for soil structure with respect to suction change;} \\
G &= \text{shear modulus, } G = E/2(1 - \mu) .
\end{aligned}$$

The constitutive matrices \mathbf{D} , \mathbf{H} , and \mathbf{h} corresponding to Eq. (9) can be promptly written. Some nonlinear strain characteristics can be accounted for by using incremental analysis and the state surface concept (Matyas and Radakrishna, 1968). Using coefficients of compressibility obtained from the volume the void ratio state surface, the values of E and H can be obtained for each incremental step as follows:

$$E = \frac{3(1-2\mu)}{m_1^s} \tag{11}$$

$$H = \frac{3}{m_2^s} \tag{12}$$

where:

$$\begin{aligned}
 m_1^s &= \frac{d\varepsilon_v}{d(\sigma_{mean} - u_a)} = \frac{1}{1 + e_0} \frac{de}{d(\sigma_{mean} - u_a)}; \\
 m_2^s &= \frac{d\varepsilon_v}{d(u_a - u_w)} = \frac{1}{1 + e_0} \frac{de}{d(u_a - u_w)}; \\
 d\varepsilon_v &= \frac{dV}{V_0}; \\
 d\varepsilon_v &= m_1^s d(\sigma_{mean} - u_a) + m_2^s d(u_a - u_w); \\
 \sigma_{mean} &= \text{total mean stress, } \sigma_{mean} = (\sigma_x + \sigma_y + \sigma_z)/3; \\
 e_0 &= \text{initial void ratio;} \\
 e &= \text{state surface for void ratio, } e = f(\sigma_{mean} - u_a, u_a - u_w).
 \end{aligned}$$

Equations (11) and (12) are based on the assumption that the volume change of unsaturated soils is a function of changes in net mean stress and soil suction. Equation (11) alone does not provide a way of computing μ . The value of Poisson's ratio must be estimated or obtained from other means. For instance, μ can be obtained through triaxial or oedometric tests with measurement of lateral strains of lateral stresses, respectively.

The stress-induced anisotropy notably found in highly collapsible soils can be considered by using a stress-dependent Poisson's ratio and anisotropy coefficients applied to the H_i modulus (Pereira and Fredlund, 2000). Shear strength can be addressed by using a hyperbolic curve (Duncan and Chang, 1970) for the unsaturated soil Young modulus near failure. Elastic models can be considered generally appropriate for the analysis of monotonic net stress and suction paths. However, elastic models may not be accurate when non-monotonic paths take place because the distinction between recoverable and irrecoverable strains is not considered.

6.1.2 Elastoplastic models

Elastoplastic models (right main branch in Fig. 4) may be employed in order to address features of soil behaviour such as yield and irrecoverable strains. Most elastoplastic models found in the literature are generally based on the same fundamental principles, but use different yield criteria, flow rules, and compressibility functions. Figure 4 lists several yield criteria used by perfect plastic models. Perfect plastic formulations for saturated soils can be extended to unsaturated soils by using the generalised Hooke's law and by incorporating the effect of soil suction into the yield criterion (Pereira, 1996).

Yield surfaces can be combined with hardening rules and cap surfaces. Hardening rules are used in order to reproduce changes in the size of the yield surface (isotropic hardening) or shifts in the yield surface position (kinematic hardening). Cap surfaces are used in order to account for yield that occurs at stress states below failure conditions.

Numerous models have been proposed for unsaturated soils based on a critical state framework. Some of the early model were proposed by Karube and Kato (1989), Alonso et al. (1990), Wheeler and Sivakumar (1995), and Cui and Delage (1996), among others. Great emphasis has been given to soils compacted at collapsible conditions. Most models are based on isotropic hardening laws and on yield surfaces that expand for increasing soil suctions. Collapse is reproduced by using appropriate modes of expansion of the yield curves and appropriate variations in soil compressibility for different suctions. Research continues to be undertaken in order to refine elastoplastic models for unsaturated soils.

Lloret and Ledesma (1993) present the manner how the elastoplastic stress-strain relationship can be written for unsaturated soils. The yield functions and corresponding flow rules

proposed by Alonso et al. (1990) were considered. The general stress-strain relationship takes the following form:

$$\begin{cases} \text{if } F_1 \leq 0 \text{ and } F_2 \leq 0 & d(\boldsymbol{\sigma} - u_a \boldsymbol{\delta}) = \mathbf{D}^e d\boldsymbol{\varepsilon} - \mathbf{h}^e d(u_a - u_w) \\ \text{if } F_1 > 0 \text{ or } F_2 > 0 & d(\boldsymbol{\sigma} - u_a \boldsymbol{\delta}) = \mathbf{D}^{ep} d\boldsymbol{\varepsilon} - \mathbf{h}^{ep} d(u_a - u_w) \end{cases} \quad (13)$$

where:

$$\begin{aligned} F_1 &= \text{yield function for load or suction decrease,} \\ &F_1 = f(\boldsymbol{\sigma} - u_a, u_a - u_w, \Gamma); \\ F_2 &= \text{yield function for suction increase,} \\ &F_2 = f(\boldsymbol{\sigma} - u_a, u_a - u_w, \Gamma); \\ \mathbf{D}^e, \mathbf{H}^e &= \text{elastic constitutive matrices, defined according to Eq. (10);} \\ \mathbf{D}^{ep}, \mathbf{H}^{ep} &= \text{elastoplastic constitutive matrices;} \\ \mathbf{D}^{ep} &= \mathbf{D}^e - \frac{1}{A - A_{cr}} \mathbf{D}^e \frac{\partial G_1}{\partial(\boldsymbol{\sigma} - u_a)} \left(\frac{\partial F_1}{\partial(\boldsymbol{\sigma} - u_a)} \right)^T \mathbf{D}^e; \\ &\mathbf{D}^e \mathbf{H}_s + \\ \mathbf{h}^{ep} &= \left[- \left(\frac{\partial F_1}{\partial(\boldsymbol{\sigma} - u_a)} \right)^T \mathbf{D}^e \mathbf{H}_s + \frac{\partial F_1}{\partial(u_a - u_w)} \right] \frac{1}{A - A_{cr}} \mathbf{D}^e \frac{\partial G_1}{\partial(\boldsymbol{\sigma} - u_a)}; \\ \mathbf{H}_s &= \begin{cases} \text{if } F_2 \leq 0 & \mathbf{H}^e \\ \text{if } F_2 > 0 & \mathbf{H}^e + \mathbf{H}^{ep} \end{cases}; \\ A &= - \frac{\partial F_1}{\partial \Gamma} \left(\frac{\partial \Gamma}{\partial \boldsymbol{\varepsilon}^p} \right)^T \frac{\partial G_1}{\partial(\boldsymbol{\sigma} - u_a)}; \\ A_{cr} &= - \left(\frac{\partial F_1}{\partial(\boldsymbol{\sigma} - u_a)} \right)^T \mathbf{D}^e \frac{\partial G_1}{\partial(\boldsymbol{\sigma} - u_a)}; \\ G_1 &= \text{flow rule, } G_1 = f(\boldsymbol{\sigma} - u_a, u_a - u_w, \Gamma); \\ \Gamma &= \text{hardening parameter;} \\ \left(\frac{\partial F_1}{\partial(\boldsymbol{\sigma} - u_a)} \right)^T &= \left[\frac{\partial F_1}{\partial(\sigma_x - u_a)} \quad \frac{\partial F_1}{\partial(\sigma_y - u_a)} \quad \frac{\partial F_1}{\partial(\sigma_z - u_a)} \quad \frac{\partial F_1}{\partial \tau_{xy}} \quad \frac{\partial F_1}{\partial \tau_{xz}} \quad \frac{\partial F_1}{\partial \tau_{yz}} \right]; \\ \left(\frac{\partial G_1}{\partial(\boldsymbol{\sigma} - u_a)} \right)^T &= \left[\frac{\partial G_1}{\partial(\sigma_x - u_a)} \quad \frac{\partial G_1}{\partial(\sigma_y - u_a)} \quad \frac{\partial G_1}{\partial(\sigma_z - u_a)} \quad \frac{\partial G_1}{\partial \tau_{xy}} \quad \frac{\partial G_1}{\partial \tau_{xz}} \quad \frac{\partial G_1}{\partial \tau_{yz}} \right]. \end{aligned}$$

The term Γ is generally taken as equal to the pre-consolidation stress for saturated conditions. Different functions for F_1 , F_2 , G_1 , G_2 and for the soil compressibility are defined by each model found in the literature. The original references should be consulted for further details.

Equations (8) and (9) can be used to provide generic equations to be used in the derivation of the partial differential equations governing unsaturated soil behaviour. Nevertheless, Eq. (10) will be employed herein for the derivation of the governing PDE's. The selection of Eq. (10) was based on its simplicity and straightforward relation with the soil compressibility coefficients.

6.2 Shear strength

Shear strength characteristics may be incorporated into the PDE's governing unsaturated soil behaviour through modification to the \mathbf{D} , \mathbf{H} , and \mathbf{h} matrices. For instance, shear strength is used by the Hyperbolic-type models to control the shape of the Young modulus function

(Duncan and Chang, 1970). The shear strength equations can also be used to define the yield criteria used by elastoplastic models.

Several shear strength equations were listed in Fig. 4, such as the Tresca, Von Mises, and Mohr-Coulomb equations. Extensions of the Mohr-Coulomb criterion for saturated soils are widely used to represent the shear strength for an unsaturated soil, τ_{ff} . Fredlund et al. (1996) proposed the following equation based on the Mohr-Coulomb criterion:

$$\tau_{ff} = c' + (\sigma_n - u_a)_f \tan \phi' + (u_a - u_w) \Theta^\kappa \tan \phi' \quad (14)$$

where:

τ_{ff}	=	shear stress at failure, acting on the failure plane;
$(\sigma_n - u_a)_f$	=	net normal stress acting on the failure plane;
c'	=	cohesion;
ϕ'	=	friction angle;
Θ	=	dimensionless parameter to account for the wetter area of contact;
κ	=	fitting parameter to account for any non-linearity between the area and volume representation of the amount of water contributing to the shear strength.

The shear strength for an unsaturated soil can be predicted using the soil-water characteristic curve and the saturated shear strength parameters, c' and ϕ' . According to Fredlund et al. (1996), Θ can be assumed as equal to the degree of saturation, S . Experimental evidence shows that the slope of the plot of shear strength versus soil suction begins to deviate from the effective angle of internal friction as the soil desaturates. This reduced slope is associated with the reduction in the wetted area of contact past the air-entry value.

Vanapalli et al. (1996) presents a slightly modified procedure, defining $\Theta = \Theta_n = (S - S_{res}) / (1 - S_{res})$ and making $\kappa = 1$. This second procedure, based on normalised (or effective) water content, renders the envelope potentially less flexible if the fitting parameter κ is not used.

6.3 Water phase volume change

The constitutive relationship for the amount of water store in the soil pores is usually given in terms of volume of water. Water compressibility is generally neglected. The change in volume of water stored in the soil pores can be written as function of elastic coefficients of compressibility, m_1^w and m_2^w , or volumetric modulus, E_w and H_w , as follows:

$$\begin{aligned} \frac{dV_w}{V_0} &= m_1^w d(\sigma_{mean} - u_a) + m_2^w d(u_a - u_w) \\ &= \frac{3}{E_w} d(\sigma_{mean} - u_a) + \frac{1}{H_w} d(u_a - u_w) \end{aligned} \quad (15)$$

where:

$$\begin{aligned} m_1^w &= \frac{S}{1 + e_0} \frac{de}{d(\sigma_{mean} - u_a)} + \frac{e}{1 + e_0} \frac{dS}{d(\sigma_{mean} - u_a)}; \\ m_2^w &= \frac{S}{1 + e_0} \frac{de}{d(u_a - u_w)} + \frac{e}{1 + e_0} \frac{dS}{d(u_a - u_w)}; \\ S &= \text{degree of saturation, } S = f(\sigma_{mean} - u_a, u_a - u_w); \end{aligned}$$

$$\begin{aligned}
e &= \text{void ratio, } e = f(\sigma_{mean} - u_a, u_a - u_w); \\
E_w &= 3/m_1^w; \\
H_w &= 1/m_2^w.
\end{aligned}$$

Equation (15) is based on the assumption that changes in the volume of pore-water stored in the soil are a function of changes in net mean stress and soil suction and are independent of changes in shear stresses. The use of state surfaces for void ratio and degree of saturation provides an effective method for computing E_w and H_w . Hysteretic characteristics of the pore-water storage can be addressed using more sophisticated relationships. However, the simple elastic relationships based on state surfaces can adequately reproduce monotonic stress paths.

Coupled PDE systems are often written in terms of displacements and pore pressures. Changes in $(\sigma_{mean} - u_a)$ present in Eq. (15) can be written in terms of changes in $(u_a - u_w)$ and strains using Eq. (10), as follows:

$$\frac{dV_w}{V_0} = \beta_1^w d\varepsilon_v + \beta_1^w d(u_a - u_w) \quad (16)$$

where:

$$\begin{aligned}
\beta_1^w &= \frac{m_1^w}{m_1^s} = \frac{E}{E_w(1-2\mu)}; \\
\beta_2^w &= m_2^w - \frac{m_1^w m_2^s}{m_1^s} = \frac{1}{H_w} - \frac{3}{E_w} \frac{E}{H(1-2\mu)}.
\end{aligned}$$

Equation (16) results in a smooth transition between saturated and unsaturated conditions, provided that appropriate constitutive coefficients are employed. As the soil saturates the effects of changes in soil suction and net stresses become equal (i.e., $m_1^s = m_2^s = m_1^w = m_2^w$). Consequently, Eq. (16) shows that for saturated conditions water volume changes are equal to changes in void ratio.

6.4 Air phase volume change

The characterisation of the air phase volume change requires the determination of three of the following variables; namely, V_a , M_a , and ρ_a . The air phase is highly compressible, and its density is given by the following equation:

$$\rho_a = \frac{M_a}{V_a} = \frac{W_a}{RT} \bar{u}_a \quad (17)$$

where:

$$\begin{aligned}
\rho_a &= \text{density of the bulk air phase, } \rho_a = W_a \bar{u}_a / (RT), \text{ kg/m}^3; \\
W_a &= \text{molecular weight of pore-air, 28.966 kg/kmol}; \\
\bar{u}_a &= \text{total pressure in the bulk air phase, } u_a + u_{atm}, \text{ kPa}; \\
u_a &= \text{pore-air pressure, kPa}; \\
u_{atm} &= \text{atmospheric pressure, 101.325 kPa};
\end{aligned}$$

Three volume change measurements can be made for an unsaturated soil; namely, overall, pore-water, and pore-air volume change. The combination of any two of these three volume change measurements provides a complete description of volume change within an

unsaturated soil. Pore-air volume changes have proven more difficult to measure than those of the pore-water phase. Therefore, it has become common practice to measure overall and pore-water volume changes. The volume of pore-air may be computed as follows:

$$\begin{aligned} \frac{V_a}{V_0} &= \frac{V_v}{V_o} - \frac{V_w}{V_o}(1-H_c) \\ &= n(1-S + SH_c) \end{aligned} \quad (18)$$

where:

$$\begin{aligned} H_c &= \text{Henry's volumetric coefficient of solubility, } V_{ad}/V_w; \\ V_{ad} &= \text{volume of air dissolved in the pore-water.} \end{aligned}$$

H_c is also known as the volumetric coefficient of solubility. At a constant temperature, the volume of dissolved air is a constant for different pressures. Dorsey (1940) cited by Fredlund and Rahadjo (1993) presents values of H_c for various temperatures. The density is assumed as being the same for the free air and for dissolved air.

The volume change constitutive relationship for the water phase can be obtained by taking an incremental form of Eq. (18) and using the constitutive relationship for pore-water volume change:

$$\frac{dV_a}{V_0} = \beta_1^a d\varepsilon_v + \beta_2^a d(u_a - u_w) \quad (19)$$

where:

$$\begin{aligned} \beta_1^a &= 1 - \beta_1^w(1 - H_c); \\ \beta_2^a &= -\beta_2^w(1 - H_c). \end{aligned}$$

Equation (19) shows how the volume change characteristics of the air phase can be directly obtained from the volume change characteristics of the water phase and soil skeleton.

6.5 Flow laws

Table 1 presents an overview of flow laws traditionally used for modelling unsaturated soil flow behaviour. 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). The several flow equations have the same format, but distinct potentials and properties. The flow laws presented in Table 1 are well established equations that have been experimentally verified.

Pore-air and pore-water have both miscible and immiscible mixture characteristics. Pore-air can flow as free air, as dissolved air diffusing through the liquid water, or as dissolved air carried by the liquid water. Pore-water can flow as liquid water, as water vapour diffusing through the free air-phase, or as water vapour carried by moving free air-phase. Some flow mechanisms are essential in the modelling of certain air and water flow conditions. For instance, evaporation cannot be properly reproduced without consideration of the water vapour flow (Wilson, 1990). Similarly, the air flow that takes place through saturated high air-entry value ceramics cannot be understood without consideration of the movement of dissolved air through the liquid water phase (Fredlund and Rahardjo, 1993).

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

Type of flow (1)	Flow mechanism (2)	Driving Potential (3)	Flow Law (4)
	Liquid water, v^{wl}	Hydraulic head, h (m)	Darcy's law
Flow of water, v^w	Water vapour diffusion, v^{vd}	Mass concentration of vapour per unit volume of soil, C_v (kg/m ³)	Modified Fick's law
	Water vapour carried by bulk air flow, v^{va}	Mass concentration of air per unit volume of soil, C_a (kg/m ³)	Modified Fick's law
Interphase liquid-vapour flow	Thermodynamic equilibrium	--- (*)	Lord Kelvin's equation
	Free air, v^{af}	Mass concentration of air per unit volume of soil, C_a (kg/m ³)	Modified Fick's law
Flow of air, v^a	Dissolved air diffusion, v^{ad}	Mass concentration of dissolved air per unit volume of soil, C_{ad} (kg/m ³)	Modified Fick's law
	Dissolved air carried by liquid water flow, v^{aa}	Hydraulic head, h (m)	Darcy's law
Flow of heat, q^h	Heat by conduction, q^c	Temperature, T (°C)	Fourier's law
	Latent heat	--- (*)	Interphase liquid-vapour flow

(*) local thermodynamic equilibrium assumed; function of the rate of vapour flow.

The following sections present a concise description of the flow laws listed in Table 1. All flow equations presented in this section were written for the y -direction (i.e., the direction corresponding to elevation) and considering isotropic conditions. Similar equations can be written for the x - and z -directions by using the appropriate gradient directions. Anisotropy can be easily incorporated into the flow equations by using conductivity ellipsoids. These ellipsoids can be defined by an anisotropy ratio and by the direction of “principal conductivities”, as shown by Bear (1972) and Freeze and Cherry (1979).

6.5.1 Flow of liquid water

The flow rate of liquid water in saturated/unsaturated soils can be described by using a generalisation of Darcy's Law (Bear et al., 1968), where the driving mechanism is the total head gradient and the hydraulic conductivity varies with matric suction, $(u_a - u_w)$. The generalised Darcy's law can be written as follows:

$$v_y^{wl} = -k^w \frac{\partial h}{\partial y} \quad (20)$$

where:

$$v_y^{wl} = \text{liquid pore-water flow rate in the } y\text{-direction across a unit area of the soil due to hydraulic head gradients, m/s;}$$

k^w	=	hydraulic conductivity, $k^w = f(u_a - u_w)$, m/s;
h	=	hydraulic head, m;
h	=	$\frac{u_w}{\gamma_w} + y$;
u_w	=	pore-water pressure, kPa;
γ_w	=	unit weight of water, ≈ 9.81 kN/m ³ ;
y	=	elevation, m.

The hydraulic conductivity function (i.e., the function giving the value of k^w for any value of $(u_a - u_w)$) may be obtained experimentally using laboratory or field tests, or estimated using the saturated hydraulic conductivity and the soil-water characteristic curve (Fredlund et al., 1994). The use of a continuous k^w function provides a smooth transition between the saturated and unsaturated condition.

6.5.2 Flow of water vapour

Water vapour flow through soils takes place by two mechanisms. Pore-water vapour may flow independently from the pore-air phase, driven by gradients in vapour concentration. Water vapour flow driven by vapour concentration may take place even if the bulk pore-air is at rest. Pore-water vapour may also be carried by the bulk pore-air phase, which may flow driven by gradients in the total pore-air pressure. The sum of these two vapour flow components results in the total water vapour flow, v^v .

The flow rate of water vapour due to gradients in vapour concentration can be described by a modified form of Fick's law (Philip and de Vries, 1957 and Dakshanamurthy and Fredlund, 1981):

$$v_y^{vd} = -\frac{D^v}{\rho_w} \frac{\partial C_v}{\partial y} = -\frac{D^v}{\rho_w} \frac{\partial C_v}{\partial p_v} \frac{\partial p_v}{\partial y} = -\frac{D^{v*}}{\rho_w} \frac{\partial p_v}{\partial y} \quad (21)$$

where:

v_y^{vd}	=	pore-water vapour flow rate in the y-direction across a unit area of the soil due to vapour concentration gradients, m/s;
D^v	=	molecular diffusivity of vapour through soil, m ² /s;
ρ_w	=	density of water, ≈ 1000.0 kg/m ³ ;
C_v	=	concentration of water vapour in terms of the mass of vapour per <u>unit volume of soil</u> , $C_v = \rho_v(1 - S)n$, kg/m ³ ;
ρ_v	=	density of the water vapour, $\rho_v = W_v p_v / (RT)$, kg/m ³ ;
W_v	=	molecular weight of water vapour, 18.016 kg/kmol;
p_v	=	partial pressure of water vapour, kPa;
R	=	universal gas constant, 8.314 J/(mol.K);
T	=	temperature, K;
S	=	degree of saturation, $S = V_w/V_v$;
n	=	porosity, $n = V_v/V_0$;
V_w, V_v	=	volume of water and voids in the elemental volume, respectively, m ³ ;
D^{v*}	=	$(1 - S)nD^v W_v / RT$, (kg.m)/(kN.s).

The soil properties D^v and D^{v*} can be directly measured or reasonably estimated by using the value of molecular diffusivity of vapour through air $(0.229 \times 10^{-4} (1 + T/273.15)^{1.75} \text{ m}^2/\text{s})$, Kimball et al., 1976) and combining that value with a tortuosity factor. Ebrahimi-B et al.

(2004) presents a summary of tortuosity coefficient functions proposed in the literature and shows that most existing functions result in similar values for the ranges of soil suction where vapour flow predominates over liquid flow.

The flow rate of water vapour due to bulk pore-air flow may also be described by a modified form of Fick's law (Philip and de Vries, 1957 and Dakshanamurthy and Fredlund, 1981). Using the fraction ρ_v/ρ_a in order to obtain the fraction of water vapour present in the pore-air, the following equation can be written:

$$\begin{aligned} v_y^{va} &= -\frac{\rho_v}{\rho_a} \frac{D^a}{\rho_w} \frac{\partial C_a}{\partial y} \\ &= -\frac{\rho_v}{\rho_a} \frac{D^a}{\rho_w} \frac{\partial C_a}{\partial \bar{u}_a} \frac{\partial \bar{u}_a}{\partial y} = -\frac{\rho_v}{\rho_a} \frac{D^{a*}}{\rho_w} \frac{\partial \bar{u}_a}{\partial y} \end{aligned} \quad (22)$$

where:

$$\begin{aligned} v_y^{va} &= \text{pore-water vapour flow rate in the } y\text{-direction across a unit area} \\ &\quad \text{of the soil due to bulk air-phase flow, m/s;} \\ \rho_a &= \text{density of the bulk air phase, } \rho_a = W_a \bar{u}_a / (RT), \text{ kg/m}^3; \\ D^a &= \text{coefficient of transmission of air, m}^2/\text{s}; \\ C_a &= \text{concentration of air in terms of the mass of vapour per } \underline{\text{unit}} \\ &\quad \underline{\text{volume of soil}}, C_a = \rho_a(1 - S)n; \\ D^{a*} &= (1 - S)nD^a W_a / RT, (\text{kg.m})/(\text{kN.s}). \end{aligned}$$

The soil properties D^a and D^{a*} can be directly measured or estimated using the same approach that was described above for D^v and D^{v*} . The total flow of water vapour is obtained by summing v_y^{vd} and v_y^{va} , given by Eqs. (22) and (23). Taking the sum of the two vapour flow components and neglecting gradients of atmospheric pressure, the following equation is obtained:

$$v_y^v = v_y^{vd} + v_y^{va} = -\frac{D^{v*}}{\rho_w} \frac{\partial p_v}{\partial y} - \frac{\rho_v}{\rho_a} \frac{D^{a*}}{\rho_w} \frac{\partial \bar{u}_a}{\partial y} \quad (23)$$

6.5.3 Mass transfer between liquid pore-water and pore-water vapour

Local thermodynamic equilibrium can be assumed between liquid pore-water and pore-water vapour at any time and at any point in the soil. This assumption means that a change in any of the state variables; namely, partial vapour pressure, p_v , temperature, T , or the total potential of the liquid pore-water, ψ , results in an immediate change of the other state variables towards equilibrium of the liquid-vapour system. The assumption of local thermodynamic equilibrium provides a way of quantifying mass transfer between liquid and vapour water. The following relationship between p_v , ψ , and T can be derived by assuming local thermodynamic equilibrium (Edlefsen and Anderson, 1943):

$$p_v = p_{vsat} e^{\frac{-\psi W_v}{\rho_w R(T+273.15)}} \quad (24)$$

where:

$$\begin{aligned} p_{vsat} &= \text{saturation vapour pressure of the soil water at temperature } T, \text{ kPa;} \\ \psi &= \text{total suction, kPa;} \\ W_v &= \text{molecular weight of water, 18.016 kg/kmol;} \end{aligned}$$

$$\begin{aligned} \rho_w &= \text{water density, } \approx 1000 \text{ kg/m}^3; \\ R &= \text{universal gas constant, } 8.314 \text{ J/(mol.K)}; \\ T &= \text{temperature, } ^\circ\text{C}. \end{aligned}$$

Values of saturation vapour pressure, p_{vsat} , are well established and depend primarily on the vapour temperature (i.e., the vaporization curve). Equation (24) shows that the partial vapour pressure is equal to the saturation vapour pressure when $\psi = 0$ kPa and zero when $\psi \approx 1 \times 10^6$ kPa. Changes in p_v due to changes in ψ at any given fixed temperature are negligible when $\psi < 1500$ kPa. As a result, the use of SWCC's formed by combining matric and total suction values (Fredlund, 2002) does not affect the value of p_v computed using Eq. (24).

It will be shown in the next sections that it is convenient to replace the gradients of p_v in Eq. (23) by gradients of suction, ψ , and temperature, T . A relationship between the gradients of p_v and the gradients of the other two variables, ψ and T , can be determined by deriving Eq. (24) using the chain rule:

$$\frac{\partial p_v}{\partial y} = \frac{W_v p_v}{\rho_w R (T + 273.15)} \left(\frac{\psi}{(T + 273.15)} \frac{\partial T}{\partial y} - \frac{\partial \psi}{\partial y} \right) \quad (25)$$

Soil-water characteristic curve data is generally plotted combining matric suction values up to 1500 kPa and total suction values beyond this value. In order to make Eqs. (24) and (25) consistent with the "hybrid" SWCC plot, the water potential, ψ , in Eqs. (24) and (25) can be assumed as equal to the soil suction obtained from the SWCC. Therefore, the term ψ corresponds to the total suction when values of ψ are larger than 1500 kPa and to matric suction when values of ψ are lower than 1500 kPa. Assuming that the effect of pore-air pressure changes is negligible in the computation of vapour pressures, and replacing the term ψ by $-u_w$, Eq. (25) can be re-written as follows:

$$\frac{\partial p_v}{\partial y} = \frac{W_v p_v}{\rho_w R (T + 273.15)} \left(\frac{\partial u_w}{\partial y} - \frac{u_w}{(T + 273.15)} \frac{\partial T}{\partial y} \right) \quad (26)$$

The following equation is obtained by substituting Eq. (26) into Eq. (23):

$$v_y^v = v_y^{vd} + v_y^{va} = -\frac{k^{vd}}{\gamma_w} \frac{\partial u_w}{\partial y} + \frac{k^{vd}}{\gamma_w} \frac{u_w}{(T + 273.15)} \frac{\partial T}{\partial y} - \frac{k^{va}}{\gamma_a} \frac{\partial u_a}{\partial y} \quad (27)$$

where:

$$\begin{aligned} k^{vd} &= \text{pore-water vapour conductivity by vapour diffusion within the air phase;} \\ k^{vd} &= \gamma_w \frac{W_v p_v}{\rho_w R (T + 273.15)} \frac{D^{v*}}{\rho_w}, \text{ m/s;} \\ k^{va} &= \text{pore-water vapour conductivity by advection within the free pore-air;} \\ k^{va} &= \gamma_a \frac{\rho_v}{\rho_a} \frac{D^{a*}}{\rho_w}, \text{ m/s;} \\ \gamma_w &= \text{unit weight of water, kN/m}^3; \\ \gamma_a &= \text{unit weight of air, kN/m}^3. \end{aligned}$$

6.5.4 Flow of dry air

Pore-air flow takes place primarily by two mechanisms. Pore-air may flow as free air driven by gradients in its concentration. Pore-air may also flow within the liquid pore-water, as dissolved pore-air. Dissolved pore-air may be carried by water flow (i.e., advection) or may flow by pore-air diffusion, driven by gradients in dissolved pore-air concentration.

The mass flux of free pore-air may be described by a modified form of Fick's law:

$$\begin{aligned} v_y^{af} &= -\frac{D^a}{\rho_a} \frac{\partial C_a}{\partial y} \\ &= -\frac{D^a}{\rho_a} \frac{\partial C_a}{\partial \bar{u}_a} \frac{\partial \bar{u}_a}{\partial y} = -\frac{D^{a*}}{\rho_a} \frac{\partial \bar{u}_a}{\partial y} \end{aligned} \quad (28)$$

where:

$$\begin{aligned} v_y^{va} &= \text{pore-air flow rate in the } y\text{-direction across a unit area of the soil due to pore-air concentration gradients, m/s;} \\ D^a &= \text{coefficient of transmission of air, m}^2\text{/s;} \\ \rho_a &= \text{density of the bulk air phase, } \rho_a = W_a \bar{u}_a / (RT), \text{ kg/m}^3\text{;} \\ C_a &= \text{concentration of air in terms of the mass of vapour per } \underline{\text{unit volume of soil}}, C_a = \rho_a(1-S)n\text{;} \\ D^{a*} &= (1-S)nD^aW_a / RT, \text{ (kg.m)/(kN.s).} \end{aligned}$$

All variables and soil properties presented in Eq. (28) have been defined previously. The soil properties D^a and D^{a*} can be directly measured or estimated using the same approach that was described above for D^v and D^{v*} , using a tortuosity coefficient.

The flow of dissolved pore-air driven by gradients in dissolved pore-air concentration may be described by a modified form of Fick's law:

$$\begin{aligned} v_y^{ad} &= -\frac{D^{ad}}{\rho_a} \frac{\partial C_{ad}}{\partial y} \\ &= -\frac{D^{ad}}{\rho_a} \frac{\partial C_{ad}}{\partial \bar{u}_a} \frac{\partial \bar{u}_a}{\partial y} = -\frac{D^{ad*}}{\rho_a} \frac{\partial \bar{u}_a}{\partial y} \end{aligned} \quad (29)$$

where:

$$\begin{aligned} v_y^{ad} &= \text{dissolved pore-air flow rate of in the } y\text{-direction across a unit area of the soil due to pore-air concentration gradients, m/s.} \\ D^{ad} &= \text{molecular diffusivity of dissolved air through water, m}^2\text{/s;} \\ C_{ad} &= \text{concentration of dissolved air in terms of the mass per } \underline{\text{unit volume of soil}}, C_{ad} = \rho_a S n H_c\text{;} \\ D^{ad*} &= n S H_c D^{ad} W_a / RT, \text{ (kg.m)/(kN.s).} \end{aligned}$$

The values of D^{ad*} can be directly measured or estimated. Values of D^{ad} and H_c found in the literature are summarised by Fredlund and Rahardjo (1993). As the soil desaturates, the diffusion of dissolved air through the liquid pore-water decreases and becomes insignificant when compared with the flow of free pore-air. The decrease in v^{ad} due to desaturation can be incorporated into the prediction of D^{ad*} by using a tortuosity coefficient.

The flow of dissolved pore-air carried by water flow (i.e., advection) may be described by

Darcy's law and taking the amount of dissolved air:

$$v_y^{aa} = -H_c k^w \frac{\partial h}{\partial y} \quad (30)$$

where:

$$v_y^{aa} = \text{flow rate of dissolved pore-air in the } y\text{-direction across a unit area of the soil due to bulk pore-liquid water flow, m/s.}$$

The total flow of pore-air is obtained by summing the three flow mechanisms, given by Eqs. (28), (29), and (30):

$$v_y^a = v_y^{af} + v_y^{ad} + v_y^{aa} = -\frac{k^a}{\gamma_a} \frac{\partial u_a}{\partial y} - \frac{k^{ad}}{\gamma_a} \frac{\partial u_a}{\partial y} - H_c k^w \frac{\partial h}{\partial y} \quad (31)$$

where:

$$\begin{aligned} k^a &= \text{pore-air conductivity;} \\ k^a &= \gamma_a \frac{D^{a*}}{\rho_a}, \text{ m/s;} \\ k^{ad} &= \text{pore-air conductivity by diffusion within the pore-liquid water;} \\ k^{ad} &= \gamma_a \frac{D^{ad*}}{u_a}, \text{ m/s;} \\ \gamma_a &= \text{unit weight of air, kN/m}^3. \end{aligned}$$

Equation (31) provides a smooth transition between unsaturated and saturated conditions. As suction decreases, the soil saturates and k^a decreases, eventually reaching zero, for the saturated condition. However, the flow of air does not cease for saturated conditions. The pore-air conductivity by diffusion within the pore-liquid water and the flow of dissolved air carried by bulk liquid-water flow increase for increasing saturation.

6.5.5 Flow of heat by conduction

Heat transfer in soils occurs by three primary mechanisms, namely: conduction; convection; and latent heat due to phase change. Heat transfer by convection of the pore-fluid in soils is considerably smaller than conductive heat transfer (Milly, 1984) and is generally neglected. Changes of phase can take place as vaporization/condensation. Freeze and thawing are of concern in some unsaturated soil mechanics problems, but are omitted herein.

The conductive heat flow, q_y^c , can be written as a function of the thermal conductivity of the soil and the temperature gradient, as follows:

$$q_y^c = -\lambda \frac{\partial T}{\partial y} \quad (32)$$

where:

$$\begin{aligned} q_y^c &= \text{heat flow rate in the } y\text{-direction across a unit area of the soil due to heat conduction, J/s;} \\ T &= \text{temperature, } ^\circ\text{C;} \\ \lambda &= \text{thermal conductivity, } \lambda = f(u_a - u_w), \text{ J/(m s } ^\circ\text{C)}. \end{aligned}$$

The latent heat flow can be obtained by multiplying the latent heat of vaporization and condensation, L_v , by the amount of vapour flow, given by Eq. (27).

7 Partial differential equations for stress analysis

Partial differential equation for stress-deformation analysis can be written by combining the equilibrium equations, Eq. (2) with Hooke's generalised stress-strain law, Eq. (10). Expressing strains in terms of small displacements (u , v , and w for the x -, y -, and z -directions, respectively), the following PDE's are obtained:

$$\begin{aligned} \frac{\partial}{\partial x} \left[D_{11} \frac{\partial u}{\partial x} + D_{12} \frac{\partial v}{\partial y} + D_{12} \frac{\partial w}{\partial z} \right] + \frac{\partial}{\partial y} \left[D_{44} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ + \frac{\partial}{\partial z} \left[D_{44} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] - \frac{\partial}{\partial x} [h(u_a - u_w)] + \frac{\partial u_a}{\partial x} = 0 \end{aligned} \quad \begin{array}{l} \text{(x-direction)} \\ (33) \end{array}$$

$$\begin{aligned} \frac{\partial}{\partial x} \left[D_{44} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[D_{12} \frac{\partial u}{\partial x} + D_{11} \frac{\partial v}{\partial y} + D_{12} \frac{\partial w}{\partial z} \right] \\ + \frac{\partial}{\partial z} \left[D_{44} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] - \frac{\partial}{\partial y} [h(u_a - u_w)] + \frac{\partial u_a}{\partial y} = -\gamma_{nat} \end{aligned} \quad \begin{array}{l} \text{(y-direction)} \\ (34) \end{array}$$

$$\begin{aligned} \frac{\partial}{\partial x} \left[D_{44} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[D_{44} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] \\ + \frac{\partial}{\partial z} \left[D_{12} \frac{\partial u}{\partial x} + D_{12} \frac{\partial v}{\partial y} + D_{11} \frac{\partial w}{\partial z} \right] - \frac{\partial}{\partial z} [h(u_a - u_w)] + \frac{\partial u_a}{\partial z} = 0 \end{aligned} \quad \begin{array}{l} \text{(z-direction)} \\ (35) \end{array}$$

where:

$$\begin{aligned} D_{11} &= E(1-\mu)/[(1+\mu)(1-2\mu)]; \\ D_{12} &= E\mu/[(1+\mu)(1-2\mu)]; \\ D_{44} &= E/[2(1+\mu)]; \\ h &= E/[H(1-2\mu)]; \\ \gamma_{nat} &= \text{body force acting downward}; \\ \gamma_{nat} &= \gamma_s(1-n) + \gamma_w nS, \text{ kN/m}^3; \\ \gamma_s &= \text{specific weight of soil particles, kN/m}^3. \end{aligned}$$

Body forces are zero, with exception of the vertical body force, equal to the unit weight of the soil, γ_{nat} . Total volume change due to changes in pore-water pressure is neglected in Eqs. # and #. If total volume change due to changes in pore-water pressure is to be determined, the relationship between total volume change and pore-water pressure would have to be considered and Eqs. # and # should be solved in a coupled manner with Eqs. # and #. The primary variable of interest in the W-GHA model is the change in pore-water pressure and net stresses in response to the atmospheric boundary conditions. Therefore, the equilibrium-moisture flow coupling was assumed as not essential. This may not be the case for soils with large volume change characteristics, such as expansive and collapsible soils (Pereira, 1996).

8 Partial differential equations for water flow

In order to obtain the partial differential equation that governs the conservation and flow of liquid and vapour water through soils the flow law equations (Eqs. # and #) and a water volume change constitutive equation are combined with the continuity of water mass equation (Eq.). Considering the reference volume V_0 constant, the water phase and the soil structure incompressible, and assuming that the pore-air pressure is constant, the following equation is

obtained:

The PDE governing moisture flow can be modified using Eq. # in order to express gradients of p_v as function of the gradients of u_w and T . As a result, Eq. # can be re-written as follows:

$$\begin{aligned}
 & \frac{\partial}{\partial x} \left[k^w \frac{\partial h}{\partial x} + \frac{k^{vd}}{\gamma_w} \frac{\partial u_w}{\partial x} - \frac{k^{vd}}{\gamma_w} \frac{u_w}{(T+273.15)} \frac{\partial T}{\partial x} + \frac{k^{va}}{\gamma_a} \frac{\partial u_a}{\partial x} \right] \\
 & + \frac{\partial}{\partial y} \left[k^w \frac{\partial h}{\partial y} + \frac{k^{vd}}{\gamma_w} \frac{\partial u_w}{\partial y} - \frac{k^{vd}}{\gamma_w} \frac{u_w}{(T+273.15)} \frac{\partial T}{\partial y} + \frac{k^{va}}{\gamma_a} \frac{\partial u_a}{\partial y} \right] \\
 & + \frac{\partial}{\partial z} \left[k^w \frac{\partial h}{\partial z} + \frac{k^{vd}}{\gamma_w} \frac{\partial u_w}{\partial z} - \frac{k^{vd}}{\gamma_w} \frac{u_w}{(T+273.15)} \frac{\partial T}{\partial z} + \frac{k^{va}}{\gamma_a} \frac{\partial u_a}{\partial z} \right] \\
 & = \beta_1^w \frac{d}{dt} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \beta_1^w \frac{d(u_a - u_w)}{dt}
 \end{aligned} \tag{36}$$

Equation # is the final PDE governing the flow of moisture by liquid water and water vapour flow. Temperature gradients required to render this equation solvable can be obtained by solving a PDE governing conservation of thermal energy. Three unsaturated soil property functions can be identified in Eq. #; namely: the hydraulic conductivity, the vapour conductivity, and the soil-water characteristic curve. These soil properties functions vary with soil suction, and therefore, the PDE is physically non-linear.

9 Partial differential equations for air flow

Present the general equation, and several degrees of simplification, always describing in which situations the several PDE forms should be used. The general equation should be transient, and take into account the air dissolved in the water and the compressibility of the soil structure. Describe the boundary and initial conditions applicable to this equation.

$$\begin{aligned}
 & \frac{\partial}{\partial x} \left[\frac{k^a}{g} \frac{\partial u_a}{\partial x} + \frac{k^{ad}}{g} \frac{\partial u_a}{\partial x} + \rho_a H_c k^w \frac{\partial h}{\partial x} \right] \\
 & + \frac{\partial}{\partial y} \left[\frac{k^a}{g} \frac{\partial u_a}{\partial y} + \frac{k^{ad}}{g} \frac{\partial u_a}{\partial y} + \rho_a H_c k^w \frac{\partial h}{\partial y} \right] \\
 & + \frac{\partial}{\partial z} \left[\frac{k^a}{g} \frac{\partial u_a}{\partial z} + \frac{k^{ad}}{g} \frac{\partial u_a}{\partial z} + \rho_a H_c k^w \frac{\partial h}{\partial z} \right] \\
 & = \frac{W_a}{RT} \bar{u}_a \beta_1^a \frac{\partial}{\partial t} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \frac{W_a}{RT} \bar{u}_a \beta_1^a \frac{\partial (u_a - u_w)}{\partial t} + (1-S)n \frac{W_a}{RT} \frac{\partial u_a}{\partial t}
 \end{aligned} \tag{37}$$

where:

- n = soil porosity;
- S = degree of saturation, obtained from the soil-water characteristic curve.

10 Partial differential equations for heat flow

In order to obtain the partial differential equation that governs the conservation and flow of heat through soils, the equation of conservation of heat (Eq. #) must be combined with the heat flow equations (Eqs. # multiplied by L_v , and Eqs. #). Furthermore, the total amount of heat within the REV must be written as a function of the volumetric specific heat of the soil. The following results:

$$\begin{aligned} & \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} + L_v \frac{\bar{u}_a + p_v}{\bar{u}_a} D^{v*} \frac{\partial p_v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} + L_v \frac{\bar{u}_a + p_v}{\bar{u}_a} D^{v*} \frac{\partial p_v}{\partial y} \right) \\ & + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} + L_v \frac{\bar{u}_a + p_v}{\bar{u}_a} D^{v*} \frac{\partial p_v}{\partial z} \right) = \zeta \frac{\partial T}{\partial t} \end{aligned} \quad (38)$$

where:

$$\begin{aligned} T &= \text{temperature, } ^\circ\text{C}; \\ L_v &= \text{latent heat of vaporization/condensation, } 4.187 \times 10^3 \times (591 - 0.51 \times T), \text{ J/kg}; \\ \zeta &= \text{volumetric specific heat of soil, } \zeta = \gamma_{nat} c = f(u_a - u_w), \text{ J/(m}^3 \text{ } ^\circ\text{C)}. \end{aligned}$$

Expressing the gradients of partial vapour pressure in Eq. # in terms of gradients of pore-water pressure and temperature (using Eq. #), the following PDE is obtained:

$$\begin{aligned} & \frac{\partial}{\partial x} \left[\left(\lambda - L_v k^v \frac{\rho_w}{\gamma_w} \frac{u_w}{T + 273.15} \right) \frac{\partial T}{\partial x} + L_v k^v \frac{\rho_w}{\gamma_w} \frac{\partial u_w}{\partial x} \right] \\ & + \frac{\partial}{\partial y} \left[\left(\lambda - L_v k^v \frac{\rho_w}{\gamma_w} \frac{u_w}{T + 273.15} \right) \frac{\partial T}{\partial y} + L_v k^v \frac{\rho_w}{\gamma_w} \frac{\partial u_w}{\partial y} \right] \\ & + \frac{\partial}{\partial z} \left[\left(\lambda - L_v k^v \frac{\rho_w}{\gamma_w} \frac{u_w}{T + 273.15} \right) \frac{\partial T}{\partial z} + L_v k^v \frac{\rho_w}{\gamma_w} \frac{\partial u_w}{\partial z} \right] = \zeta \frac{\partial T}{\partial t} \end{aligned} \quad (39)$$

Equation # is the final PDE governing the flow of heat. Equation # must be solved in a coupled manner, along with Eq. #. The primary variables are u_w and T . These two PDE's can be solved using some numerical approximations, such as the *Finite Element* and the *Finite Difference* methods. Two new unsaturated soil property functions can be identified in Eq. #; namely: the thermal conductivity function and the volumetric specific heat. These soil properties functions also vary with soil suction, rendering the PDE physically non-linear. All of the above-mentioned unsaturated soil property functions bear a relationship to the SWCC.

11 General coupled partial differential equations

This section will present diagrams showing the above PDE's (in their general forms, without simplifications), and showing how they are coupled. I intend to produce great figures for this section that could be used in the book.

Moisture moves through soils driven by gradients of total head and/or partial pressures for each of the moisture phases (i.e., both liquid water and water vapour). The ratio between the flow of liquid water and water vapour depends mainly on the *temperature* and degree of saturation of the soil. Consequently, the transient temperature gradients need to be determined and heat transfer must be taken into account when simulating the flow of moisture (Philip and de Vries, 1957 and Wilson et al., 1990). Several physical processes are involved in the analysis of moisture and heat flow. In order to obtain the equations governing heat and

moisture transfer, constitutive flow laws and water volume change constitutive laws are combined with the mass and heat conservation equations. Appropriate equations for the soil-atmosphere flux boundary conditions are required. The two-dimensional PDE's used herein are extensions of the one-dimensional formulations presented by Philip and de Vries (1957) and Wilson et al. (1990).

Coupling terms show indirect processes. Make table.

12 Concluding remarks

13 References

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We may have to explain this:

It has become conventional practice to plot soil-water characteristic curves using matric suction data for $(u_a - u_w) < 1500$ kPa and total suction data otherwise. Fredlund (2002) presents a detailed justification for why this apparently inconsistent approach is adequate in geotechnical engineering practice. Capillary effects dominate in the "low" suction range, while osmotic potential becomes of importance in the "high" suction range. Quoting Fredlund (2002), "*it is anticipated that this [the above manner] will continue to be the manner in which the soil-water characteristic curve is plotted and utilized in geotechnical engineering*". The plot of the SWCC combining matric and total suction was adopted throughout this paper. This combined plot provides an effective approach for unifying theories developed for the capillary and residual saturation conditions.

PAPER OUTLINE

- 1 Relevance of partial differential equations to unsaturated soil mechanics**
- 2 Assumptions traditionally adopted in the derivation of partial differential equations governing unsaturated soil behaviour**
- 3 Stress state variables**
- 4 Differential conservation equations for unsaturated soils**
 - 4.1 Conservation of linear and angular momentum**
 - 4.2 Conservation of mass and heat energy**
- 5 Strain-displacement relationships and compatibility equations**
- 6 Constitutive laws for unsaturated soils**
 - 6.1 Stress-strain relationship**
 - 6.1.1 Elastic models**
 - 6.1.2 Elastoplastic models**
 - 6.2 Shear strength**
 - 6.3 Water phase volume change**
 - 6.4 Air phase volume change**
 - 6.5 Flow laws**
 - 6.5.1 Flow of liquid water**
 - 6.5.2 Flow of water vapour**
 - 6.5.3 Mass transfer between liquid pore-water and pore-water vapour**
 - 6.5.4 Flow of dry air**
 - 6.5.5 Flow of heat by conduction**
- 7 Partial differential equations for stress analysis**

- 8 **Partial differential equations for water flow**
- 9 **Partial differential equations for air flow**
- 10 **Partial differential equations for heat flow**
- 11 **General coupled partial differential equations**
- 12 **Concluding remarks**
- 13 **References**

Appendices: equations using tensor notation, physical constants, etc.?