UNIVERSITAT POLITÈCNICA DE CATALUNYA

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CONSTITUTIVE MODELS FOR UNSATURATED SOILS. A THERMODYNAMIC APPROACH

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ABSTRACT

Unsaturated soils are particular instances of porous materials, which are characterized by a solid skeleton and a number of fluids that can flow through the skeleton. At the microscale, a porous material is made of interacting entities of various dimensions (3D phases, 2D interfaces, 1D common lines, 0D common points), which contain various species (mineral, water, air, …). If representative volume elements (REV) can be defined, averaging yields a set of macroscale interacting continua, which can be modeled using mixture theory. After averaging, the microscale geometric features of the entities and the microscale distributions of thermodynamic properties within the entities are lost. In order to recover part of this information, macroscale geometric variables (e.g. volume, area, length or number of points of each entity per REV volume) and macroscale density variables (e.g. mass of each species in each entity per unit REV) are defined. Additional macroscale variables can be defined in order to characterize the anisotropy of the porous material (e.g. structure tensors).

The state of a porous material is assumed to be given by the deformation of the solid skeleton, the measure (volume, area, length, number of points) of each microscale entity per unit REV, the mass of each species in each microscale entity per unit REV, the temperature and a set of internal variables, which encapsulate the history of the material. The number of state variables can be significantly reduced by assuming that the evolution of the porous material is along local equilibrium states. These states are such that, for prescribed values of the strain tensor of the solid skeleton, the total mass of each species per unit reference volume, the temperature and the internal variables, the measure of each microscale entity per unit REV and of the mass of each species in each microscale entity per unit REV take unique values, such that the total free energy per unit reference volume is minimum. As a result, the state of a porous material is given by the strain tensor of the solid skeleton, the total mass of each species per unit reference volume, the temperature and the internal variables.

The constitutive model of a porous material is derived using the framework of thermodynamics with internal variables, in which the porous material is considered to be an open thermodynamic system. The state equations are derived from the free energy and the evolutions of the internal variables are derived from the dissipation or the dissipation potential. For unsaturated soils, additional simplifying assumptions are made: (1) small strains of the solid skeleton; (2) isothermal atmospheric conditions; (3) three species: solid mineral, water and gas; and (4) elastoplastic response of the deformation of the solid skeleton and of the water mass content.

Eventually, short-range interaction forces bond water to the solid skeleton. Vicinal water is bond to the solid skeleton, whereas free water is not. The behavior of free water is as if it were outside the soil, so that microscale pressure distributions are uniform (neglecting gravity) and a macroscale pressure can be related to chemical potentials and temperature. In contrast, the behavior of vicinal water is influenced by interaction forces, so that microscale pressure distributions are not uniform. The behavior of a soil is assumed to be given by three different regimes: (1) saturated (fixed vicinal water, variable free water, no gas phase); (2) capillary (fixed vicinal water, variable free water, gas phase), with an hysteretic water retention curve; and (3) dry (variable vicinal water, no free water, gas phase). At each of these regimes a different constitutive model for the soil is used. Generic examples of these models are given: elastoplastic for the saturated regime, elastoplastic with water content hysteresis for the capillary regime and elastoplastic for the dry regime.

1 INTRODUCTION

Unsaturated soils exhibit particular features, such as reversible shrinking and hardening upon drying or irreversible collapse upon wetting. This might have led to consider unsaturated soils as special problem soils with respect to the more well understood saturated soils (Alonso et al. 1987). However, available field data of moisture content distribution with depth in regions with arid and semi-arid climates shows that total saturation is never reached in the upper soil layers, so that there is a need of an appropriate understanding of the behavior of unsaturated soils. In fact, complete saturation should be considered as a particular state of a soil (Gens 2010). The particular features of unsaturated soils are the result of complex interactions between solid particles and pore water (Low 1951, 1961), which bond the pore water to the soil. It is therefore expected that a measure of these interactions plays an important role in unsaturated soil mechanics.

In soil science, the attraction of the solid for water in a moist soil was considered in the pioneering work of Buckingham (1907). He defined the capillary potential as "the work required per centigram to pull water away from the mass of soil", which he considered to be a function of the gravimetric water content of the soil. Soil science applied thermodynamics to soil moisture (Edlefsen and Anderson 1943; Bolt and Frissel 1960; Babcock 1963; Sposito 1981), and used the concept of chemical potential of water. Sposito (1981) notes that the chemical potential of water has units of energy per unit mass, but it can be expressed in pressure units by multiplication by the liquid water density at a reference state and is called soil water pressure. He further remarks that "The chemical potential of soil water is no more a pressure physically after multiplication by the mass density of pure liquid water than it was before".

In soil mechanics, Terzaghi's principle of effective stress for saturated soils was an important landmark (Terzaghi 1923; Terzaghi 1936; Clayton et al. 1995). This principle was shown to result from the incompressibility of the solid grains and the independence of the yield stress in the grain material of the confining pressure. A generalization of this principle for soils containing two pore fluids at different pressures was proposed by Bishop, which depended on the pressure of both fluids (Bishop and Blight 1963). Subsequently, based on experimental evidence and theoretical developments, it was proposed that the stress state of an unsaturated soil requires two stress variables, such as net stress and matric suction (Fredlund and Morgenstern 1977; Houlsby 1997). Constitutive models for unsaturated soils based on a state surface were developed (Lloret and Alonso 1985), which give volumetric deformations induced by monotonic changes in net stress and suction. An important progress was achieved by the Barcelona Basic Model (Alonso et al. 1990), which extended the modified Cam clay model to unsaturated soils and was able to reproduce irreversible deformations induced by changes in net stress and suction. Based on this model with two stress state variables, a number of models for unsaturated soils have been proposed. On the other hand, models for unsaturated soils with one state variable (a generalized effective stress reducing to the Terzaghi's effective stress at saturation) have also been proposed (i.e. Wheeler et al. 2003; Li 2007a, 2007b).

Classical irreversible thermodynamics extended equilibrium thermodynamics by using the local equilibrium state assumption (de Groot and Mazur 1984; Kestin 1990). Rational thermodynamics was used to ensure the compatibility of constitutive laws with the second law of thermodynamics (Coleman and Noll 1963). Classical irreversible thermodynamics was enhanced with internal state variables to take into account the previous history (Coleman and Gurtin 1967; Lubliner 1973; Maugin 1999). Mixture theory was developed in order to describe the interactions of bodies composed of identifiable constituents (Bowen 1976; Truesdell 1984, Lecture 5) and has been used to develop constitutive models for porous materials such as soils (e.g. Bowen 1980, 1982).

Available constitutive models for unsaturated soils are able to reproduce many salient features of unsaturated soils. There are however conceptual issues in many of these models, such as not having a thermodynamic basis or using exceedingly large negative water pressures (Korevaar et al. 1983; Gray and Hassanizadeh 1991; Nitao and Bear 1996; Coussy 2004). It should be mentioned that the physics of unsaturated soils has also been considered in the scientific literature, but often leading to extremely complex models (Gray and Miller 2014).

The object of the present work is to propose a general framework for constitutive models for unsaturated soils. The conceptual approach employed is summarized below.

At the microscale (Gray and Miller 2014) soils are considered to be made of interacting entities (3D phases, 2D interfaces, 1D common lines and, if there are more than 3 phases, 0D common points), which contain various species (mineral, water, air, …). Each entity is considered to be a mixture of the interacting continua associated to each of its species (e.g. a 3D gas phase is considered a mixture of its gas components). If the conditions for the existence of a representative elementary volume (REV) are satisfied (Bear and Bachmat 1990), then averaging of these microscale interacting continua yields corresponding macroscale 3D interacting continua (Gray and Miller 2014).

After averaging, the microscale geometric features of the entities and the microscale distributions of thermodynamic properties within the entities are lost. In order to recover part of this information, macroscopic geometric variables are defined, such as the quotient of the measure of each entity (volume, area, length, number of points) and the volume of the REV. Similarly, macroscopic density variables are defined, such as the quotient of the mass of each species in each entity and the volume of the REV. A macroscale continuum is assigned to each species in the soil, which is equivalent to the set of the macroscopic continua assigned to the considered species in each entity (e.g. the macroscale continuum associated to water is the set of the macroscale continua associated to water in liquid phase, water in gas phase, water in liquid-gas interface, …), so that the soil is considered to be the mixture of these macroscopic interacting continua associated to each species (e.g. continua associated to mineral, water, air, …).

The hypothesis of local accompanying state (Callen 1985; Kestin 1990; Maugin 1999; Coussy 2004) allows to extend equilibrium thermodynamics to non-uniform systems. This hypothesis can be adopted provided that the considered evolutions of the soil are sufficiently slow so that at all times the soil in each REV can be considered to be approximately in equilibrium. The thermodynamic state is assumed to be given by the deformation of the skeleton, the macroscopic geometric and density variables, temperature and a set of internal variables, which account for the previous history. Recall that internal variables are observable but not controllable (Maugin 1999).

Furthermore, it is also assumed that, for given values of the skeleton deformation, total mass of each species, temperature and a set of internal variables, the macroscopic geometric and density variables can be obtained by minimization of the total free energy. In this case, the thermodynamic state is defined by the skeleton deformation, the mass of each species per unit volume, the temperature and a set of internal variables. Constitutive equations of the soil can be derived from the free energy and the dissipation or dissipation potential functions (Edelen 1974; Halphen and Nguyen 1975; Ziegler 1983; Maugin 1999; Coussy 2004; Houlsby and Puzrin 2006).

Using this thermodynamic framework, derivation of the free energy yields the total stress tensor and the chemical potentials of the constituents. If short-range interaction forces bond the liquid water to the solid particles (Low 1951), it is not possible to define the pressure of liquid water, because within a REV the distribution of liquid pressure is not uniform. However, it may occur that, away from the solid particles, there is fluid not subjected to interaction forces (free fluid), so that throughout the free fluid the pressure is uniform (neglecting gravity forces). In this case the pressure of the free liquid can be given as a function of the chemical potentials of its components and the temperature, as if the free liquid were outside the soil.

In the unsaturated soil mechanics literature, often exceedingly high negative liquid water pressures are used, whereas in those conditions water should be in fact in gas phase (Gray and Hassanizadeh 1991). While it is widely acknowledged that those high negative liquid water pressures are in fact bonding energies per unit volume (Gens 2010), results including liquid pressures, such as the work input to a soil (Houlsby 1997; Coussy 2004), are used to develop constitutive models for unsaturated soils in which those high negative liquid pressures occur (i.e. energies per unit volume and pressures are used interchangeably).

Features of the soil at the microscale, such as the presence of liquid-gas interfaces or the presence of free liquid (not bonded to the solid particles), have an impact on the behavior of the soil. In this sense, we can define 3 regimes in a soil: (1) saturated (free liquid, no free gas); (2) capillary (free liquid, free gas); and (3) dry (no free liquid, free gas). In the saturated regime, under certain conditions (solid particles and vicinal liquid (bonded to the solid particles) are incompressible, no phase change), Terzaghi's effective stress principle applies. In the capillary regime, the soil water characteristic curve exhibits hysteresis, and no (general) effective stress principle seems to apply. In the dry regime, drying progressively removes bonded liquid, leading to shrinking of eventually present solid-liquid aggregates. Because each of these regimes have different features, from the modeling point of view it seems appropriate to model each of these regimes separately. However, the state variables deformation of the solid skeleton, mass of each species and temperature are common to all regimes.

The following chapters are organized as follows. Chapter 2 Thermodynamic Framework presents the general balance equation of a continuum and gives several alternative expressions of it. They are used to establish the fundamental balance equations for a single continuum and for a material with identifiable constituents. Chapter 3 Porous Materials first presents the modeling framework for porous materials, describes their structure at the microscale, the variables and balance equations at the macroscale and introduces the concept of local equilibrium state. Then it presents the general form of the constitutive equations, the resulting entropy inequality, its general solution and the dissipative mechanisms. Finally, it discusses the pressures of free fluids within a porous material and the effective stresses. Chapter 4 Unsaturated Soils first presents the basic assumptions made for modeling unsaturated soils and gives a brief summary of convex analysis. Next it presents the elastoplastic framework used, with the general forms of the free energy and dissipation functions, Ziegler's orthogonality principle and the application of the framework of multisurface plasticity. Next it discusses the three regimes considered for the behavior of unsaturated soils, namely saturated, capillary and dry, and shows a generic example of a constitutive model for each of them. The capillary regime model includes the hysteresis of the water characteristic curve. Finally, additional topics are addressed, namely negative pore water pressures in the context of the work input and matrix suction, and an example of the implicit use of the concept of local equilibrium state in saturated porous materials. Chapter 5 Conclusions presents a summary of the general modeling approach used, the soil regimes and discusses some features of the proposed formulation.

2 THERMODYNAMIC FRAMEWORK

2.1 GENERAL BALANCE EQUATION OF A CONTINUUM

Balance equations are used to express fundamental physical principles, such as balance of mass, balance of momentum, balance of moment of momentum, balance of energy and balance of entropy. The main forms in which the general balance equation of a continuum can be stated are given below.

2.1.1 Basic forms of the general balance equation

The general balance equation of a continuum is stated in integral form. Additional regularity assumptions allow to express the general balance equation of a continuum in differential and jump forms.

2.1.1.1 Integral form

The balance equation of an extensive property ξ in a material volume $\mathcal{V}_t$ of a continuum states that the rate of change of ξ in $\mathcal{V}_t$ equals the sum of the supply of ξ through the boundary $\partial\mathcal{V}_t$ of $\mathcal{V}_t$ plus the supply of ξ within $\mathcal{V}_t$. The integral form of the general balance equation (in Cartesian coordinates) is

$$\frac{d}{dt}\left(\int_{\mathcal{V}_t} \xi^{\cdots}_{\cdots} dv\right) = \int_{\partial\mathcal{V}_t} \phi^{\cdots i}_{\cdots} n_i da + \int_{\mathcal{V}_t} \zeta^{\cdots}_{\cdots} dv\,, \tag{2.1}$$

where $\phi^{\cdots i}_{\cdots}$ is the flux of $\xi^{\cdots}_{\cdots}$ through $\partial\mathcal{V}_t$, n_i is the outer unit normal to $\partial\mathcal{V}_t$ and $\zeta^{\cdots}_{\cdots}$ is the supply of $\xi^{\cdots}_{\cdots}$ within $\mathcal{V}_t$ per unit volume (Truesdell and Toupin 1960, Sect. 157).

2.1.1.2 Differential form

If (2.1) holds for all sufficiently regular volumes $\mathcal{V}_t$ and the fields $(\xi^{\cdots}_{\cdots})_{,t}$, $(\xi^{\cdots}_{\cdots})_{,i}$, $(v^i)_{,i}$, $(\phi^{\cdots i}_{\cdots})_{,i}$ and $\zeta^{\cdots}_{\cdots}$ are continuous, where v^i is the velocity field of the continuum, then it follows the differential form of (2.1)

$$(\xi^{\cdots}_{\cdots})_{,t} + \left(\xi^{\cdots}_{\cdots} v^i - \phi^{\cdots i}_{\cdots}\right)_{,i} = \zeta^{\cdots}_{\cdots} \tag{2.2}$$

(Truesdell and Toupin 1960, Sect. 157).

2.1.1.3 Jump form

If (2.1) holds for all sufficiently regular material volumes $\mathcal{V}_t$ and there is a persistent (not necessarily material) singular surface $\mathcal{S}_t$ with respect to $\xi^{\cdots}_{\cdots}$ and possibly also with respect to v^i in it such that $(\xi^{\cdots}_{\cdots})_{,t}$ and $\zeta^{\cdots}_{\cdots}$ are bounded and on each side of $\mathcal{S}_t$ and $\xi^{\cdots}_{\cdots}$, $v^i n_i$ and $\phi^{\cdots i}_{\cdots} n_i$, where n_i is the unit normal to $\mathcal{S}_t$, approach limits that are continuous functions of position on $\mathcal{S}_t$, then it follows the jump form of (2.1) on $\mathcal{S}_t$

$$\left[\!\left[\xi^{\cdots}_{\cdots}\left(v^i - u^i\right)n_i - \phi^{\cdots i}_{\cdots} n_i\right]\!\right] = 0 \tag{2.3}$$

where $[\![(\cdot)]\!]$ denotes the difference of the limits of $(\cdot)$ as $\mathcal{S}_t$ is approached on both sides and $u^i = un^i$ is the velocity of S_t (Truesdell and Toupin 1960, Sect. 193).

For interacting continua, it will be convenient to split the supply ζ as the sum of the supply as if the continuum were alone σ and the supply due to interactions with the other continua π (Kelly 1964). In this case (2.2) can be rewritten in the form

$$(\xi^{\cdots}_{\cdots})_{,t} + \left(\xi^{\cdots}_{\cdots} v^i - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots} = \pi^{\cdots}_{\cdots} \tag{2.4}$$

while (2.3) remains unchanged.

2.1.2 Alternative expressions of the general balance equation

There are equivalent expressions of the differential balance equation (2.4) and of the jump balance equation (2.3), which can be interpreted by considering a motion $x = \bar{\chi}(\bar{X}, t) = \bar{\chi}_t(\bar{X})$, which is a time-dependent smooth invertible map from a reference space with Cartesian coordinates $\{X^I\}$ to the physical space with Cartesian coordinates $\{x^i\}$. The velocity of the motion is $\bar{v}^i(\bar{X}, t\,) = \left(\partial\bar{\chi}^i/\partial t\right)(\bar{X}, t)$ and the deformation gradient of the motion is $\bar{F}^i{}_I(\bar{X}, t) = \left(\partial\bar{\chi}^i/\partial\bar{X}^I\right)(\bar{X}, t)$.

The inverse map $\bar{X} = \bar{\chi}_t^{-1}(x)$ assigns to the volume $\mathcal{V}$ or the surface $\mathcal{S}$ in the physical space the volume $\bar{\mathcal{V}} = \bar{\chi}_t^{-1}(\mathcal{V})$ or the surface $\bar{\mathcal{S}} = \bar{\chi}_t^{-1}(\mathcal{S})$ in the reference space and, vice versa, the map $x = \bar{\chi}_t(\bar{X})$ assigns to the volume $\bar{\mathcal{V}}$ or the surface $\bar{\mathcal{S}}$ in the reference space the volume $\mathcal{V} = \bar{\chi}_t(\bar{\mathcal{V}})$ or the surface $\mathcal{S} = \bar{\chi}_t(\mathcal{S})$ in the physical space. Similarly, the map $x = \bar{\chi}_t(\bar{X})$ assigns to the Eulerian field $g_E(x, t)$ the Lagrangian field $g_L(\bar{X}, t) = g_E(\bar{\chi}_t(\bar{X}), t)$ and, vice versa, the inverse map $\bar{X} = \chi_t^{-1}(x)$ assigns to the Lagrangian field $g_L(\bar{X}, t)$ the Eulerian field $g_E(x, t) = g_L(\chi_t^{-1}(x), t)$. By notational convenience, both fields g_E and g_L will be denoted by the same symbol g, leaving to the context which field is meant.

2.1.2.1 Differential form in Eulerian description

Let $\bar{v}^i(x, t) = \left(\partial\bar{\chi}^i/\partial t\right)(\bar{\chi}_t^{-1}(x), t)$ be the spatial velocity of the motion $x = \bar{\chi}_t(\bar{X})$. Then (2.4) can be rewritten as follows:

$$\begin{aligned}
\pi^{\cdots}_{\cdots} &= (\xi^{\cdots}_{\cdots})_{,t} + \left(\xi^{\cdots}_{\cdots} v^i - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots} \\
&= (\xi^{\cdots}_{\cdots})_{,t} + \left(\xi^{\cdots}_{\cdots}\bar{v}^i + \xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right) - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots} \\
&= (\xi^{\cdots}_{\cdots})_{,t} + (\xi^{\cdots}_{\cdots})_{,i}\bar{v}^i + \xi^{\cdots}_{\cdots}\left(\bar{v}^i\right)_{,i} + \left(\xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right) - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots}
\end{aligned}$$

and, using the definition $D^{\bar{v}}(\xi^{\cdots}_{\cdots})(x, t) = (\xi^{\cdots}_{\cdots})_{,t}(x, t) + (\xi^{\cdots}_{\cdots})_{,k}(x, t)\bar{v}^k(x, t)$, it becomes

$$D^{\bar{v}}(\xi^{\cdots}_{\cdots}) + \xi^{\cdots}_{\cdots}\left(\bar{v}^i\right)_{,i} + \left(\xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right) - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots} = \pi^{\cdots}_{\cdots} \tag{2.5}$$

Note that $D^{\bar{v}}(\xi^{\cdots}_{\cdots}) + \xi^{\cdots}_{\cdots}\left(\bar{v}^i{}_i\right)_{,i}$ is the rate of change of ξ in the elementary volume with motion $x = \bar{\chi}_t(\bar{X})$ and $\left(\xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right)\right)_{,i}$ is the flux of ξ that leaves the elementary volume with motion $x = \bar{\chi}_t(\bar{X})$.

2.1.2.2 Differential form in Lagrangian description

Multiplication of (2.5) by $\bar{J} = dv/d\bar{V}$, where dv is the element of volume in the current configuration and $d\bar{V}$ is the corresponding element of volume in the reference configuration, yields

$$\bar{J}\{D^{\bar{v}}(\xi^{\cdots}_{\cdots}) + \xi^{\cdots}_{\cdots}\left(\bar{v}^i\right)_{,i} + \left(\xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right) - \phi^{\cdots i}_{\cdots}\right)_{,i} - \sigma^{\cdots}_{\cdots}\} = \bar{J}\{\pi^{\cdots}_{\cdots}\}$$

and use Euler's formula $D^{\bar{v}}(J)(x, t) = J(x, t)\left(\bar{v}^i\right)_{,i}(x, t)$ (Truesdell and Toupin 1960, Sect. 20) yields

$$D^{\bar{v}}(\bar{J}\xi^{\cdots}_{\cdots}) + \bar{J}\left(\xi^{\cdots}_{\cdots}\left(v^i - \bar{v}^i\right) - \phi^{\cdots i}_{\cdots}\right)_{,i} - \bar{J}\sigma^{\cdots}_{\cdots} = \bar{J}\pi^{\cdots}_{\cdots}$$

where all variables are considered to be Eulerian fields depending on (x, t). Further, using the relation $D^{\bar{v}}(\xi^{\cdots}_{\cdots})(\bar{\chi}(\bar{X}, t), t) = (\xi^{\cdots}_{\cdots})_{,t}(\bar{X}, t)$ and the Piola identity $\left(\bar{J}y^i(\bar{F}^{-1})^I{}_i\right)_{,I} = \bar{J}\left(y^i\right)_{,i}$, where y^i is a vector field in the physical space and its Piola transform $Y^I = \bar J y^i (\bar F^{-1})^I{}_i$ is a vector field in the reference space (Marsden and Hughes 1994, p. 116), yields

$$(\bar J \xi^{\cdots}_{\cdots})_{,t} + \left(\bar J (\bar F^{-1})^I{}_i \left(\xi^{\cdots}_{\cdots}(v^i - \bar v^i) - \phi^{\cdots i}_{\cdots}\right)\right)_{,I} - \bar J \sigma^{\cdots}_{\cdots} = \bar J \pi^{\cdots}_{\cdots}$$

where all variables are considered to be Lagrangian fields depending on $(\bar X, t)$. This can be written in the form

$$(\Xi^{\cdots}_{\cdots})_{,t} + (\Xi^{\cdots}_{\cdots}(V^I - \bar V^I) - \Phi^{\cdots I}_{\cdots})_{,I} - \Sigma^{\cdots}_{\cdots} = \Pi^{\cdots}_{\cdots} \tag{2.6}$$

where the Lagrangian fields $\Xi^{\cdots}_{\cdots}(\bar X, t)$, $V^I(\bar X, t)$, $\bar V^I(\bar X, t)$, $\Phi^{\cdots I}_{\cdots}(\bar X, t)$, $\Sigma^{\cdots}_{\cdots}(\bar X, t)$ and $\Pi^{\cdots}_{\cdots}(\bar X, t)$ are defined in terms of the Eulerian fields $\xi^{\cdots}_{\cdots}(x, t)$, $v^i(x, t)$, $\bar v^i(x, t)$, $\phi^{\cdots i}_{\cdots}(x, t)$, $\sigma^{\cdots}_{\cdots}(x, t)$ and $\pi^{\cdots}_{\cdots}(x, t)$ by the relations

$$\begin{aligned}
\Xi^{\cdots}_{\cdots}(\bar X, t) &= \bar J(\bar X, t)\xi^{\cdots}_{\cdots}(\bar\chi(\bar X, t), t) \\
V^I(\bar X, t) &= (\bar F^{-1})^I{}_i(\bar X, t) v^i(\bar\chi(\bar X, t), t) \\
\bar V^I(\bar X, t) &= (\bar F^{-1})^I{}_i(\bar X, t) \bar v^i(\bar\chi(\bar X, t), t) \\
\Phi^{\cdots I}_{\cdots}(\bar X, t) &= \bar J(\bar X, t)(\bar F^{-1})^I{}_i\big((\bar X, t), t\big)\phi^{\cdots i}_{\cdots}(\bar\chi(\bar X, t), t) \\
\Sigma^{\cdots}_{\cdots}(\bar X, t) &= \bar J(\bar X, t)\sigma^{\cdots}_{\cdots}(\bar\chi(\bar X, t), t) \\
\Pi^{\cdots}_{\cdots}(\bar X, t) &= \bar J(\bar X, t)\pi^{\cdots}_{\cdots}(\bar\chi(\bar X, t), t)
\end{aligned} \tag{2.7}$$

2.1.2.3 Jump form in Eulerian description

Let $\bar v^i(x, t) = \left(\partial \bar\chi^i / \partial t\right)((\bar\chi_t)^{-1}(x), t)$ be the spatial velocity of the motion $x = \bar\chi_t(\bar X)$. Then (2.3) can be rewritten as follows:

$$\begin{aligned}
0 &= \llbracket \xi^{\cdots}_{\cdots}(v^i - u^i) n_i - \phi^{\cdots i}_{\cdots} n_i \rrbracket \\
&= \llbracket \xi^{\cdots}_{\cdots}(\bar v^i - u^i) n_i + \xi^{\cdots}_{\cdots}(v^i - \bar v^i) n_i - \phi^{\cdots i}_{\cdots} n_i \rrbracket
\end{aligned}$$

so that it becomes

$$\llbracket \xi^{\cdots}_{\cdots}(\bar v^i - u^i) n_i \rrbracket + \llbracket \xi^{\cdots}_{\cdots}(v^i - \bar v^i) n_i - \phi^{\cdots i}_{\cdots} n_i \rrbracket = 0 \tag{2.8}$$

where all variables are considered to be Eulerian fields on $\mathcal{S}_t$ depending on (x, t).

2.1.2.4 Jump form in Lagrangian description

Multiplication of (2.8) by $\bar J_s = da/d\bar A$, where da is the element of area in the current configuration and $d\bar A$ is the element of area in the reference configuration, yields

$$\bar J_s \{ \llbracket \xi^{\cdots}_{\cdots}(\bar v^i - u^i) n_i \rrbracket + \llbracket \xi^{\cdots}_{\cdots}(v^i - \bar v^i) n_i - \phi^{\cdots i}_{\cdots} n_i \rrbracket \} = 0$$

and using $\llbracket \bar J_s \rrbracket = 0$ yields

$$\llbracket \bar J_s \xi^{\cdots}_{\cdots}(\bar v^i - u^i) n_i \rrbracket + \llbracket \bar J_s \xi^{\cdots}_{\cdots}(v^i - \bar v^i) n_i - \bar J_s \phi^{\cdots i}_{\cdots} n_i \rrbracket = 0$$

From Nanson's formula $n_i da = \bar J(\bar F^{-1})^I{}_i N_I d\bar A$, where n_i is the unit normal to the element of surface in the current configuration and N_I is the unit normal to the corresponding element of surface in the reference configuration (Truesdell and Toupin 1960, Sect. 20), it follows $n_i = \bar J_s^{-1} \bar J (\bar F^{-1})^I{}_i N_I$. As in definitions (2.7), define the Lagrangian field $U^I(\bar X, t)$ in terms of the Eulerian field $u^i(x, t)$ by the relation

$$U^I(\bar{X},t) = (\bar{F}^{-1})^I{}_i(\bar{X},t)u^i(\bar{\chi}(\bar{X},t),t) \tag{2.9}$$

From this definition and definitions (2.7) it follows $\xi_{\cdots}^{\cdots} = \bar{J}^{-1}\Xi_{\cdots}^{\cdots}$, $v^i = \bar{F}^i{}_I V^I$, $\bar{v}^i = \bar{F}^i{}_I \bar{V}^I$, $\phi_{\cdots}^{\cdots i} = \bar{J}^{-1}\bar{F}^i{}_I \Phi_{\cdots}^{\cdots I}$. and $u^i = \bar{F}^i{}_I U^I$. Using these relations yields

$$\begin{aligned}
\bar{J}_s \xi_{\cdots}^{\cdots}\left(\bar{v}^i - u^i\right)n_i &= \bar{J}_s \bar{J}^{-1}\Xi_{\cdots}^{\cdots}\left(\bar{F}^i{}_I \bar{V}^I - \bar{F}^i{}_I U^I\right)\bar{J}_s^{-1}\bar{J}(\bar{F}^{-1})^J{}_i N_J \\
&= \Xi_{\cdots}^{\cdots}\left(\delta_I^J \bar{V}^I - \delta_I^J U^I\right)N_J \\
&= \Xi_{\cdots}^{\cdots}(\bar{V}^I - U^I)N_I
\end{aligned}$$

$$\begin{aligned}
\bar{J}_s \xi_{\cdots}^{\cdots}\left(v^i - \bar{v}^i\right)n_i &= \bar{J}_s \bar{J}^{-1}\Xi_{\cdots}^{\cdots}\left(\bar{F}^i{}_I V^I - \bar{F}^i{}_I \bar{V}^I\right)\bar{J}_s^{-1}\bar{J}(\bar{F}^{-1})^J{}_i N_J \\
&= \Xi_{\cdots}^{\cdots}\left(\delta_I^J V^I - \delta_I^J \bar{V}^I\right)N_J \\
&= \Xi_{\cdots}^{\cdots}(V^I - \bar{V}^I)N_I
\end{aligned}$$

$$\begin{aligned}
\bar{J}_s \phi_{\cdots}^{\cdots i} n_i &= \bar{J}_s \bar{J}^{-1}\bar{F}^i{}_I \Phi_{\cdots}^{\cdots I}\bar{J}_s^{-1}\bar{J}(\bar{F}^{-1})^J{}_i N_J \\
&= \delta_I^J \Phi_{\cdots}^{\cdots I} N_J \\
&= \Phi_{\cdots}^{\cdots I} N_I
\end{aligned}$$

Using these results it follows

$$[\![\Xi_{\cdots}^{\cdots}(\bar{V}^I - U^I)N_I]\!] + [\![\Xi_{\cdots}^{\cdots}(V^I - \bar{V}^I)N_I - \Phi_{\cdots}^{\cdots I}N_I]\!] = 0 \tag{2.10}$$

where all variables are considered to be Lagrangian fields on $\bar{\mathcal{S}}$ depending on $(\bar{X},t)$.

2.2 FUNDAMENTAL BALANCE EQUATIONS

Balance of mass, momentum, moment of momentum, energy and entropy express fundamental physical principles, so that they hold independently of the material type.

2.2.1 Balance equations for a single continuum

The balance equations of mass, momentum, moment of momentum, energy and entropy are obtained by replacing in the differential balance equation (2.4) and in the jump balance equation (2.3) the general variables $\xi_{\cdots}^{\cdots}$, $\phi_{\cdots}^{\cdots i}$, $\sigma_{\cdots}^{\cdots}$ and $\pi_{\cdots}^{\cdots}$ by the variables indicated in Table 2.1.

Table 2.1. Variables used in the balance equations: ρ is the mass density, $\hat{\rho}$ is the supply of mass per unit volume, v^j is the velocity, T^{ji} is the Cauchy stress tensor, b^j is the body force per unit mass, $\hat{p}^j$ is the supply of momentum per unit volume, $\hat{m}^j$ is the supply of moment of momentum per unit volume, ε is the internal energy per unit mass, q^i is the heat flux, r is the body heat supply per unit mass, $\hat{\varepsilon}$ is the supply of energy per unit volume, η is the entropy per unit mass, φ^i is the entropy flux, ς is the entropy supply per unit mass and $\hat{\eta}$ is the supply of entropy per unit volume (ε_{jkl} is the permutation symbol).

balance of	$\xi_{\cdots}^{\cdots}$	$\phi_{\cdots}^{\cdots i}$	$\sigma_{\cdots}^{\cdots}$	$\pi_{\cdots}^{\cdots}$
mass	ρ	$-$	$-$	$\hat{\rho}$
momentum	ρv^j	T^{ji}	ρb^j	$\hat{p}^j$
moment of momentum	$\varepsilon^j{}_{kl} x^k \rho v^l$	$\varepsilon^j{}_{kl} x^k T^{li}$	$\varepsilon^j{}_{kl} x^k \rho b^l$	$\hat{m}^j$
energy	$\rho\left(\varepsilon+\frac{1}{2}v_k v^k\right)$	$T_k{}^i v^k - q^i$	$\rho\left(b_k v^k + r\right)$	$\hat{\varepsilon}$
entropy	$\rho\eta$	$-\varphi^i$	$\rho\varsigma$	$\hat{\eta}$

The resulting balance equations and some transformations of them are given below.

2.2.1.1 Balance of mass

- Differential form

$$(\rho)_{,t} + \left(\rho v^i\right)_{,i} = \hat{\rho} \tag{2.11}$$

This relation can be transformed as follows

$$\left((\rho)_{,t} + (\rho)_{,i} v^i\right) + \rho\left(v^i\right)_{,i} = \hat{\rho} \tag{2.12}$$

which, since the expression in the first parenthesis is the material derivative of the density ρ, can be rewritten as

$$D^v(\rho) + \rho\left(v^i\right)_{,i} = \hat{\rho} \tag{2.13}$$

- Jump form

$$[\![\rho\left(v^i - u^i\right) n_i]\!] = 0 \tag{2.14}$$

This relation states that the flow of mass that enters one side of the surface of discontinuity is equal to the flow of mass that exits the surface of discontinuity on the other side (cf. Wilmański 1998, Eq. (4.63)).

2.2.1.2 Balance of momentum

- Differential form

$$\left(\rho v^j\right)_{,t} + \left(\rho v^j v^i - T^{ji}\right)_{,i} - \rho b^j = \hat{p}^j \tag{2.15}$$

This relation can be transformed as follows

$$\begin{aligned}
\hat{p}^j &= \left(\rho v^j\right)_{,t} + \left(\rho v^j v^i - T^{ji}\right)_{,i} - \rho b^j \\
&= \rho\left(v^j\right)_{,t} + (\rho)_{,t} v^j + \left(\rho v^i\right)_{,i} v^j + \rho v^i \left(v^j\right)_{,i} - \left(T^{ji}\right)_{,i} - \rho b^j \\
&= \rho\left(\left(v^j\right)_{,t} + v^i\left(v^j\right)_{,i}\right) + \left((\rho)_{,t} + \left(\rho v^i\right)_{,i}\right) v^j - \left(T^{ji}\right)_{,i} - \rho b^j \\
&= \rho\left(\left(v^j\right)_{,t} + \left(v^j\right)_{,i} v^i\right) + \hat{\rho} v^j - \left(T^{ji}\right)_{,i} - \rho b^j
\end{aligned}$$

where the balance of mass (2.11) has been used in the last equation. Consequently, by use of the balance of mass, the balance of momentum becomes

$$\rho\left(\left(v^j\right)_{,t} + \left(v^j\right)_{,i} v^i\right) - \left(T^{ji}\right)_{,i} - \rho b^j = \hat{p}^j - \hat{\rho} v^j \tag{2.16}$$

which, since the expression in the first parenthesis is the material derivative of the velocity v^j (i.e., the acceleration), can be rewritten as

$$\rho D^v\left(v^j\right) - \left(T^{ji}\right)_{,i} - \rho b^j = \hat{p}^j - \hat{\rho} v^j \tag{2.17}$$

- Jump form

$$\left[\!\left[\rho v^j\left(v^i - u^i\right) n_i - T^{ji} n_i\right]\!\right] = 0 \tag{2.18}$$

This relation can be transformed as follows

$$\begin{aligned}
0 &= \left[\!\left[\rho v^j\left(v^i - u^i\right) n_i - T^{ji} n_i\right]\!\right] \\
&= \rho\left(v^i - u^i\right) n_i \left[\!\left[v^j\right]\!\right] - \left[\!\left[T^{ji}\right]\!\right] n_i
\end{aligned}$$

where in the last equation the jump balance of mass (2.14) has been used. Consequently, by use of the jump balance of mass, the jump balance of momentum becomes (cf. Wilmański 1998, Eq. (4.79))

$$\rho\left(v^i - u^i\right) n_i \left[\!\left[v^j\right]\!\right] - \left[\!\left[T^{ji}\right]\!\right] n_i = 0 \tag{2.19}$$

Note that if $\rho\left(v^i - u^i\right) n_i = 0$ this relation reduces to $\left[\!\left[T^{ji}\right]\!\right] n_i$, which is the continuity of the traction vector $T^{ji} n_i$ across the surface of discontinuity.

2.2.1.3 *Balance of moment of momentum*

- Differential form

$$\left(\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}\right)_{,t} + \left(\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}v^{i} - \varepsilon^{j}{}_{kl}x^{k}T^{li}\right)_{,i} - \varepsilon^{j}{}_{kl}x^{k}\rho b^{l} = \widehat{m}^{j} \tag{2.20}$$

This relation can be transformed as follows

$$\begin{aligned}
\widehat{m}^{j} &= \left(\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}\right)_{,t} + \left(\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}v^{i} - \varepsilon^{j}{}_{kl}x^{k}T^{li}\right)_{,i} - \varepsilon^{j}{}_{kl}x^{k}\rho b^{l} \\
&= \varepsilon^{j}{}_{kl}x^{k}\left(\rho v^{l}\right)_{,t} + \varepsilon^{j}{}_{kl}\delta^{k}_{i}\left(\rho v^{l}v^{i} - T^{li}\right) + \varepsilon^{j}{}_{kl}x^{k}\left(\rho v^{l}v^{i} - T^{li}\right)_{,i} - \varepsilon^{j}{}_{kl}x^{k}\rho b^{l} \\
&= \varepsilon^{j}{}_{kl}x^{k}\left(\left(\rho v^{l}\right)_{,t} + \left(\rho v^{l}v^{i} - T^{li}\right)_{,i} - \rho b^{l}\right) + \varepsilon^{j}{}_{kl}\left(\rho v^{l}v^{k} - T^{lk}\right) \\
&= \varepsilon^{j}{}_{kl}x^{l}\hat{p}^{k} - \varepsilon^{j}{}_{kl}T^{lk}
\end{aligned}$$

where in the last equation the balance of momentum (2.15) and the identity $\varepsilon^{j}{}_{kl}v^{l}v^{k} = 0$ have been used. Consequently, by the use of the balance of momentum, the balance of moment of momentum becomes

$$\varepsilon^{j}{}_{kl}T^{kl} = \widehat{m}^{j} + \varepsilon^{j}{}_{kl}x^{k}\hat{p}^{l} \tag{2.21}$$

Note that if $\widehat{m}^{j} + \varepsilon^{j}{}_{kl}x^{k}\hat{p}^{l} = 0$ this relation reduces to $\varepsilon^{j}{}_{kl}T^{kl} = 0$, which is equivalent to the symmetry of the Cauchy stress tensor $T^{kl} = T^{lk}$.

- Jump form

$$\left[\!\left[\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}\left(v^{i} - u^{i}\right)n_{i} - \varepsilon^{j}{}_{kl}x^{k}T^{li}n_{i}\right]\!\right] = 0 \tag{2.22}$$

This relation can be transformed as follows

$$\begin{aligned}
0 &= \left[\!\left[\varepsilon^{j}{}_{kl}x^{k}\rho v^{l}\left(v^{i} - u^{i}\right)n_{i} - \varepsilon^{j}{}_{kl}x^{k}T^{li}n_{i}\right]\!\right] \\
&= \varepsilon^{j}{}_{kl}x^{k}\left[\!\left[\rho v^{l}\left(v^{i} - u^{i}\right)n_{i} - T^{li}n_{i}\right]\!\right]
\end{aligned}$$

Consequently, the jump balance of moment of momentum is equivalent to the jump balance of momentum.

2.2.1.4 *Balance of energy*

- Differential form

$$\left(\rho\left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)\right)_{,t} + \left(\rho\left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)v^{i} - \left(T_{k}{}^{i}v^{k} - q^{i}\right)\right)_{,i} - \rho\left(b_{k}v^{k} + r\right) = \hat{\varepsilon} \tag{2.23}$$

This relation can be transformed as follows

$$\begin{aligned}
\hat{\varepsilon} &= \left(\rho\left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)\right)_{,t} + \left(\rho\left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)v^{i} - \left(T_{k}{}^{i}v^{k} - q^{i}\right)\right)_{,i} - \rho\left(b_{k}v^{k} + r\right) \\
&= \rho\left((\varepsilon)_{,t} + (v_{k})_{,t}v^{k}\right) + \left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)(\rho)_{,t} + \left((\varepsilon)_{,i} + (v_{k})_{,i}v^{k}\right)\rho v^{i} + \left(\varepsilon + \tfrac{1}{2}v_{k}v^{k}\right)\left(\rho v^{i}\right)_{,i} \\
&\qquad - \left(T_{k}{}^{i}\right)_{,i}v^{k} - T_{k}{}^{i}\left(v^{k}\right)_{,i} + \left(q^{i}\right)_{,i} - \rho\left(b_{k}v^{k} + r\right)
\end{aligned}$$

$$
\begin{aligned}
&= \rho\big((\varepsilon)_{,t} + (\varepsilon)_{,i} v^i\big) + \left(\varepsilon + \tfrac{1}{2} v_k v^k\right)\left((\rho)_{,t} + \left(\rho v^i\right)_{,i}\right) + v^k \left(\rho\big((v_k)_{,t} + (v_k)_{,i} v^i\big) - \left(T_k{}^i\right)_{,i} - \rho b_k\right) \\
&\qquad - T_k{}^i \left(v^k\right)_{,i} + \left(q^i\right)_{,i} - \rho r \\
&= \rho\big((\varepsilon)_{,t} + (\varepsilon)_{,i} v^i\big) + \left(\varepsilon + \tfrac{1}{2} v_k v^k\right)\hat{\rho} + v^k(\hat{p}_k - \hat{\rho} v_k) - T_k{}^i \left(v^k\right)_{,i} + \left(q^i\right)_{,i} - \rho r
\end{aligned}
$$

where the balance of mass (2.11) and the balance of momentum (2.16) (in which the balance of mass (2.11) has been used) have been used in the last equation. Consequently, by use of the balance of mass and the balance of momentum, the balance of energy becomes

$$
\rho\big((\varepsilon)_{,t} + (\varepsilon)_{,i} v^i\big) - T_k{}^i \left(v^k\right)_{,i} + \left(q^i\right)_{,i} - \rho r = \hat{\varepsilon} - \left(\varepsilon - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k \tag{2.24}
$$

which, since the expression in the first parenthesis is the material derivative of the specific internal energy ε, can be rewritten as (cf. Truesdell 1984, Eq. $(5.11)_4$)

$$
\rho D^v(\varepsilon) - T_k{}^i \left(v^k\right)_{,i} + \left(q^i\right)_{,i} - \rho r = \hat{\varepsilon} - \left(\varepsilon - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k \tag{2.25}
$$

Furthermore, if the Cauchy stress tensor is symmetric, the second term on the l. h. s. can be rewritten as $T^{ki} D_{ki}$, where D_{ki} is the rate of deformation tensor (i.e., the symmetric part of the velocity gradient tensor), so that

$$
\rho D^v(\varepsilon) - T^{ki} D_{ki} + \left(q^i\right)_{,i} - \rho r = \hat{\varepsilon} - \left(\varepsilon - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k \tag{2.26}
$$

- Jump form

$$
\left[\!\left[\rho \left(\varepsilon + \tfrac{1}{2} v_k v^k\right)\left(v^i - u^i\right) n_i - \left(T_k{}^i v^k - q^i\right) n_i\right]\!\right] = 0 \tag{2.27}
$$

This relation can be transformed as follows

$$
\begin{aligned}
0 &= \left[\!\left[\rho \left(\varepsilon + \tfrac{1}{2} v_k v^k\right)\left(v^i - u^i\right) n_i - \left(T_k{}^i v^k - q^i\right) n_i\right]\!\right] \\
&= \rho\left(v^i - u^i\right) n_i \left[\!\left[\varepsilon + \tfrac{1}{2} v_k v^k\right]\!\right] - \left[\!\left[T_k{}^i v^k - q^i\right]\!\right] n_i
\end{aligned}
$$

where in the last equation the jump balance of mass (2.14) has been used. Consequently, by use of the jump balance of mass, the jump balance of momentum becomes (cf. Wilmański 1998, Eq. (4.87))

$$
\rho\left(v^i - u^i\right) n_i \left[\!\left[\varepsilon + \tfrac{1}{2} v_k v^k\right]\!\right] - \left[\!\left[T_k{}^i v^k - q^i\right]\!\right] n_i = 0 \tag{2.28}
$$

2.2.1.5 Balance of entropy

- Differential form

$$
(\rho\eta)_{,t} + \left(\rho\eta v^i + \varphi^i\right)_{,i} - \rho\varsigma = \hat{\eta} \tag{2.29}
$$

This equation can be transformed as follows

$$
\begin{aligned}
\hat{\eta} &= (\rho\eta)_{,t} + \left(\rho\eta v^i + \varphi^i\right)_{,i} - \rho\varsigma \\
&= \rho(\eta)_{,t} + (\rho)_{,t}\eta + \left(\rho v^i\right)_{,i}\eta + \rho v^i (\eta)_{,i} + \left(\varphi^i\right)_{,i} - \rho\varsigma \\
&= \rho\big((\eta)_{,t} + (\eta)_{,i} v^i\big) + \eta\left((\rho)_{,t} + \left(\rho v^i\right)_{,i}\right) + \left(\varphi^i\right)_{,i} - \rho\varsigma
\end{aligned}
$$

$$= \rho\big((\eta)_{,t} + (\eta)_{,i} v^i\big) + \eta\hat{\rho} + \left(\varphi^i\right)_{,i} - \rho\varsigma$$

where the balance of mass (2.11) has been used in the last equation. Consequently, by use of the balance of mass, the balance of entropy becomes

$$\rho\big((\eta)_{,t} + (\eta)_{,i} v^i\big) + \left(\varphi^i\right)_{,i} - \rho\varsigma = \hat{\eta} - \eta\hat{\rho} \tag{2.30}$$

which, since the expression in the first parenthesis is the material derivative of the specific entropy η, can be rewritten as

$$\rho D^v(\eta) + \left(\varphi^i\right)_{,i} - \rho\varsigma = \hat{\eta} - \eta\hat{\rho} \tag{2.31}$$

- Jump form

$$\llbracket \rho\eta\left(v^i - u^i\right)n_i + \varphi^i n_i \rrbracket = 0 \tag{2.32}$$

This relation can be transformed as follows

$$\begin{aligned} 0 &= \llbracket \rho\eta\left(v^i - u^i\right)n_i + \varphi^i n_i \rrbracket \\ &= \rho\left(v^i - u^i\right)n_i \llbracket \eta \rrbracket + \llbracket \varphi^i \rrbracket n_i \end{aligned}$$

where in the last equation the jump balance of mass (2.14) has been used. Consequently, by use of the jump balance of mass, the jump balance of entropy becomes

$$\rho\left(v^i - u^i\right)n_i \llbracket \eta \rrbracket + \llbracket \varphi^i \rrbracket n_i = 0 \tag{2.33}$$

It will be further assumed that

$$\begin{aligned} \varphi^i &= \frac{1}{\theta} q^i \\ \varsigma &= \frac{1}{\theta} r \end{aligned} \tag{2.34}$$

where θ is the temperature. In this case, (2.31) becomes (cf. Truesdell 1984, Eq. (5.18))

$$\rho D^v(\eta) + \left(\frac{1}{\theta} q^i\right)_{,i} - \frac{1}{\theta}\rho r = \hat{\eta} - \eta\hat{\rho} \tag{2.35}$$

which can be transformed as follows

$$\begin{aligned} &\hat{\eta} - \eta\hat{\rho} = \\ &= \rho D^v(\eta) + \left(\frac{1}{\theta} q^i\right)_{,i} - \frac{1}{\theta}\rho r \\ &= \rho D^v(\eta) - \frac{1}{\theta^2} q^i (\theta)_{,i} + \frac{1}{\theta}\left(\left(q^i\right)_{,i} - \rho r\right) \\ &= \rho D^v(\eta) - \frac{1}{\theta^2} q^i (\theta)_{,i} + \frac{1}{\theta}\left(\hat{\varepsilon} - \left(\varepsilon - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k - \rho D^v(\varepsilon) + T_k{}^i \left(v^k\right)_{,i}\right) \end{aligned}$$

where the balance of energy (2.25) has been used. Defining the free energy per unit mass ψ by

$$\psi = \varepsilon - \theta\eta \tag{2.36}$$

it follows that

$$
\begin{aligned}
&\hat{\eta} - \eta\hat{\rho} = \\
&= \rho D^v(\eta) - \frac{1}{\theta^2} q^i(\theta)_{,i} + \frac{1}{\theta}\left(\hat{\varepsilon} - \left(\psi + \theta\eta - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k - \rho D^v(\psi + \theta\eta) + T_k{}^i \left(v^k\right)_{,i}\right) \\
&= -\frac{1}{\theta^2} q^i(\theta)_{,i} - \eta\hat{\rho} + \frac{1}{\theta}\left(\hat{\varepsilon} - \left(\psi - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k - \rho D^v(\psi) - \rho\eta D^v(\theta) + T_k{}^i \left(v^k\right)_{,i}\right)
\end{aligned}
$$

and the balance of entropy becomes

$$
\hat{\eta} = \frac{1}{\theta} T_k{}^i \left(v^k\right)_{,i} - \frac{1}{\theta^2} q^i(\theta)_{,i} - \frac{1}{\theta}\rho\left(\eta D^v(\theta) + D^v(\psi)\right) + \frac{1}{\theta}\left(\hat{\varepsilon} - \left(\psi - \tfrac{1}{2} v_k v^k\right)\hat{\rho} - v^k \hat{p}_k\right) \tag{2.37}
$$

2.2.2 Balance equations for a material with identifiable constituents

We consider a material composed of n identifiable constituents, which are modelled as interacting continua with their own motions and thermodynamic properties (Bowen 1976; Truesdell 1984, Lecture 5). Constituents are denoted by lowercase Fraktur letters. Variables pertaining to a constituent are denoted by a subscript with the constituent symbol, while variables pertaining to the material as a whole do not have such a subscript.

Balance of mass, momentum, moment of momentum, energy and entropy are postulated at two levels: (1) for each constituent, a balance equation as for a single medium, but including a term to take into account the interaction with the other constituents, and (2) for the material as a whole, assuming that the interactions between the constituents are exchanges, so that the sum over all constituents of the interaction terms vanish. As a result, the sum over all constituents of a balance equation yields the corresponding balance equation for the material as a whole, without the interaction terms. It is also possible to define thermodynamic properties for the material as a whole in terms of the thermodynamic properties of the constituents so that the balance equations are those of a single medium.

2.2.2.1 Balance of mass

The balance of mass for the constituent α (cf. (2.11)) reads

$$\hat{\rho}_\mathfrak{a} = (\rho_\mathfrak{a})_{,t} + \left(\rho_\mathfrak{a} v_\mathfrak{a}{}^i\right)_{,i} \tag{2.38}$$

which can be rewritten as (cf. Truesdell 1984, Eq. $(5.11)_1$)

$$\hat{\rho}_\mathfrak{a} = D^{v_\mathfrak{a}}(\rho_\mathfrak{a}) + \rho_\mathfrak{a}\left(v_\mathfrak{a}{}^i\right)_{,i} \tag{2.39}$$

The balance of mass for the material as a whole reads (cf. Truesdell 1984, Eq. $(5.12)_1$)

$$\sum_\mathfrak{a} \hat{\rho}_\mathfrak{a} = 0 \tag{2.40}$$

2.2.2.2 Balance of momentum

The balance of mass for the constituent $\mathfrak{a}$ (cf. (2.15)) reads

$$\hat{p}_\mathfrak{a}{}^j = \left(\rho v_\mathfrak{a}{}^j\right)_{,t} + \left(\rho v_\mathfrak{a}{}^j v_\mathfrak{a}{}^i - T_\mathfrak{a}{}^{ji}\right)_{,i} - \rho_\mathfrak{a} b_\mathfrak{a}{}^j \tag{2.41}$$

which, using the balance of mass, can be rewritten as (cf. Truesdell 1984, Eq. $(5.11)_2$)

$$\hat{p}_\mathfrak{a}{}^j = \rho_\mathfrak{a} D^{v_\mathfrak{a}}\left(v_\mathfrak{a}{}^j\right) - \left(T_\mathfrak{a}{}^{ji}\right)_{,i} - \rho_\mathfrak{a} b_\mathfrak{a}{}^j + \hat{\rho}_\mathfrak{a} v_\mathfrak{a}{}^j \tag{2.42}$$

The balance of momentum for the material as a whole reads (cf. Truesdell 1984, Eq. $(5.12)_2$)

$$\sum_\mathfrak{a} \hat{p}_\mathfrak{a}{}^j = 0 \tag{2.43}$$

2.2.2.3 Balance of moment of momentum

The balance of momentum for the constituent $\mathfrak{a}$ (cf. (2.20)) reads

$$\hat{m}_{\mathfrak{a}}{}^{j} = \left(\varepsilon^{j}{}_{kl} x^{k} \rho_{\mathfrak{a}} v_{\mathfrak{a}}{}^{l}\right)_{,t} + \left(\varepsilon^{j}{}_{kl} x^{k} \rho_{\mathfrak{a}} v_{\mathfrak{a}}{}^{l} v_{\mathfrak{a}}{}^{i} - \varepsilon^{j}{}_{kl} x^{k} T_{\mathfrak{a}}{}^{li}\right)_{,i} - \varepsilon^{j}{}_{kl} x^{k} \rho_{\mathfrak{a}} b_{\mathfrak{a}}{}^{l} \tag{2.44}$$

which, using the balance of momentum, can be rewritten as (cf. Truesdell 1984, Eq. (5.11)$_3$)

$$\hat{m}_{\mathfrak{a}}{}^{j} = \varepsilon^{j}{}_{kl} T_{\mathfrak{a}}{}^{kl} - \varepsilon^{j}{}_{kl} x^{k} \hat{p}_{\mathfrak{a}}{}^{l} \tag{2.45}$$

The balance of moment of momentum for the material as a whole reads (cf. Truesdell 1984, Eq. (5.12)$_3$)

$$\sum_{\mathfrak{a}} \hat{m}_{\mathfrak{a}}{}^{j} = 0 \tag{2.46}$$

2.2.2.4 Balance of energy

The balance of energy for the constituent $\mathfrak{a}$ (cf. (2.23)) reads

$$\hat{\varepsilon}_{\mathfrak{a}} = \left(\rho_{\mathfrak{a}}\left(\varepsilon_{\mathfrak{a}} + \tfrac{1}{2} v_{\mathfrak{a}k} v_{\mathfrak{a}}{}^{k}\right)\right)_{,t} + \left(\rho_{\mathfrak{a}}\left(\varepsilon_{\mathfrak{a}} + \tfrac{1}{2} v_{\mathfrak{a}k} v_{\alpha}{}^{k}\right) v_{\mathfrak{a}}{}^{i} - \left(T_{\mathfrak{a}k}{}^{i} v_{\mathfrak{a}}{}^{k} - q_{\mathfrak{a}}{}^{i}\right)\right)_{,i} - \rho_{\mathfrak{a}}\left(b_{\mathfrak{a}k} v_{\mathfrak{a}}{}^{k} + r_{\mathfrak{a}}\right) \tag{2.47}$$

which, using the balance of mass and the balance of momentum, can be rewritten as (cf. Truesdell 1984, Eq. (5.11)$_4$)

$$\hat{\varepsilon}_{\mathfrak{a}} = \rho_{\mathfrak{a}} D^{v_{\mathfrak{a}}}(\varepsilon_{\mathfrak{a}}) - T_{\mathfrak{a}k}{}^{i}\left(v_{\mathfrak{a}}{}^{k}\right)_{,i} + \left(q_{\mathfrak{a}}{}^{i}\right)_{,i} - \rho_{\mathfrak{a}} r_{\mathfrak{a}} + \left(\varepsilon_{\mathfrak{a}} - \tfrac{1}{2} v_{\mathfrak{a}k} v_{\mathfrak{a}}{}^{k}\right)\hat{\rho}_{\mathfrak{a}} + v_{\mathfrak{a}}{}^{k} \hat{p}_{\mathfrak{a}k} \tag{2.48}$$

The balance of energy for the material as a whole reads (cf. Truesdell 1984, Eq. (5.12)$_4$)

$$\sum_{\mathfrak{a}} \hat{\varepsilon}_{\mathfrak{a}} = 0 \tag{2.49}$$

2.2.2.5 Balance of entropy

The balance of entropy for the constituent $\mathfrak{a}$ (cf. (2.29)) with the assumptions (2.34) reads

$$\hat{\eta}_{\mathfrak{a}} = (\rho\eta)_{,t} + \left(\rho\eta v^{i} + \frac{1}{\theta_{\mathfrak{a}}} q_{\mathfrak{a}}{}^{i}\right)_{,i} - \rho_{\mathfrak{a}} \frac{r_{\mathfrak{a}}}{\theta_{\mathfrak{a}}} \tag{2.50}$$

which, using the balance of mass, can be rewritten as (cf. Truesdell 1984, Eq. (5.11)$_2$)

$$\hat{\eta}_{\mathfrak{a}} = \rho_{\mathfrak{a}} D^{v_{\mathfrak{a}}}(\eta_{\mathfrak{a}}) + \left(\frac{1}{\theta_{\mathfrak{a}}} q_{\mathfrak{a}}{}^{i}\right)_{,i} - \frac{1}{\theta_{\mathfrak{a}}} \rho_{\mathfrak{a}} r_{\mathfrak{a}} + \eta_{\mathfrak{a}} \hat{\rho}_{\mathfrak{a}} \tag{2.51}$$

and using the balance of energy becomes (cf. Truesdell 1984, Eq. (5.26))

$$\hat{\eta}_{\mathfrak{a}} = \frac{1}{\theta_{\mathfrak{a}}} T_{\mathfrak{a}k}{}^{i}\left(v_{\mathfrak{a}}{}^{k}\right)_{,i} - \frac{1}{\theta_{\mathfrak{a}}^{2}} q_{\mathfrak{a}}{}^{i} (\theta_{\mathfrak{a}})_{,i} - \frac{1}{\theta_{\mathfrak{a}}} \rho_{\mathfrak{a}}\left(\eta_{\mathfrak{a}} D^{v_{\mathfrak{a}}}(\theta_{\mathfrak{a}}) + D^{v_{\mathfrak{a}}}(\psi_{\mathfrak{a}})\right) \tag{2.52}$$

$$+\frac{1}{\theta_\mathfrak{a}}\left(\hat{\varepsilon}_\mathfrak{a}-\left(\psi_\mathfrak{a}-\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\right)\hat{\rho}_\mathfrak{a}-v_\mathfrak{a}{}^k\hat{p}_{\mathfrak{a}k}\right)$$

The balance of entropy for the material as a whole reads (cf. Truesdell 1984, Eq. (5.20))

$$\sum_\mathfrak{a}\hat{\eta}_\mathfrak{a}\geq 0 \tag{2.53}$$

which, using (2.52), becomes (cf. Truesdell 1984, Eq. (5.27))

$$\begin{aligned}\sum_\mathfrak{a}\Bigg\{&\frac{1}{\theta_\mathfrak{a}}T_{\mathfrak{a}k}{}^i\left(v_\mathfrak{a}{}^k\right)_{,i}-\frac{1}{\theta_\mathfrak{a}{}^2}q_\mathfrak{a}{}^i(\theta_\mathfrak{a})_{,i}-\frac{1}{\theta_\mathfrak{a}}\rho_\mathfrak{a}\left(\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta_\mathfrak{a})+D^{v_\mathfrak{a}}(\psi_\mathfrak{a})\right)\\ &+\frac{1}{\theta_\mathfrak{a}}\left(\hat{\varepsilon}_\mathfrak{a}-\left(\psi_\mathfrak{a}-\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\right)\hat{\rho}_\mathfrak{a}-v_\mathfrak{a}{}^k\hat{p}_{\mathfrak{a}k}\right)\Bigg\}\geq 0\end{aligned} \tag{2.54}$$

If all constituents have the same temperature $\theta_\mathfrak{a}=\theta$, then using (2.49) and multiplying by θ (which is positive), it follows

$$\begin{aligned}\sum_\mathfrak{a}\Bigg\{&T_{\mathfrak{a}k}{}^i\left(v_\mathfrak{a}{}^k\right)_{,i}-\frac{1}{\theta}q_\mathfrak{a}{}^i(\theta)_{,i}-\rho_\mathfrak{a}\left(\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta)+D^{v_\mathfrak{a}}(\psi_\alpha)\right)\\ &-\left(\psi_\mathfrak{a}-\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\right)\hat{\rho}_\mathfrak{a}-v_\mathfrak{a}{}^k\hat{p}_{\mathfrak{a}k}\Bigg\}\geq 0\end{aligned} \tag{2.55}$$

This inequality can be transformed as follows

$$\begin{aligned}\sum_\mathfrak{a}\Bigg\{&T_{\mathfrak{a}k}{}^i\left(v_\mathfrak{a}{}^k\right)_{,i}-\frac{1}{\theta}q_\mathfrak{a}{}^i(\theta)_{,i}-\rho_\mathfrak{a}\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta)-D^{v_\mathfrak{a}}(\rho_\mathfrak{a}\psi_\mathfrak{a})+\psi_\mathfrak{a}D^{v_\mathfrak{a}}(\rho_\mathfrak{a})\\ &\qquad\qquad\qquad\qquad-\left(\psi_\mathfrak{a}-\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\right)\hat{\rho}_\mathfrak{a}-v_\mathfrak{a}{}^k\hat{p}_{\mathfrak{a}k}\Bigg\}\geq 0\end{aligned}$$

$$\begin{aligned}\sum_\mathfrak{a}\Bigg\{&T_{\mathfrak{a}k}{}^i\left(v_\mathfrak{a}{}^k\right)_{,i}-\frac{1}{\theta}q_\mathfrak{a}{}^i(\theta)_{,i}-\rho_\mathfrak{a}\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta)-D^{v_\mathfrak{a}}(\rho_\mathfrak{a}\psi_\mathfrak{a})+\psi_\mathfrak{a}\left(\hat{\rho}_\mathfrak{a}-\rho_\mathfrak{a}\left(v_\mathfrak{a}{}^i\right)_{,i}\right)\\ &\qquad\qquad\qquad\qquad-\left(\psi_\mathfrak{a}-\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\right)\hat{\rho}_\mathfrak{a}-v_\mathfrak{a}{}^k\hat{p}_{\mathfrak{a}k}\Bigg\}\geq 0\end{aligned}$$

and, using the balance of mass for constituent $\mathfrak{a}$, yields

$$\begin{aligned}-&\sum_\mathfrak{a}D^{v_\mathfrak{a}}(\rho_\mathfrak{a}\psi_\mathfrak{a})-\sum_\mathfrak{a}\rho_\mathfrak{a}\psi_\mathfrak{a}\left(v_\mathfrak{a}{}^i\right)_{,i}+\sum_\mathfrak{a}T_\mathfrak{a}{}^{ki}(v_{\mathfrak{a}k})_{,i}\\ &\qquad-\sum_\mathfrak{a}\rho_\mathfrak{a}\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta)-\frac{1}{\theta}(\theta)_{,i}\sum_\mathfrak{a}q_\mathfrak{a}{}^i+\sum_\mathfrak{a}\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\hat{\rho}_\mathfrak{a}-\sum_\mathfrak{a}\hat{p}_{\mathfrak{a}k}v_\mathfrak{a}{}^k\geq 0\end{aligned}$$

$$\begin{aligned}-&\sum_\mathfrak{a}D^{v_\mathfrak{a}}(\rho_\mathfrak{a}\psi_\mathfrak{a})-\sum_\mathfrak{a}\left(\rho_\mathfrak{a}\psi_\mathfrak{a}\delta^{ki}-T_\mathfrak{a}{}^{ki}\right)(v_{\mathfrak{a}k})_{,i}\\ &\qquad-\sum_\mathfrak{a}\rho_\mathfrak{a}\eta_\mathfrak{a}D^{v_\mathfrak{a}}(\theta)-\frac{1}{\theta}(\theta)_{,i}\sum_\mathfrak{a}q_\mathfrak{a}{}^i+\sum_\mathfrak{a}\tfrac{1}{2}v_{\mathfrak{a}k}v_\mathfrak{a}{}^k\hat{\rho}_\mathfrak{a}-\sum_\mathfrak{a}\hat{p}_{\mathfrak{a}k}v_\mathfrak{a}{}^k\geq 0\end{aligned} \tag{2.56}$$

Introducing a reference velocity $\bar{v}^i$, this expression can be transformed as follows

$$\begin{aligned}-&\sum_\mathfrak{a}D^{v_\mathfrak{a}}(\rho_\mathfrak{a}\psi_\mathfrak{a})-\sum_\mathfrak{a}\left(\rho_\mathfrak{a}\psi_\mathfrak{a}\delta^{ki}-T_\mathfrak{a}{}^{ki}\right)(v_{\mathfrak{a}k})_{,i}-\sum_\mathfrak{a}\rho_\mathfrak{a}\eta_\mathfrak{a}\left(D^{\bar{v}}(\theta)+(\theta)_{,i}\left(v_\mathfrak{a}{}^i-\bar{v}^i\right)\right)\\ &-\frac{1}{\theta}(\theta)_{,i}\sum_\mathfrak{a}q_\mathfrak{a}{}^i+\sum_\mathfrak{a}\tfrac{1}{2}(\bar{v}_k+(v_{\mathfrak{a}k}-\bar{v}_k))\left(\bar{v}^k+(v_\mathfrak{a}{}^k-\bar{v}^k)\right)\hat{\rho}_\mathfrak{a}-\sum_\mathfrak{a}\hat{p}_{\mathfrak{a}k}\left(\bar{v}^k+(v_\mathfrak{a}{}^k-\bar{v}^k)\right)\geq 0\end{aligned}$$

$$
\begin{aligned}
&-\sum_\alpha D^{v_\alpha}(\rho_\alpha\psi_\alpha)-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)(v_{\alpha k})_{,i}-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)-\sum_\alpha\rho_\alpha\eta_\alpha(\theta)_{,i}\left(v_\alpha{}^i-\bar v^i\right)\\
&-\frac{1}{\theta}(\theta)_{,i}\sum_\alpha q_\alpha{}^i+\tfrac{1}{2}\bar v_k\bar v^k\sum_\alpha\hat\rho_\alpha+\bar v^k\sum_\alpha(v_{\alpha k}-\bar v_k)\hat\rho_\alpha+\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-\bar v_k)\left(v_\alpha{}^k-\bar v^k\right)\hat\rho_\alpha\\
&-\bar v^k\sum_\alpha\hat p_{\alpha k}-\sum_\alpha\hat p_{\alpha k}(v_\alpha{}^k-\bar v^k)\geq 0
\end{aligned}
$$

using $\sum_\alpha\hat\rho_\alpha=0$ and $\sum_\alpha\hat p_{\alpha k}=0$, and further transforming the resulting expression yields

$$
\begin{aligned}
&-\sum_\alpha D^{v_\alpha}(\rho_\alpha\psi_\alpha)-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)(v_{\alpha k})_{,i}-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)-\sum_\alpha\rho_\alpha\eta_\alpha(\theta)_{,i}\left(v_\alpha{}^i-\bar v^i\right)\\
&-\frac{1}{\theta}(\theta)_{,i}\sum_\alpha q_\alpha{}^i+\sum_\alpha(v_{\alpha k}-\bar v_k)\bar v^k\hat\rho_\alpha+\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-\bar v_k)\left(v_\alpha{}^k-\bar v^k\right)\hat\rho_\alpha\\
&-\sum_\alpha(\hat p_{\alpha k}-\hat\rho_\alpha v_{\alpha k}+\hat\rho_\alpha v_{\alpha k})(v_\alpha{}^k-\bar v^k)\geq 0
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_\alpha D^{v_\alpha}(\rho_\alpha\psi_\alpha)-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)(v_{\alpha k})_{,i}-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)-\sum_\alpha\rho_\alpha\eta_\alpha(\theta)_{,i}\left(v_\alpha{}^i-\bar v^i\right)\\
&-\frac{1}{\theta}(\theta)_{,i}\sum_\alpha q_\alpha{}^i-\sum_\alpha(v_{\alpha k}-\bar v_k)(v_\alpha{}^k-\bar v^k)\hat\rho_\alpha+\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-\bar v_k)\left(v_\alpha{}^k-\bar v^k\right)\hat\rho_\alpha\\
&-\sum_\alpha(\hat p_{\alpha k}-\hat\rho_\alpha v_{\alpha k})(v_\alpha{}^k-\bar v^k)\geq 0
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_\alpha D^{v_\alpha}(\rho_\alpha\psi_\alpha)-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)(v_{\alpha k})_{,i}\\
&-\left(\sum_\alpha\left(q_\alpha{}^i+\rho_\alpha\eta_\alpha\theta\left(v_\alpha^i-\bar v^i\right)\right)\right)\frac{1}{\theta}(\theta)_{,i}-\sum_\alpha(\hat p_{\alpha k}-\hat\rho_\alpha v_{\alpha k})\left(v_\alpha{}^k-\bar v^k\right)\\
&-\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-\bar v_k)\left(v_\alpha{}^k-\bar v^k\right)\hat\rho_\alpha\geq 0
\end{aligned}
\tag{2.57}
$$

Setting $\bar v^i$ equal to the barycentric velocity v^i, which is defined by

$$
v^i\left(\sum_\alpha\rho_\alpha\right)=\sum_\alpha\rho_\alpha v_\alpha^i
$$

we get (cf. Bowen 1969, Eq. (4.10); Bowen 1975, Eq. (1.6.30))

$$
\begin{aligned}
&-\sum_\alpha D^{v_\alpha}(\rho_\alpha\psi_\alpha)-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{v}(\theta)-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)(v_{\alpha k})_{,i}\\
&-\left(\sum_\alpha\left(q_\alpha{}^i+\rho_\alpha\eta_\alpha\theta\left(v_\alpha^i-v^i\right)\right)\right)\frac{1}{\theta}(\theta)_{,i}-\sum_\alpha(\hat p_{\alpha k}-\hat\rho_\alpha v_{\alpha k})\left(v_\alpha{}^k-v^k\right)\\
&-\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-v_k)\left(v_\alpha{}^k-v^k\right)\hat\rho_\alpha\geq 0
\end{aligned}
\tag{2.58}
$$

The inequality (2.57) can be further transformed as follows

$$
\begin{aligned}
&-\sum_\alpha\left(D^{\bar v}(\rho_\alpha\psi_\alpha)+(\rho_\alpha\psi_\alpha)_{,i}\left(v_\alpha{}^i-\bar v^i\right)\right)-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)\\
&-\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)\left((\bar v_k)_{,i}+(v_{\alpha k}-\bar v_k)_{,i}\right)-\left(\sum_\alpha q_\alpha{}^i\right)\frac{1}{\theta}(\theta)_{,i}-\left(\sum_\alpha\rho_\alpha\eta_\alpha(\theta)_{,i}\left(v_\alpha^i-\bar v^i\right)\right)\\
&-\sum_\alpha(\hat p_{\alpha k}-\hat\rho_\alpha v_{\alpha k})\left(v_\alpha{}^k-\bar v^k\right)-\sum_\alpha\tfrac{1}{2}(v_{\alpha k}-\bar v_k)\left(v_\alpha{}^k-\bar v^k\right)\hat\rho_\alpha\geq 0
\end{aligned}
$$

$$
-D^{\bar v}\left(\sum_\alpha\rho_\alpha\psi_\alpha\right)-\sum_\alpha(\rho_\alpha\psi_\alpha)_{,i}\left(v_\alpha{}^i-\bar v^i\right)-\left(\sum_\alpha\rho_\alpha\eta_\alpha\right)D^{\bar v}(\theta)-\left(\sum_\alpha\left(\rho_\alpha\psi_\alpha\delta^{ki}-T_\alpha{}^{ki}\right)\right)(\bar v_k)_{,i}
$$

$$\begin{aligned}
&-\sum\nolimits_{\mathfrak{a}}\left(\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\delta^{ki}-T_{\mathfrak{a}}{}^{ki}\right)\left(v_{\mathfrak{a}k}-\bar{v}_k\right)_{,i}-\left(\sum\nolimits_{\mathfrak{a}}q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\left(\left(\hat{p}_{\mathfrak{a}k}-\hat{\rho}_{\mathfrak{a}}v_{\mathfrak{a}k}\right)+\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}(\theta)_{,k}\right)-\sum\nolimits_{\mathfrak{a}}\tfrac{1}{2}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\hat{\rho}_{\mathfrak{a}}\geq 0
\end{aligned}$$

$$\begin{aligned}
&-D^{\bar{v}}\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)-\sum\nolimits_{\mathfrak{a}}\left(\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)_{,i}\left(v_{\mathfrak{a}}{}^{i}-\bar{v}^{i}\right)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right)D^{\bar{v}}(\theta)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)\left(\bar{v}^{i}\right)_{,i}\\
&+\left(\sum\nolimits_{\mathfrak{a}}T_{\mathfrak{a}}{}^{ki}\right)(\bar{v}_k)_{,i}-\sum\nolimits_{\mathfrak{a}}\left(\left(\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\delta^{ki}-T_{\mathfrak{a}}{}^{ki}\right)\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\right)_{,i}+\\
&+\sum\nolimits_{\mathfrak{a}}\left(\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\delta^{ki}-T_{\mathfrak{a}}{}^{ki}\right)_{,i}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)-\left(\sum\nolimits_{\mathfrak{a}}q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\left(\left(\hat{p}_{\mathfrak{a}k}-\hat{\rho}_{\mathfrak{a}}v_{\mathfrak{a}k}\right)+\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}(\theta)_{,k}\right)-\sum\nolimits_{\mathfrak{a}}\tfrac{1}{2}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\hat{\rho}_{\mathfrak{a}}\geq 0
\end{aligned}$$

$$\begin{aligned}
&-D^{\bar{v}}\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right)D^{\bar{v}}(\theta)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)\left(\bar{v}^{i}\right)_{,i}+\left(\sum\nolimits_{\mathfrak{a}}T_{\mathfrak{a}}{}^{ki}\right)(\bar{v}_k)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\left(\psi_{\mathfrak{a}}\delta^{ki}-\frac{1}{\rho_{\mathfrak{a}}}T_{\mathfrak{a}}{}^{ki}\right)\left(\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\right)_{,i}-\sum\nolimits_{\mathfrak{a}}\left(\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\right)\left(\psi_{\mathfrak{a}}\delta^{ki}-\frac{1}{\rho_{\mathfrak{a}}}T_{\mathfrak{a}}{}^{ki}\right)_{,i}\\
&-\left(\sum\nolimits_{\mathfrak{a}}q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i}-\sum\nolimits_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\left(\left(\hat{p}_{\mathfrak{a}k}-\hat{\rho}_{\mathfrak{a}}v_{\mathfrak{a}k}\right)+\left(T_{\mathfrak{a}k}{}^{i}\right)_{,i}+\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}(\theta)_{,k}\right)\\
&-\sum\nolimits_{\mathfrak{a}}\tfrac{1}{2}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\hat{\rho}_{\mathfrak{a}}\geq 0
\end{aligned}$$

and using the balance of momentum and rearranging yields

$$\begin{aligned}
&-\left(D^{\bar{v}}\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)+\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)\left(\bar{v}^{i}\right)_{,i}\right)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right)D^{\bar{v}}(\theta)+\left(\sum\nolimits_{\mathfrak{a}}T_{\mathfrak{a}}{}^{ki}\right)(\bar{v}_k)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\left(\psi_{\mathfrak{a}}\delta^{ki}-\frac{1}{\rho_{\mathfrak{a}}}T_{\mathfrak{a}}{}^{ki}\right)\left(\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\right)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\left(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}k})-b_{\mathfrak{a}k}+\left(\psi_{\mathfrak{a}}\delta^{ki}-\frac{1}{\rho_{\mathfrak{a}}}T_{\mathfrak{a}}{}^{ki}\right)_{,i}+\eta_{\mathfrak{a}}(\theta)_{,k}\right)\\
&-\left(\sum\nolimits_{\mathfrak{a}}q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i}\\
&-\sum\nolimits_{\mathfrak{a}}\tfrac{1}{2}\left(v_{\mathfrak{a}k}-\bar{v}_k\right)\left(v_{\mathfrak{a}}{}^{k}-\bar{v}^{k}\right)\hat{\rho}_{\mathfrak{a}}\geq 0
\end{aligned}\tag{2.59}$$

Setting $\bar{v}^{i}$ equal to the velocity of a constituent $v_{\mathfrak{s}}{}^{i}$ and assuming that the Cauchy stress tensors of the other constituents are spherical, such that

$$\psi_{\mathfrak{a}}\delta^{ki}-\frac{1}{\rho_{\mathfrak{a}}}T_{\mathfrak{a}}{}^{ki}=\mu_{\mathfrak{a}}\delta^{ki}\quad(\mathfrak{a}\neq\mathfrak{s})$$

yields

$$\begin{aligned}
&-\left(D^{v_{\mathfrak{s}}}\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)+\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)\left(v_{\mathfrak{s}}{}^{i}\right)_{,i}\right)-\left(\sum\nolimits_{\mathfrak{a}}\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right)D^{v_{\mathfrak{s}}}(\theta)+\left(\sum\nolimits_{\mathfrak{a}}T_{\mathfrak{a}}{}^{ki}\right)(v_{\mathfrak{s}k})_{,i}\\
&-\sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}}\mu_{\mathfrak{a}}\left(\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{i}-v_{\mathfrak{s}}{}^{i}\right)\right)_{,i}-\sum\nolimits_{\alpha\neq\mathfrak{s}}\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k}-v_{\mathfrak{s}}{}^{k}\right)\left(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}k})-b_{\mathfrak{a}k}+(\mu_{\mathfrak{a}})_{,k}+\eta_{\mathfrak{a}}(\theta)_{,k}\right)\\
&-\left(\sum\nolimits_{\mathfrak{a}}q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i}-\sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}}\tfrac{1}{2}\left(v_{\mathfrak{a}k}-v_{\mathfrak{s}k}\right)\left(v_{\mathfrak{a}}{}^{k}-v_{\mathfrak{s}}{}^{k}\right)\hat{\rho}_{\mathfrak{a}}\geq 0
\end{aligned}\tag{2.60}$$

The balance of mass for constituent $\mathfrak{a}$ can be transformed as follows:

$$
\begin{aligned}
\hat{\rho}_{\mathfrak{a}} &= D^{v_{\mathfrak{a}}}(\rho_{\mathfrak{a}}) + \rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{i}\right)_{,i} \\
&= D^{\bar{v}}(\rho_{\mathfrak{a}}) + (\rho_{\mathfrak{a}})_{,i}(v_{\mathfrak{a}}^{i} - \bar{v}^{i}) + \rho_{\mathfrak{a}}\left(\bar{v}^{i} + (v_{\mathfrak{a}}{}^{i} - \bar{v}^{i})\right)_{,i} \\
&= D^{\bar{v}}(\rho_{\mathfrak{a}}) + \left(\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}^{i} - \bar{v}^{i}\right)\right)_{,i} + \rho_{\mathfrak{a}}\left(\bar{v}^{i}\right)_{,i}
\end{aligned}
$$

and using this result with $\bar{v}^{i} = v_{\mathfrak{s}}{}^{i}$ and rearranging yields

$$
\begin{aligned}
&-\left(D^{v_{\mathfrak{s}}}\left(\sum\nolimits_{\mathfrak{a}} \rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right) + \left(\sum\nolimits_{\mathfrak{a}} \rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right)\left(v_{\mathfrak{s}}{}^{i}\right)_{,i}\right) - \left(\sum\nolimits_{\mathfrak{a}} \rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right) D^{v_{\mathfrak{s}}}(\theta) + \left(\sum\nolimits_{\mathfrak{a}} T_{\mathfrak{a}}{}^{ki}\right)(v_{\mathfrak{s}k})_{,i} \\
&+ \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \mu_{\mathfrak{a}}\left(D^{v_{\mathfrak{s}}}(\rho_{\mathfrak{a}}) + \rho_{\mathfrak{a}}\left(v_{\mathfrak{s}}{}^{i}\right)_{,i}\right) \\
&- \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\left(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}k}) - b_{\mathfrak{a}k} + (\mu_{\mathfrak{a}})_{,k} + \eta_{\mathfrak{a}}(\theta)_{,k}\right) \\
&- \left(\sum\nolimits_{\mathfrak{a}} q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i} - \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \left(\mu_{\mathfrak{a}} + \tfrac{1}{2}(v_{\mathfrak{a}k} - v_{\mathfrak{s}k})\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\right)\hat{\rho}_{\mathfrak{a}} \geq 0
\end{aligned}
\tag{2.61}
$$

Multiplication of this relation by $J_{\mathfrak{s}}$, the Jacobian of the motion of constituent $\mathfrak{s}$, (which is positive) and using the identity $D^{v_{\mathfrak{s}}}(J_{\mathfrak{s}}) = J_{\mathfrak{s}}\left(v_{\mathfrak{s}}{}^{i}\right)_{,i}$ yields (cf. Coussy 2004, Eqs. (3.26), (3.104), (6.16), (6.28))

$$
\begin{aligned}
&-D^{v_{\mathfrak{s}}}\left(\sum\nolimits_{\mathfrak{a}} J_{\mathfrak{s}}\rho_{\mathfrak{a}}\psi_{\mathfrak{a}}\right) - \left(\sum\nolimits_{\mathfrak{a}} J_{\mathfrak{s}}\rho_{\mathfrak{a}}\eta_{\mathfrak{a}}\right) D^{v_{\mathfrak{s}}}(\theta) + J_{\mathfrak{s}}\left(\sum\nolimits_{\mathfrak{a}} T_{\mathfrak{a}}{}^{ki}\right)(v_{\mathfrak{s}k})_{,i} + \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \mu_{\mathfrak{a}} D^{v_{\mathfrak{s}}}(J_{\mathfrak{s}}\rho_{\mathfrak{a}}) \\
&- \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} J_{\mathfrak{s}}\rho_{\mathfrak{a}}\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\left(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}k}) - b_{\mathfrak{a}k} + (\mu_{\mathfrak{a}})_{,k} + \eta_{\mathfrak{a}}(\theta)_{,k}\right) \\
&- J_{\mathfrak{s}}\left(\sum\nolimits_{\mathfrak{a}} q_{\mathfrak{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i} - \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} J_{\mathfrak{s}}\left(\mu_{\mathfrak{a}} + \tfrac{1}{2}(v_{\mathfrak{a}k} - v_{\mathfrak{s}k})\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\right)\hat{\rho}_{\mathfrak{a}} \geq 0
\end{aligned}
\tag{2.62}
$$

Using the motion of constituent $\mathfrak{s}$, we can define the following Lagrangian variables

$\Psi = J_{\mathfrak{s}}\sum\nolimits_{\alpha} \rho_{\mathfrak{a}}\psi_{\mathfrak{a}}$	Total (inner) free energy per unit reference volume
$\mathrm{H} = J_{\mathfrak{s}}\sum\nolimits_{\mathfrak{a}} \rho_{\mathfrak{a}}\eta_{\mathfrak{a}}$	Total entropy per unit reference volume
$S^{IJ} = J_{\mathfrak{s}}(F_{\mathfrak{s}}^{-1})^{I}_{i}(F_{\mathfrak{s}}^{-1})^{J}_{j}\sum\nolimits_{\alpha} T_{\mathfrak{a}}{}^{ij}$	Total (inner) 2nd Piola-Kirchhoff stress tensor
$E_{\mathfrak{s}IJ} = \frac{1}{2}(F^{i}_{\mathfrak{s}I}F^{j}_{\mathfrak{s}J}\delta_{ij} - \delta_{IJ})$	Green-Lagrange strain tensor of constituent $\mathfrak{s}$
$m_{\mathfrak{a}} = J_{\mathfrak{s}}\rho_{\mathfrak{a}}$	Mass of constituent $\mathfrak{a}$ per unit reference volume
$M_{\mathfrak{a}}{}^{I} = J_{\mathfrak{s}}\rho_{\mathfrak{a}}(F_{\mathfrak{s}}^{-1})^{I}_{i}(v_{\mathfrak{a}}{}^{i} - v_{\mathfrak{s}}{}^{i})$	Lagrangian mass flux of constituent $\mathfrak{a}$ w.r.t. constituent $\mathfrak{s}$
$Q^{I} = J_{\mathfrak{s}}(F_{\mathfrak{s}}^{-1})^{I}_{i}\sum\nolimits_{\alpha} q_{\mathfrak{a}}{}^{i}$	Lagrangian total (inner) heat flux
$\hat{m}_{\mathfrak{a}} = J_{\mathfrak{s}}\hat{\rho}_{\mathfrak{a}}$	Lagrangian supply of mass of constituent $\mathfrak{a}$

With these definitions the dissipation inequality (2.62) becomes (Coussy 2004)

$$
\begin{aligned}
&-D^{v_{\mathfrak{s}}}(\Psi) - \mathrm{H}D^{v_{\mathfrak{s}}}(\theta) + S^{IJ}D^{v_{\mathfrak{s}}}\left(E_{\mathfrak{s}IJ}\right) + \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \mu_{\mathfrak{a}} D^{v_{\mathfrak{s}}}(m_{\mathfrak{a}}) \\
&- \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} M_{\mathfrak{a}}{}^{I}\left(F^{i}_{\mathfrak{s}I}(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}i}) - b_{\mathfrak{a}i}) + (\mu_{\mathfrak{a}})_{,I} + \eta_{\mathfrak{a}}(\theta)_{,I}\right) \\
&- Q^{I}\frac{1}{\theta}(\theta)_{,I} - \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \left(\mu_{\mathfrak{a}} + \tfrac{1}{2}(v_{\mathfrak{a}k} - v_{\mathfrak{s}k})\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\right)\hat{m}_{\mathfrak{a}} \geq 0
\end{aligned}
\tag{2.63}
$$

where $(\cdot)_{,I} = \left(F^{i}_{\mathfrak{s}I}\right)(\cdot)_{,i}$ denotes the partial derivative of $(\cdot)$ with respect to the I-th Lagrangian coordinate.

Remarks

- The Lagrangian formulation for porous materials is used in Biot (1972), and is also used in Coussy (2004) and Wilmański (1998).

- In the formulation of Coussy (2004) it is assumed that the components are fluids that behave as if they were outside the porous material. In our formulation we have not made use of this assumption.

The dissipation is the sum of the following groups of terms

$$
\begin{aligned}
&-D^{v_{\mathfrak{s}}}(\Psi) - \mathrm{H}D^{v_{\mathfrak{s}}}(\theta) + S^{IJ}D^{v_{\mathfrak{s}}}\left(E_{\mathfrak{s}IJ}\right) + \sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} \mu_{\mathfrak{a}} D^{v_{\mathfrak{s}}}(m_{\mathfrak{a}}) && \text{intrinsic dissipation}\\
&-\sum\nolimits_{\mathfrak{a}\neq\mathfrak{s}} M_{\mathfrak{a}}{}^{I}\left(F_{\mathfrak{s}\,I}^{i}(D^{v_{\mathfrak{a}}}(v_{\mathfrak{a}i}) - b_{\mathfrak{a}i}) + (\mu_{\mathfrak{a}})_{,I} + \eta_{\mathfrak{a}}(\theta)_{,I}\right) && \text{fluids dissipation}\\
&-Q^{I}\frac{1}{\theta}(\theta)_{,I} && \text{thermal dissipation}\\
&-\sum\nolimits_{\mathfrak{a}\neq s}\left(\mu_{\mathfrak{a}} + \tfrac{1}{2}(v_{\mathfrak{a}k} - v_{sk})\left(v_{\mathfrak{a}}{}^{k} - v_{\mathfrak{s}}{}^{k}\right)\right)\widehat{m}_{\mathfrak{a}} && \text{phase change dissipation}
\end{aligned}
$$

Although the dissipation inequality requires the non-negativity of the sum of these four groups of terms, often the non-negativity of each group of terms is required.

Note that the form of the dissipation inequality (2.63) is based on the following assumptions:

- All constituents have the same temperature.
- All constituents have mass.
- For each constituent, the entropy flux and body entropy source are the heat flux and body heat source divided by the temperature, so that the corresponding balance of entropy is given by (2.50).
- All constituents are non-polar, so that their respective Cauchy stress tensors are symmetric.
- Except for constituent $\mathfrak{s}$, the Cauchy stress tensors of all constituents are spherical.

3 POROUS MATERIALS

3.1 MODELLING FRAMEWORK

3.1.1 Structure of a porous material

Porous materials are characterized by the presence of a solid skeleton and a number of fluids, which can flow through the solid skeleton. The solid skeleton and the fluids occupy 3D regions (volumes) of the space, are eventually made of various species and have thermodynamic properties, such as mass, momentum, energy and entropy. In general, the solid skeleton and the fluids are subjected to interactions, so that they may exchange thermodynamic properties.

Short-range interactions between 3D regions give rise to 2D regions (surfaces) with thermodynamic properties at the common boundary of the 3D regions. Similarly, short-range interactions between 2D regions give rise to 1D regions (lines) with thermodynamic properties at the common boundary of the 2D regions, and short-range interactions between 1D regions give rise to 0D regions (points) with thermodynamic properties at the common boundary of the 1D regions.

Eventually, between the solid skeleton and a neighboring fluid strong interaction forces exist that bond the fluid to the solid skeleton (Low 1951). Fluid particles in the regions subjected to these interaction forces have properties, such as density or viscosity, that are different from those of fluid particles not subjected to those interactions. The former will be referred to as vicinal fluid and the later as free fluid. Because of their strong bonding to the solid skeleton, the regions containing vicinal fluids will be considered to be part of the solid skeleton.

The structure of porous materials can be complex and some porous material can exhibit several structural levels. For instance, clay particles and vicinal water can form aggregates, which can be considered as larger particles which form a larger structure and the space left is occupied by free fluids, which in turn are mixtures of various species (Alonso et al. 1987). Further, the solid skeleton can be cemented by the presence of certain substances and can become unstable by changes in the concentrations of certain cations or in the pH of water (Koorevaar et al. 1983).

3.1.2 Microscale and macroscale continua

Modeling of a porous material as a continuous medium, implicitly assumes an averaging process. Averaging is based on the existence of representative element volumes (REV) that must satisfy certain conditions (Bear and Bachmat 1990; Whitaker 1999; Gray and Miller 2014). On the one hand, the REV must be large enough with respect to the characteristic dimensions of the details of the structure of the porous material so that averaging yields results independent of the REV size. On the other hand, the REV must be small enough with respect to the characteristic dimensions of the region analyzed so that it can be considered a macroscale point.

We assume that the material in a given region α of a certain dimension (3D, 2D, 1D, 0D) containing a number of species can be modeled as a mixture of microscale interacting continua $c_{\alpha\mathrm{a}}$. The interacting continuum $c_{\alpha\mathrm{a}}$ corresponds to the species a contained in the region α, and has microscale thermodynamic properties subjected to microscale balance equations, which include interaction terms with the other microscale continua such that their sum over all $c_{\alpha\mathrm{a}}$ vanishes. Averaging associates to each microscale continuum $c_{\alpha\mathrm{a}}$ a macroscale continuum $\mathcal{C}_{\alpha\mathrm{a}}$, with macroscale thermodynamic properties subjected to macroscale balance equations, which include interaction terms with the other macroscale continua such that their sum over all $\mathcal{C}_{\alpha\mathrm{a}}$ vanishes.

Macroscale thermodynamic properties at a macroscale space point are defined by integration of microscale properties over the microscale region α within the REV centered at the considered macroscale point. Macroscale balance equations are obtained by integration of microscale balance equations over the microscale region α within the REV and use of averaging theorems (Gray and Miller 2014). Note that, whereas the microscale continua $c_{\alpha\mathrm{a}}$ that model the behaviour of the material in a microscale region α of a certain dimension are defined only on that microscale region, the corresponding macroscale continua $\mathcal{C}_{\alpha\mathrm{a}}$ are defined on macroscale 3D regions. The porous material can be modelled as the mixture of all macroscale continua $\mathcal{C}_{\alpha\mathrm{a}}$ as in mixture theory (Truesdell 1984, Lecture 5).

Averaging of microscale distributions of extensive thermodynamic variables, such as mass or momentum, is conceptually clear, because of the extensive nature of these variables. Averaging of microscale distributions of intensive thermodynamic variables, such as pressure, chemical potential or temperature, requires the multiplication of the intensive variable by a weighting function that yields an extensive variable (Gray and Miller 2014), and it should be mentioned that for the same intensive variables different weighting functions have been used by different authors. However, averaging of microscale uniform distributions of intensive thermodynamic properties should give this uniform value, independently of the weighting function used.

While microscale continua occupy space regions of various dimensions, macroscale continua occupy 3D space regions, so that microscale geometric information is lost after averaging. Part of this geometric information can be recovered by macroscale variables defined as the measure of a microscale region (volume, area, length, number of points) within the REV divided by the volume of the REV. For instance, in geomechanics several variables are functions of the volume fractions of the solid skeleton and the fluids. These additional macroscale variables will be referred to as geometric variables. They increase the number of variables and require additional constitutive equations. These geometric variables are not independent (for instance, the sum of all volume fractions must be one). Moreover, the variations of the geometric variables are not independent (for instance, the variation of the volume of a spherical bubble is not independent of the variation of its surface). Approximate relations between the variations of the geometric variables have been proposed (Gray and Miller 2014). Additional geometric variables can be defined from the geometry of the microscale regions, giving rise to structure tensors. These variables can be used to describe the anisotropy of the porous material.

For many practical problems, the aforementioned modeling of a porous material is too detailed. This detail can be reduced in several ways (Gray and Miller 2014). For instance, some properties of a microscale continuum, such as mass or momentum, can be neglected so that the corresponding balance equations become boundary conditions between the microscale continua in the neighboring regions, or several regions can be grouped into a larger region, with appropriately defined macroscale thermodynamic properties.

In what follows the porous material will be modeled as the mixture $\mathcal{C}$ of the species-based macroscale continua $\mathcal{C}_{\mathrm{a}}$, where a ranges over all species, which we symbolically denote by $\mathcal{C} = \bigcup_{\mathrm{a}} \mathcal{C}_{\mathrm{a}}$. The macroscale continuum $\mathcal{C}_{\mathrm{a}}$ associated to species a is the mixture of the macroscale continua $\mathcal{C}_{\alpha\mathrm{a}}$ associated to species a in region α, where α ranges over all the regions that contain species a, which we symbolically denote by $\mathcal{C}_{\mathrm{a}} = \bigcup_{\alpha} \mathcal{C}_{\alpha\mathrm{a}}$.

3.1.3 Balance equations in Eulerian and Lagrangian descriptions

The postulated balance equations are those of mixture theory (Truesdell 1984, Lecture 5) presented in section 2.2.2, where the distinguishable constituents are the aforementioned macroscale continua. Since no chemical reactions will be considered, all mass exchange terms will be set to zero. We assume that (1) for each constituent, the entropy flux and the entropy supply per unit mass are equal to the heat flux and the heat supply divided by the temperature; (2) all constituents have the same temperature; (3) the Cauchy stress tensors of all constituents are non-polar; and (4) the Cauchy stress tensors of all constituents except the solid mineral are spherical.

Notation. In order to simplify the notation, in what follows the following changes will be made

$$\begin{gathered}
\mathfrak{a} \rightarrow \mathrm{a} \\
\mathfrak{s} \rightarrow \mathrm{s} \\
D^{v_{\mathfrak{s}}}(\cdot) \rightarrow (\cdot)^{\cdot} \\
F_{\mathfrak{s}}{}^{i}{}_{J} \rightarrow F^{i}_{J} \\
v^{i}_{\mathfrak{s}} \rightarrow v^{i} \\
E_{\mathfrak{s}\,IJ} \rightarrow E_{IJ}
\end{gathered}$$

Assuming that the microscale 3D region occupied by the solid particles contains only the species s (solid mineral) and that species s is not contained in any other microscale region, it follows that the motion of the constituent s coincides with the motion of the solid skeleton. Recall that the solid skeleton contains the solid particles and the tightly bonded vicinal fluids.

With the assumptions

$$\begin{gathered}
\hat{\rho}_{\mathrm{a}} = 0 \\
\theta_{\mathrm{a}} = \theta \\
T_{\mathrm{a}}{}^{ij} = T_{\mathrm{a}}{}^{ji} \\
T^{ij}_{\mathrm{a}} = -p_{\mathrm{a}}\delta^{ij} \quad \mathrm{a} \neq \mathrm{s} \\
\varphi_{\mathrm{a}}{}^{i} = q^{i}_{\mathrm{a}}/\theta \\
\varsigma_{\mathrm{a}} = r_{\mathrm{a}}/\theta
\end{gathered} \tag{3.1}$$

the balance equations can be transformed relative to the skeleton motion, both in Eulerian and in Lagrangian descriptions.

3.1.3.1 Balance of mass for a species

Equation (2.39) becomes

$$\begin{aligned}
0 &= (\rho_{\mathrm{a}})^{\cdot} + (\rho_{\mathrm{a}})_{,i}\left(v^{i}_{\mathrm{a}} - v^{i}\right) + \rho_{\mathrm{a}}\left(v_{\mathrm{a}}{}^{i} - v^{i}\right)_{,i} + \rho_{\mathrm{a}}\left(v^{i}\right)_{,i} \\
&= (\rho_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\left(v^{i}\right)_{,i} + \left(\rho_{\mathrm{a}}\left(v^{i}_{\mathrm{a}} - v^{i}\right)\right)_{,i}
\end{aligned}$$

$$0 = (\rho_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\left(v^{i}\right)_{,i} + \left(\rho_{\mathrm{a}}\left(v^{i}_{\mathrm{a}} - v^{i}\right)\right)_{,i} \tag{3.2}$$

Multiplication by J, use of the identity $(J)^{\cdot} = J\left(v^{i}\right)_{,i}$ and the Piola transform $\left(w^{i}\right)_{,i} = \left(J(F^{-1})^{I}_{i}w^{i}\right)$ yields

$$0 = (J\rho_{\mathrm{a}})^{\cdot} + \left(J\rho_{\mathrm{a}}(F^{-1})^{I}_{i}\left(v^{i}_{\mathrm{a}} - v^{i}\right)\right)_{,I} \tag{3.3}$$

which can be rewritten in the form (cf. Coussy 2004, Eqs. (1.67), (6.6))

$$0 = (m_{\mathrm{a}})^{\cdot} + ({M_{\mathrm{a}}}^{I})_{,I} \tag{3.4}$$

where the following Lagrangian variables have been used: m_{a} is the mass of species a per unit reference volume and ${M_{\mathrm{a}}}^{I}$ is the Lagrangian mass flux of species a relative to the solid skeleton.

3.1.3.2 Balance of mass for the mixture

Since there are no mass exchanges between species, the balance of mass for the mixture is trivial.

3.1.3.3 Balance of momentum for a species

Equation (2.42) becomes

$$\hat{p}_{\mathrm{a}}{}^{j} = \rho_{\mathrm{a}} a_{\mathrm{a}}{}^{j} - \left(T_{\mathrm{a}}{}^{ji}\right)_{,i} - \rho_{\mathrm{a}} b_{\mathrm{a}}{}^{j} \tag{3.5}$$

Multiplication by J, use of the identity $(J)^{\cdot} = J\left(v^{i}\right)_{,i}$ and the Piola transform $\left(w^{i}\right)_{,i} = \left(J(F^{-1})^{I}_{i} w^{i}\right)$ yields

$$J\hat{p}_{\mathrm{a}}{}^{j} = J\rho_{\mathrm{a}}\left(a_{\mathrm{a}}{}^{j} - b_{\mathrm{a}}{}^{j}\right) - \left(J(F^{-1})^{I}_{i} T_{\mathrm{a}}{}^{ji}\right)_{,I} \tag{3.6}$$

3.1.3.4 Balance of moment for the mixture

Addition of (3.6) over all constituents and use of $\sum_{\mathrm{a}} \hat{p}_{\mathrm{a}k} = 0$ yields

$$0 = \sum\nolimits_{\mathrm{a}} J\rho_{\mathrm{a}}\left(a_{\mathrm{a}}{}^{j} - b_{\mathrm{a}}{}^{j}\right) - \left(F^{j}_{J}\left(J(F^{-1})^{J}_{k}(F^{-1})^{I}_{i} \sum\nolimits_{\mathrm{a}} T_{\mathrm{a}}{}^{ki}\right)\right)_{,I} \tag{3.7}$$

which can be rewritten in the form (cf. Coussy 2004, Eq. (2.50))

$$0 = \sum\nolimits_{\mathrm{a}} m_{\mathrm{a}}\left(a_{\mathrm{a}}{}^{j} - b_{\mathrm{a}}{}^{j}\right) - \left(F^{j}_{J} S^{JI}\right)_{,I} \tag{3.8}$$

where the following Lagrangian variables have been used: m_{a} is the mass of species a per unit reference volume and S^{IJ} is the total 2nd Piola-Kirchhoff stress tensor.

3.1.3.5 Balance of moment of momentum for a species

Equation (2.45) becomes

$$T_{\mathrm{a}}{}^{ij} = T_{\mathrm{a}}{}^{ji}$$

$$J(F^{-1})^{J}_{k}(F^{-1})^{I}_{i} T_{\mathrm{a}}{}^{ij} = J(F^{-1})^{J}_{k}(F^{-1})^{I}_{i} T_{\mathrm{a}}{}^{ji} \tag{3.9}$$

3.1.3.6 *Balance of moment of momentum for the mixture*

Addition of (3.9) over all constituents yields

$$J(F^{-1})^J_{\ k}(F^{-1})^I_{\ i}\sum_{\mathrm{a}} T_{\mathrm{a}}^{\ ij} = J(F^{-1})^J_{\ k}(F^{-1})^I_{\ i}\sum_{\mathrm{a}} T_{\mathrm{a}}^{\ ji} \tag{3.10}$$

which can be rewritten in the form

$$S^{IJ} = S^{JI} \tag{3.11}$$

where S^{IJ} is the total 2nd Piola-Kirchhoff stress tensor.

3.1.3.7 *Balance of energy for a species*

Equation (2.48) becomes

$$\begin{aligned}
\hat{\varepsilon}_{\mathrm{a}} &= \rho_{\mathrm{a}}(\varepsilon_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}(\varepsilon_{\mathrm{a}})_{,i}\left(v_{\mathrm{a}}^i - v^i\right) - T_{\mathrm{a}k}^{\ \ i}\left(v_{\mathrm{a}}^{\ k} - v^k\right)_{,i} + T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} \\
&\quad +\left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \left(v_{\mathrm{a}}^k - v^k\right)\hat{p}_{\mathrm{a}k} + v^k\hat{p}_{\mathrm{a}k} \\
&= (\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} - (\rho_{\mathrm{a}})^{\cdot}\varepsilon_{\mathrm{a}} + \rho_{\mathrm{a}}(\varepsilon_{\mathrm{a}})_{,i}\left(v_{\mathrm{a}}^i - v^i\right) - T_{\mathrm{a}k}^{\ \ i}\left(v_{\mathrm{a}}^{\ k} - v^k\right)_{,i} + T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} \\
&\quad +\left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \left(v_{\mathrm{a}}^k - v^k\right)\left(\rho_{\mathrm{a}} a_{\mathrm{a}k} - \left(T_{\mathrm{a}k}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} b_{\mathrm{a}k}\right) + v^k\hat{p}_{\mathrm{a}k} \\
&= (\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} + \varepsilon_{\mathrm{a}}\left(\rho_{\mathrm{a}}\left(v^i\right)_{,i} + \left(\rho_{\mathrm{a}}\left(v_{\mathrm{a}}^i - v^i\right)\right)_{,i}\right) + \rho_{\mathrm{a}}(\varepsilon_{\mathrm{a}})_{,i}\left(v_{\mathrm{a}}^i - v^i\right) - \left(T_{\mathrm{a}k}^{\ \ i}\left(v_{\mathrm{a}}^{\ k} - v^k\right)\right)_{,i} \\
&\quad +T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} + \left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \rho_{\mathrm{a}}\left(v_{\mathrm{a}}^k - v^k\right)(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + v^k\hat{p}_{\mathrm{a}k} \\
&= (\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\varepsilon_{\mathrm{a}}\left(v^i\right)_{,i} + \left(\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}}\left(v_{\mathrm{a}}^i - v^i\right)\right)_{,i} - \left(-p_{\mathrm{a}}\delta_k^i\left(v_{\mathrm{a}}^{\ k} - v^k\right)\right)_{,i} \\
&\quad +T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} + \left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \rho_{\mathrm{a}}\left(v_{\mathrm{a}}^k - v^k\right)(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + v^k\hat{p}_{\mathrm{a}k} \\
&= (\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\varepsilon_{\mathrm{a}}\left(v^i\right)_{,i} + \left(\left(\varepsilon_{\mathrm{a}} + \frac{p_{\mathrm{a}}}{\rho_{\mathrm{a}}}\right)\rho_{\mathrm{a}}\left(v_{\mathrm{a}}^i - v^i\right)\right)_{,i} \\
&\quad +T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} + \left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \rho_{\mathrm{a}}\left(v_{\mathrm{a}}^k - v^k\right)(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + v^k\hat{p}_{\mathrm{a}k}
\end{aligned}$$

$$\begin{aligned}
\hat{\varepsilon}_{\mathrm{a}} &= (\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\varepsilon_{\mathrm{a}}\left(v^i\right)_{,i} + \left(\left(\varepsilon_{\mathrm{a}} + \frac{p_{\mathrm{a}}}{\rho_{\mathrm{a}}}\right)\rho_{\mathrm{a}}\left(v_{\mathrm{a}}^i - v^i\right)\right)_{,i} \\
&\quad +T_{\mathrm{a}k}^{\ \ i}\left(v^k\right)_{,i} + \left(q_{\mathrm{a}}^{\ i}\right)_{,i} - \rho_{\mathrm{a}} r_{\mathrm{a}} + \rho_{\mathrm{a}}\left(v_{\mathrm{a}}^k - v^k\right)(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + v^k\hat{p}_{\mathrm{a}k}
\end{aligned} \tag{3.12}$$

Note that we can set $T_{\mathrm{a}k}^{\ \ i}\left(v_{\mathrm{a}}^{\ k} - v^k\right) = -p_{\mathrm{a}}\delta_k^i\left(v_{\mathrm{a}}^{\ k} - v^k\right)$ because if a = s then $T_{\mathrm{s}k}^{\ \ i}\left(v_{\mathrm{a}}^{\ k} - v^k\right) = 0$ and if a ≠ s then $T_{\mathrm{a}k}^{\ \ i} = -p_{\mathrm{a}}\delta_k^i$ by assumption. Multiplication by J, use of the identity $(J)^{\cdot} = J\left(v^i\right)_{,i}$, the Piola transform $\left(w^i\right)_{,i} = \left(J(F^{-1})^I_{\ i}w^i\right)$ and the identity $D_{ij} = (F^{-1})^I_{\ i}(F^{-1})^J_{\ j}\left(E_{IJ}\right)^{\cdot}$ yields

$$\begin{aligned}
J\hat{\varepsilon}_{\mathrm{a}} &= (J\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}})^{\cdot} + \left(\mu_{\mathrm{a}} J(F^{-1})^I_{\ i}\rho_{\mathrm{a}}\left(v_{\mathrm{a}}^i - v^i\right)\right)_{,I} + J(F^{-1})^I_{\ i}(F^{-1})^J_{\ j}T_{\mathrm{a}}^{\ ij}\left(E_{IJ}\right)^{\cdot} \\
&\quad +\left(J(F^{-1})^I_{\ i}q_{\mathrm{a}}^{\ i}\right)_{,I} - J\rho_{\mathrm{a}} r_{\mathrm{a}} + J\rho_{\mathrm{a}}(F^{-1})^I_{\ i}\left(v_{\mathrm{a}}^{\ i} - v^i\right)F^k_{\ I}(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + Jv^k\hat{p}_{\mathrm{a}k}
\end{aligned} \tag{3.13}$$

where $\mu_{\mathrm{a}} = \varepsilon_{\mathrm{a}} + p_{\mathrm{a}}/\rho_{\mathrm{a}}$ (a ≠ s) is the chemical potential of species a.

3.1.3.8 *Balance of energy for the mixture*

Addition of (3.13) over all constituents, and use of $\sum_{\mathrm{a}} \hat{\varepsilon}_{\mathrm{a}} = 0$ and $\sum_{\mathrm{a}} \hat{p}_{\mathrm{a}k} = 0$ yields

$$\begin{aligned} 0 = {} & \left(\sum_{\mathrm{a}} J\rho_{\mathrm{a}}\varepsilon_{\mathrm{a}}\right)^{\cdot} + \left(\sum_{\mathrm{a}\neq\mathrm{s}} \mu_{\mathrm{a}}\rho_{\mathrm{a}} J (F^{-1})^{I}{}_{i}\left(v_{\mathrm{a}}^{i} - v^{i}\right)\right)_{,I} + \left(J(F^{-1})^{I}{}_{i} \sum_{\mathrm{a}} q_{\mathrm{a}}{}^{i}\right)_{,I} + \\ & - \sum_{\mathrm{a}} J\rho_{\mathrm{a}} r_{\mathrm{a}} - J(F^{-1})^{I}{}_{i}(F^{-1})^{J}{}_{j}\left(\sum_{\mathrm{a}} T_{\mathrm{a}}{}^{ij}\right)\left(E_{IJ}\right)^{\cdot} + \sum_{\mathrm{a}\neq\mathrm{s}} J\rho_{\mathrm{a}}(F^{-1})^{I}{}_{i}\left(v_{\mathrm{a}}{}^{i} - v^{i}\right)F^{k}{}_{I}(a_{\mathrm{a}k} - b_{\mathrm{a}k}) \end{aligned} \tag{3.14}$$

which can be rewritten in the form (cf. Coussy 2004, Eqs. (3.21), (6.11))

$$0 = (\mathrm{E})^{\cdot} + \left(\sum_{\mathrm{a}} \mu_{\mathrm{a}} M_{\mathrm{a}}{}^{I}\right)_{,I} + (Q^{I})_{,I} - R - S^{IJ}\left(E_{IJ}\right)^{\cdot} + \sum_{\mathrm{a}\neq\mathrm{s}} M_{\mathrm{a}}{}^{I} F^{k}{}_{I}(a_{\mathrm{a}k} - b_{\mathrm{a}k}) \tag{3.15}$$

where the following Lagrangian variables have been used: E is the total internal energy per unit reference volume, $M_{\mathrm{a}}{}^{I}$ is the Lagrangian mass flux of species a relative to the solid skeleton, S^{IJ} is the total 2nd Piola-Kirchhoff stress tensor, E_{IJ} is the Green-Lagrange strain tensor of the solid skeleton, R is the total heat supply and Q^{I} is the total heat flux.

3.1.3.9 *Entropy inequality for the mixture*

Equation (2.61) becomes

$$\begin{aligned} & -\left(\left(\sum_{\mathrm{a}} \rho_{\mathrm{a}}\psi_{\mathrm{a}}\right)^{\cdot} + \left(\sum_{\mathrm{a}} \rho_{\mathrm{a}}\psi_{\mathrm{a}}\right)\left(v^{i}\right)_{,i}\right) - \left(\sum_{\mathrm{a}} \rho_{\mathrm{a}}\eta_{\mathrm{a}}\right)(\theta)^{\cdot} + \left(\sum_{\mathrm{a}} T_{\mathrm{a}}{}^{ki}\right)(v_{k})_{,i} \\ & + \sum_{\mathrm{a}\neq\mathrm{s}} \mu_{\mathrm{a}}\left((\rho_{\mathrm{a}})^{\cdot} + \rho_{\mathrm{a}}\left(v^{i}\right)_{,i}\right) \\ & - \sum_{\mathrm{a}\neq\mathrm{s}} \rho_{\mathrm{a}}\left(v_{\mathrm{a}}{}^{k} - v^{k}\right)\left(a_{\mathrm{a}k} - b_{\mathrm{a}k} + (\mu_{\mathrm{a}})_{,k} + \eta_{\mathrm{a}}(\theta)_{,k}\right) \\ & - \left(\sum_{\mathrm{a}} q_{\mathrm{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,i} \geq 0 \end{aligned} \tag{3.16}$$

Multiplication by J, use of the identity $(J)^{\cdot} = J\left(v^{i}\right)_{,i}$, the Piola transform $\left(w^{i}\right)_{,i} = \left(J(F^{-1})^{I}{}_{i}w^{i}\right)$ and the identity $D_{ij} = (F^{-1})^{I}{}_{i}(F^{-1})^{J}{}_{j}\left(E_{IJ}\right)^{\cdot}$ yields

$$\begin{aligned} & -\left(\sum_{\mathrm{a}} J\rho_{\mathrm{a}}\psi_{\mathrm{a}}\right)^{\cdot} - \left(\sum_{\mathrm{a}} J\rho_{\mathrm{a}}\eta_{\mathrm{a}}\right)(\theta)^{\cdot} + J(F^{-1})^{I}{}_{i}(F^{-1})^{J}{}_{j}\left(\sum_{\mathrm{a}} T_{\mathrm{a}}{}^{ij}\right)\left(E_{IJ}\right)^{\cdot} + \sum_{\mathrm{a}\neq\mathrm{s}} \mu_{\mathrm{a}}(J\rho_{\mathrm{a}})^{\cdot} \\ & - \sum_{\mathrm{a}\neq\mathrm{s}} J\rho_{\mathrm{a}}(F^{-1})^{I}{}_{i}\left(v_{\mathrm{a}}{}^{i} - v^{i}\right)\left(F^{k}{}_{I}(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I}\right) \\ & - \left(\sum_{\mathrm{a}} J(F^{-1})^{I}{}_{i} q_{\mathrm{a}}{}^{i}\right)\frac{1}{\theta}(\theta)_{,I} \geq 0 \end{aligned} \tag{3.17}$$

which can be rewritten in the form (cf. Coussy 2004, Eqs. (3.26), (3.104), (6.16))

$$\begin{aligned} & -(\Psi)^{\cdot} - \mathrm{H}(\theta)^{\cdot} + S^{IJ}\left(E_{IJ}\right)^{\cdot} + \sum_{\mathrm{a}\neq\mathrm{s}} \mu_{\mathrm{a}}(m_{\mathrm{a}})^{\cdot} \\ & - \sum_{\mathrm{a}\neq\mathrm{s}} M_{\mathrm{a}}^{I}\left(F^{k}_{I}(a_{\mathrm{a}k} - b_{\mathrm{a}k}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I}\right) \\ & - Q^{I}\frac{1}{\theta}(\theta)_{,I} \geq 0 \end{aligned} \tag{3.18}$$

where the following Lagrangian variables have been used: Ψ is the total free energy per unit reference volume, H is the total entropy per unit reference volume, S^{IJ} is the total 2nd Piola-Kirchhoff stress tensor, E_{IJ} is the Green-Lagrange strain tensor of the solid skeleton, m_{a} is the mass of species a per unit reference volume, ${M_{\mathrm{a}}}^{I}$ is the Lagrangian mass flux of species a relative to the solid skeleton, R is the total heat supply and Q^{I} is the total heat flux.

3.1.4 State variables and local equilibrium states

The state of a porous medium will be assumed to be given by the deformation of the solid skeleton, the measure (volume, area, length, number of points) of each microscale region per unit reference volume, the mass of each species in each microscale region per unit reference volume, the temperature and a set of internal variables, which encapsulate the history of the material. In a Lagrangian formulation with respect to the motion of the solid skeleton they are

$$\left(E_{IJ}, n_{\mathrm{\alpha}}, m_{\mathrm{\alpha a}}, \theta, \xi\right) \tag{3.19}$$

where E_{IJ} is the Green-Lagrange strain tensor of the solid skeleton, $n_{\mathrm{\alpha}}$ is the measure (volume, area, length, number of points) of the microscale region α per unit reference volume, $m_{\mathrm{\alpha a}}$ is the mass of species a in the microscale region α per unit reference volume, θ is the temperature and ξ denotes a set on internal variables. Note that the sum of $n_{\mathrm{\alpha}}$ over all 3D regions is equal to the Jacobian of the motion of the solid skeleton J (i.e. the current volume per unit reference volume). Since $J = \left(\det\left(2E_{IJ} + \delta_{IJ}\right)\right)^{1/2}$ it follows that, for given E_{IJ}, the $n_{\mathrm{\alpha}}$ of all 3D regions are not independent, so that one of them can be dropped.

The number of the state variables can be significantly reduced by considering local equilibrium states. Let m_{a} be the total mass of species a per unit reference volume, so that $m_{\mathrm{a}} = \sum_{\mathrm{\alpha}} m_{\mathrm{\alpha a}}$. It will be assumed that, for prescribed values of E_{IJ}, m_{a}, θ and ξ, the variables $n_{\mathrm{\alpha}}$ and $m_{\mathrm{\alpha a}}$ take unique values $n_{\mathrm{\alpha}} = n_{\mathrm{\alpha}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ and $m_{\mathrm{\alpha a}} = m_{\mathrm{\alpha a}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ such that the total free energy per unit reference volume reaches a minimum. The state $\left(E_{IJ}, n_{\mathrm{\alpha}}, m_{\mathrm{\alpha a}}, \theta, \xi\right)$ given by

$$\left(E_{IJ}, n_{\mathrm{\alpha}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\mathrm{\alpha a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right) \tag{3.20}$$

will be called the local equilibrium state defined by $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$.

Let the total free energy per unit reference volume $\widetilde{\Psi}$ be given by

$$\widetilde{\Psi} = \widetilde{\Psi}\left(E_{IJ}, n_{\mathrm{\alpha}}, m_{\mathrm{\alpha a}}, \theta, \xi\right) \tag{3.21}$$

For fixed $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$, let us consider the conditions that satisfy the functions $n_{\mathrm{\alpha}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ and $m_{\mathrm{\alpha a}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ at a relative minimum of $\widetilde{\Psi}\left(E_{IJ}, n_{\mathrm{\alpha}}, m_{\mathrm{\alpha a}}, \theta, \xi\right)$. On the one hand, as already mentioned, for fixed E_{IJ} the variations of the $n_{\mathrm{\alpha}}$ are not independent, and some approximations have been proposed (Gray and Miller 2014). On the other hand, for fixed m_{a} the variables $m_{\mathrm{\alpha a}}$ are related by $m_{\mathrm{a}} = \sum_{\mathrm{\alpha}} m_{\mathrm{\alpha a}}$, so that $\sum_{\mathrm{\alpha}} dm_{\mathrm{\alpha a}} = 0$. Consequently, the necessary conditions read

$$\begin{gathered} \frac{\partial \widetilde{\Psi}}{\partial m_{\mathrm{\alpha a}}} = \lambda_{m_{\mathrm{a}}} \\ \sum\nolimits_{\mathrm{\alpha}} \frac{\partial \widetilde{\Psi}}{\partial n_{\mathrm{\alpha}}} dn_{\mathrm{\alpha}} = 0 \end{gathered} \tag{3.22}$$

where $\lambda_{m_{\mathrm{a}}}$ denotes the common value of $\partial\widetilde{\Psi}/\partial m_{\mathrm{\alpha a}}$, the partial derivatives of $\widetilde{\Psi}$ are evaluated at the local equilibrium state defined by the variables $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ and the variations of the geometric variables $dn_{\mathrm{\alpha}}$ are such that comply with the geometric constraints.

Since the solutions $n_{\alpha} = n_{\mathrm{\alpha}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ comply with the geometrical constraints, using the variations $dn_{\alpha} = \left(\partial n_{\alpha}/\partial E_{IJ}\right) dE_{IJ}$, $dn_{\alpha} = (\partial n_{\alpha}/\partial m_{\mathrm{a}}) dm_{\mathrm{a}}$, $dn_{\alpha} = (\partial n_{\alpha}/\partial \theta) d\theta$ and $dn_{\alpha} = (\partial n_{\alpha}/\partial \xi) d\xi$ in condition $(3.22)_2$ yields the following results

$$\sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial E_{IJ}}=0 \qquad \sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial m_{\mathrm{a}}}=0 \qquad \sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial \theta}=0 \qquad \sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial \xi}=0 \tag{3.23}$$

where the partial derivatives of $\tilde{\Psi}$ are evaluated at the local equilibrium state defined by the variables $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$, the partial derivatives of n_{α} are evaluated at $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ and the fact that dE_{IJ}, dm_{a}, $d\theta$ and $d\xi$ are independent has been used.

Notation. The evaluation of a state function $\tilde{\Xi}\left(E_{IJ}, n_{\alpha}, m_{\alpha\mathrm{a}}, \theta, \xi\right)$ at local equilibrium states defines the corresponding local equilibrium state function $\Xi\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ by

$$\Xi\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)=\tilde{\Xi}\left(E_{IJ}, n_{\alpha}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\alpha\mathrm{a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right)$$

Note that the symbol of the defined function is the same as the symbol of the original function without the superposed tilde (~).

Lemma 3.1. *Let the free energy of the porous material per unit reference volume at local equilibrium states be*

$$\Psi\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)=\tilde{\Psi}\left(E_{IJ}, n_{\alpha}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\alpha\mathrm{a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right) \tag{3.24}$$

then, at local equilibrium states, the following relations hold:

$$\frac{\partial\Psi}{\partial E_{IJ}}=\frac{\partial\tilde{\Psi}}{\partial E_{IJ}} \qquad \frac{\partial\Psi}{\partial m_{\mathrm{a}}}=\frac{\partial\tilde{\Psi}}{\partial m_{\alpha\mathrm{a}}} \qquad \frac{\partial\Psi}{\partial \theta}=\frac{\partial\tilde{\Psi}}{\partial \theta} \qquad \frac{\partial\Psi}{\partial \xi}=\frac{\partial\tilde{\Psi}}{\partial \xi} \tag{3.25}$$

where the derivatives of Ψ *are evaluated at* $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ *and the derivatives of* $\tilde{\Psi}$ *are evaluated at the local equilibrium state* $\left(E_{IJ}, n_{\alpha}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\alpha\mathrm{a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right)$*.*

Proof. Derivation of (3.24) with respect to E_{IJ} and use of the minimization conditions (3.22) and the results (3.23) yield

$$\begin{aligned}
\frac{\partial\Psi}{\partial E_{IJ}} &= \frac{\partial\tilde{\Psi}}{\partial E_{IJ}}+\sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial E_{IJ}}+\sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial m_{\alpha\mathrm{a}}}\frac{\partial m_{\alpha\mathrm{a}}}{\partial E_{IJ}}\\
&= \frac{\partial\tilde{\Psi}}{\partial E_{IJ}}+0+\sum\nolimits_{\alpha}\lambda_{m_{\mathrm{a}}}\frac{\partial m_{\alpha\mathrm{a}}}{\partial E_{IJ}}\\
&= \frac{\partial\tilde{\Psi}}{\partial E_{IJ}}+\lambda_{m_{\mathrm{a}}}\frac{\partial}{\partial E_{IJ}}\left(\sum\nolimits_{\alpha}m_{\alpha\mathrm{a}}\right)\\
&= \frac{\partial\tilde{\Psi}}{\partial E_{IJ}}+\lambda_{m_{\mathrm{a}}}\frac{\partial m_{\mathrm{a}}}{\partial E_{IJ}}\\
&= \frac{\partial\tilde{\Psi}}{\partial E_{IJ}}
\end{aligned}$$

Derivation of (3.24) with respect to m_{a} and use of the minimization conditions (3.22) and the results (3.23) yields

$$\begin{aligned}
\frac{\partial\Psi}{\partial m_{\mathrm{a}}} &= \sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial n_{\alpha}}\frac{\partial n_{\alpha}}{\partial m_{\mathrm{a}}}+\sum\nolimits_{\alpha}\frac{\partial\tilde{\Psi}}{\partial m_{\alpha\mathrm{a}}}\frac{\partial m_{\alpha\mathrm{a}}}{\partial m_{\mathrm{a}}}\\
&= 0+\sum\nolimits_{\alpha}\lambda_{m_{\mathrm{a}}}\frac{\partial m_{\alpha\mathrm{a}}}{\partial m_{\mathrm{a}}}
\end{aligned}$$

$$
\begin{aligned}
&= \lambda_{m_{\mathrm{a}}} \frac{\partial}{\partial m_{\mathrm{a}}} \left(\sum\nolimits_{\alpha} m_{\alpha \mathrm{a}} \right) \\
&= \lambda_{m_{\mathrm{a}}} \frac{\partial m_{\mathrm{a}}}{\partial m_{\mathrm{a}}} \\
&= \lambda_{m_{\mathrm{a}}}
\end{aligned}
$$

The proofs of the remaining relations follow by derivation of (3.24) with respect to θ and with respect to ξ, along the same lines as in the proof of the first relation. ■

Thus, along local equilibrium states, the variation of the free energy per unit reference volume

$$
d\widetilde{\Psi} = \frac{\partial \widetilde{\Psi}}{\partial E_{IJ}} dE_{IJ} + \sum\nolimits_{\alpha} \frac{\partial \widetilde{\Psi}}{\partial n_{\alpha}} dn_{\alpha} + \sum\nolimits_{\alpha \mathrm{a}} \frac{\partial \widetilde{\Psi}}{\partial m_{\alpha \mathrm{a}}} dm_{\alpha \mathrm{a}} + \frac{\partial \widetilde{\Psi}}{\partial \theta} d\theta + \frac{\partial \widetilde{\Psi}}{\partial \xi} d\xi
$$

reduces to

$$
d\Psi = \frac{\partial \Psi}{\partial E_{IJ}} dE_{IJ} + \sum\nolimits_{\mathrm{a}} \frac{\partial \Psi}{\partial m_{\mathrm{a}}} dm_{\mathrm{a}} + \frac{\partial \Psi}{\partial \theta} d\theta + \frac{\partial \Psi}{\partial \xi} d\xi
$$

where the partial derivatives of Ψ are evaluated at $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ and the partial derivatives of $\widetilde{\Psi}$ are evaluated at the local equilibrium state $\left(E_{IJ}, n_{\alpha}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\alpha \mathrm{a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right)$.

Remarks

- The minimum energy principle is used by Boruvka and Neumann (1977) to obtain the general conditions of equilibrium of a multicomponent multiphase fluid system, including phases, interfaces, common lines and common points.

- Gray and Miller (2014) use the minimization of the total energy of the system, including phases, interfaces, common lines and common points, to obtain the microscale equilibrium conditions.

- Bowen (1976, Sect. 2.9) studied a porous medium made of a gas and an elastic isotropic solid without using volume fractions, and proved that the total free energy is a function of the temperature, skeleton deformation and mass of the gas per unit mixture volume. This free energy might be interpreted as the combination of a free energy depending on the state variables and on the volume fractions with volume fractions depending on the state variables, so that the free energy ultimately depends on the state variables.

- Bowen (1982) considered a porous medium with a number of fluids using volume fractions, and proved that the total free energy is a function of the temperature, solid skeleton deformation, masses of the fluids per unit mixture volume and volume fractions of the fluids. He considered equilibrium states characterized by the vanishing of the partial derivatives of the total free energy with respect to volume fractions (as in our minimization assumption) and assumed that this condition could be inverted to obtain the volume fractions as a function of the temperature, skeleton deformation and masses of the fluids per unit mixture volume.

- Coussy (2004) considered a porous material saturated by one fluid, and deduced a general form of free energy, which depends on the skeleton deformation, the mass of the fluid and the temperature. Subsequently, this free energy is equated to the sum of (1) the free energy of the skeleton, which depends on the skeleton deformation, the volume of the fluid and the temperature, and (2) the free energy of the fluid, which depends on the mass of the fluid, the volume of the fluid and the temperature. From this relation it follows that the volume of the fluid is a function of the skeleton deformation, the mass of the fluid and the temperature. In section 4.4.2 we will show that this relation can be interpreted as the minimization condition that defines local equilibrium states.

3.2 CONSTITUTIVE EQUATIONS

Thermodynamics with internal variables is based on the hypothesis of a local accompanying state (Kestin 1990; Maugin 1999), which is defined by a set of state variables. This formulation will be completed by an additional assumptions concerning dissipative mechanisms. The constitutive equations will then be derived from the free energy function of the porous material and from functions associated to the considered dissipative mechanisms. The constitutive equations obtained are thermodynamically admissible. There is a large number of material models based in this approach (Halphen and Nguyen 1973; Ziegler 1983; Maugin 1999; Houlsby and Puzrin 2006).

3.2.1 State variables

According to the assumptions made, the state variables that define the local accompanying state are

$$\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right) \tag{3.26}$$

where E_{IJ} is the Green-Lagrange strain tensor of the solid skeleton (defined in the reference configuration), m_{a} is the mass of constituent a per unit reference volume, θ is the temperature and ξ is a set of internal variables.

Remark

- In finite strain plasticity (Halphen and Nguyen 1973; Maugin 1999; Lubliner 2008), in which an intermediate local configuration is introduced, the deformation gradient tensor (from the reference to the current configuration) is decomposed as the product of a plastic deformation gradient (from the reference to the intermediate configuration) and an elastic deformation gradient (from the intermediate to the current configuration). In this case, in the state variables (3.26) the Green-Lagrange strain tensor E_{IJ} (defined in the reference configuration) is replaced, by the elastic Green-Lagrange strain tensor (defined in the intermediate configuration).

The total free energy per unit reference volume is assumed to be a function of the state variables

$$\Psi = \Psi\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right) \tag{3.27}$$

which is convex in the variables E_{IJ}, m_{a} and ξ, and concave in θ.

3.2.2 Entropy inequality

Using assumption (3.27), the entropy inequality (3.18) becomes

$$\begin{aligned}\Phi = &\left(S^{IJ} - \frac{\partial\Psi}{\partial E_{IJ}}\right)\left(E_{IJ}\right)^{\cdot} - \left(\mathrm{H} + \frac{\partial\Psi}{\partial\theta}\right)(\theta)^{\cdot} + \sum\nolimits_{\mathrm{a}\neq\mathrm{s}}\left(\mu_{\mathrm{a}} - \frac{\partial\Psi}{\partial m_{\mathrm{a}}}\right)(m_{\mathrm{a}})^{\cdot} - \frac{\partial\Psi}{\partial\xi}(\xi)^{\cdot} \\ &-\sum\nolimits_{\mathrm{a}\neq\mathrm{s}} M_{\mathrm{a}}{}^{I}(F^{i}{}_{I}(a_{\mathrm{a}i} - b_{\mathrm{a}i}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I}) \\ &-Q^{I}\frac{1}{\theta}(\theta)_{,I} \geq 0\end{aligned} \tag{3.28}$$

This inequality has the form $X_{\Sigma} \cdot J_{\Sigma} \geq 0$, with

$$\begin{aligned}X &= \left(\left(E_{IJ}\right)^{\cdot}, (\theta)^{\cdot}, (m_{\mathrm{a}})^{\cdot}, -\frac{\partial\Psi}{\partial\xi}, -\frac{1}{\theta}(\theta)_{,I}, -(F^{i}_{I}(a_{\mathrm{a}i} - b_{\mathrm{a}i}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I}),\right) \\ J &= \left(S^{IJ} - \frac{\partial\Psi}{\partial E_{IJ}}, -\left(\mathrm{H} + \frac{\partial\Psi}{\partial\theta}\right), \mu_{\mathrm{a}} - \frac{\partial\Psi}{\partial m_{\mathrm{a}}}, (\xi)^{\cdot}, Q^{I}, M_{\mathrm{a}}^{I},\right)\end{aligned}$$

where X is the vector of thermodynamic forces and J is the vector of thermodynamic fluxes. Assuming thermodynamic fluxes of the general form $J = J(X; \omega)$, with

$$\omega = (E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$$

where ω is the field argument vector, the entropy inequality can be written in the form

$$X_{\Sigma} \cdot J_{\Sigma}(X, \omega) \geq 0$$

3.2.3 Solution of the entropy inequality

Edelen (1973) proved a decomposition theorem for vector-valued functions, and a corollary that has an immediate application to the general solution of the entropy inequality $X_\Sigma \cdot J_\Sigma(X,\omega) \geq 0$, namely

Theorem 3.2 (Edelen). *Let X stand for an element of an N-dimensional vector space E_N with inner product $A \cdot B$, let ω stand for an element of a p-dimensional vector space E_p, and let $J(X;\omega)$ be a mapping of $E_N \times E_p$ into E_N which is continuous in ω and of class C^1 in X. Then*

$$J_\Sigma(X;\omega) = \frac{\partial \Xi(X;\omega)}{\partial X_\Sigma} + U_\Sigma(X;\omega)$$

$$\sum_\Sigma X_\Sigma U_\Sigma(X;\omega) = 0$$

$$U_\Sigma(X;\omega) = \int_0^1 \tau X_\Gamma \left\{ \frac{\partial J_\Sigma(\tau X;\omega)}{\partial(\tau X_\Gamma)} - \frac{\partial J_\Gamma(\tau X;\omega)}{\partial(X_\Sigma)} \right\} d\tau$$

$$\Xi(X;\omega) = \int_0^1 X_\Sigma J_\Sigma(\tau X;\omega) d\tau$$

where $U(X;\omega)$ is unique, and $\Xi(X;\omega)$ is unique to within an additive function of ω. If $J(X;\omega)$ is of class C^2 in X, then $\Phi(X;\omega)$ is of class C^2 in X, and the symmetry relations

$$\frac{\partial}{\partial X_\Sigma}\{J_\Gamma(X;\omega) - U_\Gamma(X;\omega)\} = \frac{\partial}{\partial X_\Gamma}\{J_\Sigma(X;\omega) - U_\Sigma(X;\omega)\}$$

are satisfied identically in $E_N \times E_p$.

In order to define the vector $J(X;\omega)$, the following approaches have been proposed:

- **Orthogonality principle**. Ziegler proposed to derive the vector of forces $X(J;\omega)$ from a dissipation function $\Phi(J;\omega)$ which is convex in the J by the condition that $X(J;\omega)$ is orthogonal to the surfaces $\Phi(J;\omega) = const.$ (Ziegler 1958, 1983), namely

$$X_\Sigma(J;\omega) = \nu(J;\omega)\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} \qquad \nu(J;\omega) = \frac{\Phi(J;\omega)}{\frac{\partial \Phi(J;\omega)}{\partial J_\Gamma} J_\Gamma}$$

  so that $J = J(X;\omega)$ is defined implicitly by this orthogonality condition.

- **Normal dissipation**. The notion of dissipation was initially introduced by Rayleigh. Moreau studied the hypothesis of the existence of a dissipation potential in the framework of convex analysis (Moreau 1970). Halphen and Nguyen extended this approach and defined the generalised standard materials (Halphen and Nguyen 1973). The hypothesis of normal dissipation assumes the existence of a dissipation potential $\Xi(X;\omega)$ which is convex with respect to the X such that

$$J_\Sigma(X;\omega) = \frac{\partial \Xi(X;\omega)}{\partial X_\Sigma}$$

  If $J_\Sigma = J_\Sigma(X;\omega)$ can be inverted with respect to the X, so that $X_\Sigma = X_\Sigma(J;\omega)$, this is equivalent to the existence of a dissipation potential $\Xi^*(J;\omega)$ which is convex with respect to J such that

$$X_\Sigma(J;\omega) = \frac{\partial \Xi^*(J;\omega)}{\partial J_\Sigma}$$

The functions $\Xi(X;\omega)$ and $\Xi^*(J;\omega)$ are Legendre transforms of each other.

With the help of Theorem 3.2, we can analyze in which cases the orthogonality principle and the normal dissipation hypothesis are equivalent (see also Bataille et al. (1979)).

Corollary 3.3. *Let* $\Phi(J;\omega)$ *be a dissipation function and let* $X_\Sigma(J;\omega)$ *be the vector obtained using the orthogonality principle*

$$X_\Sigma(J;\omega) = \nu(J;\omega)\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} \qquad \nu(J;\omega) = \frac{\Phi(J;\omega)}{\frac{\partial \Phi(J;\omega)}{\partial J_\Gamma}J_\Gamma}$$

Then there exists a dissipation potential $\Xi^*(J;\omega)$ *for the vector* $X_\Sigma(J;\omega)$

$$X_\Sigma(J;\omega) = \frac{\partial \Xi^*(J;\omega)}{\partial J_\Sigma}$$

i.e., the orthogonality principle and the hypothesis of normal dissipation are equivalent, if and only if

$$\frac{\Phi(J;\omega)}{\frac{\partial \Phi(J;\omega)}{\partial J_\Gamma}J_\Gamma}\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} = \int_0^1 \frac{\partial \Phi(\tau J;\omega)}{\partial J_\Sigma}d\tau$$

and in this case the dissipation potential $\Xi^*(J;\omega)$ *is given by*

$$\Xi^*(J;\omega) = \int_0^1 \Phi(\tau J;\omega)\frac{d\tau}{\tau}$$

to within an additive function of ω.

Proof. By Theorem 3.2, the vector $X_\Sigma(J;\omega)$ can be decomposed as follows

$$X_\Sigma(J;\omega) = \frac{\partial \Xi^*(J;\omega)}{\partial J_\Sigma} + U_\Sigma(J;\omega)$$

where

$$\Xi^*(J;\omega) = \int_0^1 J_\Sigma X_\Sigma(\tau J;\omega)d\tau = \int_0^1 J_\Sigma \frac{\Phi(\tau J;\omega)}{\frac{\partial \Phi(\tau J;\omega)}{\partial J_\Gamma}\tau J_\Gamma}\frac{\partial \Phi(\tau J;\omega)}{\partial J_\Sigma}d\tau = \int_0^1 \Phi(\tau J;\omega)\frac{d\tau}{\tau}$$

$$U_\Sigma(J;\omega) = X_\Sigma(J;\omega) - \frac{\partial \Xi(J;\omega)}{\partial J_\Sigma} = \frac{\Phi(J;\omega)}{\frac{\partial \Phi(J;\omega)}{\partial J_\Gamma}J_\Gamma}\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} - \int_0^1 \frac{\partial \Phi(\tau J;\omega)}{\partial J_\Sigma}d\tau$$

$\Xi(J;\omega)$ is unique to within an additive function of ω and $U_\Sigma(J;\omega)$ is unique. Thus

$$X_\Sigma(J;\omega) = \frac{\partial \Xi^*(J;\omega)}{\partial J_\Sigma}$$

if and only if $U_\Sigma(J;\omega) = 0$. ■

Because of the restriction on the dissipation function $\Phi(J;\omega)$ of Corollary 3.3, in general the orthogonality principle and the hypothesis of normal dissipation are not equivalent. However, we have the following result.

Corollary 3.4. *If the dissipation function* $\Phi(J;\omega)$ *is homogeneous of degree* m *in the* J*, so that*

$$\Phi(\lambda J;\omega) = \lambda^m \Phi(J;\omega)$$

then the orthogonality principle and the hypothesis of normal dissipation are equivalent, and the dissipation potential is given by

$$\Xi^*(J;\omega) = \frac{1}{m}\Phi(J;\omega)$$

to within an additive function of ω.

Proof. Derivation of $\Phi(\lambda J;\omega) = \lambda^m \Phi(J;\omega)$ with respect to λ at $\lambda = 1$ and with respect to J_Γ yield

$$\frac{\partial \Phi(J;\omega)}{\partial J_\Gamma} J_\Gamma = m\Phi(J;\omega)$$
$$\frac{\partial \Phi(\lambda J;\omega)}{\partial J_\Sigma} = \lambda^{m-1}\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma}$$

which, when used in the expressions of $\Xi^*(J;\omega)$ and $U_\Sigma(J;\omega)$ of Corollary 3.3, yield

$$\Xi^*(J;\omega) = \int_0^1 \tau^m \Phi(J;\omega)\frac{d\tau}{\tau} = \Phi(J;\omega)\int_0^1 \tau^{m-1} d\tau = \frac{1}{m}\Phi(J;\omega)$$
$$U_\Sigma(J;\omega) = \frac{1}{m}\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} - \int_0^1 \tau^{m-1}\frac{\partial \Phi(J;\omega)}{\partial J_\Sigma} d\tau = \frac{\partial \Phi(J;\omega)}{\partial J_\Sigma}\left(\frac{1}{m} - \int_0^1 \tau^{m-1} d\tau\right) = 0$$

so that, in this case, the orthogonality principle is equivalent to the hypothesis of normal dissipation. ■

Remarks

- The orthogonality principle and the hypothesis of normal dissipation can be extended to the framework of convex analysis, whereby the dissipation function or the dissipation potential function are proper lower semicontinuous convex functions (Moreau 1970; Halphen and Nguyen 1973; Eve et al. 1990; Maugin 1999). This is the case of rate-independent materials, whose dissipation function is homogeneous of degree 1 in the X, so that it is not differentiable at $X = 0$.

- If the dissipation function $\Phi(J;\omega)$ is the sum of dissipation functions $\Phi_i(J_i;\omega)$, where the set of J_i is a partition of J, so that each $\Phi_i(J_i;\omega)$ is associated to a dissipation mechanism, then the orthogonality principle can also be applied separately to each of them.

- If the dissipation potential $\Xi(X;\omega)$ is the sum of dissipation functions $\Xi_i(X_i;\omega)$, where the set of X_i is a partition of X, so that each $\Xi_i(X_i;\omega)$ is associated to a dissipation mechanism, then the hypothesis of normal dissipation can also be applied separately to each of them.

3.2.4 Dissipative mechanisms

In the dissipation inequality (3.28), the dissipation Φ is the sum of the dissipations due to three mechanisms:

- Dissipation Φ_{CS} due to changes in the local equilibrium state (vanishes whenever $\left(E_{IJ}\right)^{\cdot}$, $(\theta)^{\cdot}$, $(m_{\mathrm{a}})^{\cdot}$ and $(\xi)^{\cdot}$ vanish).

$$\Phi_{CS} = \left(S^{IJ} - \frac{\partial\Psi}{\partial E_{IJ}}\right)\left(E_{IJ}\right)^{\cdot} - \left(\mathrm{H} + \frac{\partial\Psi}{\partial\theta}\right)(\theta)^{\cdot} + \sum\nolimits_{\mathrm{a}\neq\mathrm{s}}\left(\mu_{\mathrm{a}} - \frac{\partial\Psi}{\partial m_{\mathrm{a}}}\right)(m_{\mathrm{a}})^{\cdot} - \frac{\partial\Psi}{\partial\xi}(\xi)^{\cdot}$$

- Dissipation Φ_{MF} due to mass flow of constituent a through the solid skeleton (vanishes whenever the fluid mass flow M_{K}^{I} vanishes).

$$\Phi_{MF_{\mathrm{a}}} = -M_{\mathrm{a}}{}^{I}(F^{i}{}_{I}(a_{\mathrm{a}i} - b_{\mathrm{a}i}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I})$$

- Dissipation Φ_{HF} due to heat flow (vanishes whenever the heat flow Q^{I} vanishes).

$$\Phi_{HF} = -Q^{I}\frac{1}{\theta}(\theta)_{,I}$$

We make the following assumptions:

- The three dissipation mechanisms are uncoupled, so that the dissipation due to each of them is non-negative

$$\Phi_{CS} \geq 0 \quad \Phi_{MF\mathrm{a}} \geq 0 \quad \Phi_{HF} \geq 0$$

- In the dissipation due to changes in the local equilibrium state Φ_{CS}, only the terms corresponding to changes in the internal variables ξ produce dissipation, so that the coefficients of $\left(E_{IJ}\right)^{\cdot}$, $(\theta)^{\cdot}$ and $(m_{\mathrm{a}})^{\cdot}$ vanish. This yields the following state laws

$$\begin{aligned} S^{IJ} &= \frac{\partial\Psi}{\partial E_{IJ}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi) \\ \mathrm{H} &= -\frac{\partial\Psi}{\partial\theta}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi) \\ \mu_{\mathrm{a}} &= \frac{\partial\Psi}{\partial m_{\mathrm{a}}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi) \end{aligned} \tag{3.29}$$

  Additionally, it is assumed that $\Phi_{CS} = \Phi_{CS}\left((\xi)^{\cdot}; E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ and $\Phi_{CS}\left(\lambda(\xi)^{\cdot}; E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right) = \lambda\Phi_{CS}\left((\xi)^{\cdot}; E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ for $\lambda \geq 0$, so that the ensuing constitutive equations are rate-independent.

- The mass flow of constituent a with respect to the solid skeleton is a normal dissipative mechanism with a dissipation potential $\Xi_{MF\mathrm{a}}$ of the form

$$\Xi_{MF\mathrm{a}}\left(-\left(F^{i}_{J}(a_{\mathrm{a}i} - b_{\mathrm{a}i}) + (\mu_{\mathrm{a}})_{,J} + \eta_{\mathrm{a}}(\theta)_{,J}\right); E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right) = \\ -\frac{1}{2}\left(-(F^{i}_{I}(a_{\mathrm{a}i} - b_{\mathrm{a}i}) + (\mu_{\mathrm{a}})_{,I} + \eta_{\mathrm{a}}(\theta)_{,I})\right)K^{IJ}_{MF\mathrm{a}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)\left(-(F^{j}_{J}\left(a_{\mathrm{a}j} - b_{\mathrm{a}j}\right) + (\mu_{\mathrm{a}})_{,J} + \eta_{\mathrm{a}}(\theta)_{,J})\right)$$

  where $K^{IJ}_{MF\mathrm{a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$ is a symmetric, positive-definite matrix, so that

$$M_{a}{}^{I} = -K^{IJ}_{MF\mathrm{a}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)\left(-(F^{j}_{J}\left(a_{\mathrm{a}j} - b_{\mathrm{a}j}\right) + (\mu_{\mathrm{a}})_{,J} + \eta_{\mathrm{a}}(\theta)_{,J})\right) \tag{3.30}$$

which is analogous to Darcy's law.

- The heat flow is a normal dissipative mechanism with a dissipation potential Ξ_{HF} of the form

$$\Xi_{HF}\left(\left(-\frac{1}{\theta}(\theta)_{,I}\right);E_{IJ},m_{\mathrm{a}},\theta,\xi\right)=-\frac{1}{2}\left(-\frac{1}{\theta}(\theta)_{,I}\right)K_{HF}^{IJ}(E_{IJ},m_{\mathrm{a}},\theta,\xi)\left(-\frac{1}{\theta}(\theta)_{,J}\right)$$

  where $K_{HF}^{IJ}\left(E_{IJ},m_{\mathrm{a}},\theta,\xi\right)$ is a symmetric, positive-definite matrix, so that

$$Q^{I}=-K_{HF}^{IJ}(E_{IJ},m_{\mathrm{a}},\theta,\xi)\left(-\frac{1}{\theta}(\theta)_{,J}\right) \tag{3.31}$$

  which is analogous to Fourier's law.

It is possible to generalize these assumptions so that couplings between mass flows of constituents and heat flow would be taken into account.

3.3 PRESSURES OF FREE FLUIDS

3.3.1 Free energy of a porous material with free fluids

Free fluids are assumed to behave as if they were outside of the porous material. The free energy of the porous material with free fluids per unit reference volume is assumed to be of the form

$$\tilde{\Psi}\left(E_{IJ}, n_{\alpha}, m_{\alpha \mathrm{a}}, \theta, \xi\right) = \tilde{\Psi}_{\mathrm{sk}}\left(E_{IJ}, n_{\alpha}, m_{\alpha \mathrm{a}}, \theta, \xi\right) + \sum_{\beta} \tilde{\Psi}_{\beta}(n_{\beta}, m_{\beta \mathrm{a}}, \theta) \tag{3.32}$$

where $\tilde{\Psi}_{\mathrm{sk}}\left(E_{IJ}, n_{\alpha}, m_{\alpha \mathrm{a}}, \theta, \xi\right)$ is the free energy of the solid skeleton, interfaces, common lines and common points per unit reference volume (which does not depend on the $m_{\beta \mathrm{a}}$ of the free fluid phases), $\tilde{\Psi}_{\beta}(n_{\beta}, m_{\beta \mathrm{a}}, \theta)$ is the free energy of the fluid phase β per unit reference volume (which only depends on its own n_{β}, $m_{\beta \mathrm{a}}$ and θ) and β ranges over all the free fluid phases.

The state equations of the free fluid β follow from the free energy $\tilde{\Psi}_{\beta}(n_{\beta}, m_{\beta \mathrm{a}}, \theta_{\beta})$ (Callen 1985)

$$\begin{aligned} p_{\beta} &= -\frac{\partial \tilde{\Psi}_{\beta}}{\partial n_{\beta}}(n_{\beta}, m_{\beta \mathrm{a}}, \theta_{\beta}) \\ \mu_{\beta \mathrm{a}} &= \frac{\partial \tilde{\Psi}_{\beta}}{\partial m_{\beta \mathrm{a}}}(n_{\beta}, m_{\beta \mathrm{a}}, \theta_{\beta}) \\ \eta_{\beta} &= -\frac{\partial \tilde{\Psi}_{\beta}}{\partial \theta_{\beta}}(n_{\beta}, m_{\beta \mathrm{a}}, \theta_{\beta}) \end{aligned} \tag{3.33}$$

where p_{β} is the pressure, $\mu_{\beta \mathrm{a}}$ is the chemical potential of constituent a and η_{β} is the entropy per unit reference volume. Moreover, from these equations follow the relations $n_{\beta} = n_{\beta}(p_{\beta}, \mu_{\beta \mathrm{a}}, \theta_{\beta})$, $m_{\beta \mathrm{a}} = m_{\beta \mathrm{a}}(p_{\beta}, \mu_{\beta \mathrm{a}}, \theta_{\beta})$ and $\eta_{\beta} = \eta_{\beta}(p_{\beta}, \mu_{\beta \mathrm{a}}, \theta_{\beta})$. Use of these relations in the Gibbs-Duhem relation (Callen 1985)

$$-n_{\beta} dp_{\beta} + \sum_{\mathrm{a}} m_{\beta \mathrm{a}} d\mu_{\beta \mathrm{a}} + \eta_{\beta} d\theta_{\beta} = 0 \tag{3.34}$$

and integration of the resulting differential equation yields a relation between p_{β}, $\mu_{\beta \mathrm{a}}$ and θ_{β}, so that

$$p_{\beta} = p_{\beta}(\mu_{\beta \mathrm{a}}, \theta_{\beta}) \tag{3.35}$$

This result allows to determine the pressure of the fluid phase β from the chemical potentials of its constituents and the temperature.

3.3.2 Pressures of free fluids within a porous material

From (3.32) and $(3.33)_2$ it follows

$$\frac{\partial\widetilde{\Psi}}{\partial m_{\beta\mathrm{b}}}\left(E_{IJ}, n_\alpha, m_{\alpha\mathrm{a}}, \theta, \xi\right) = \frac{\partial\widetilde{\Psi}_\beta}{\partial m_{\beta\mathrm{b}}}\left(n_\beta, m_{\beta\mathrm{a}}, \theta\right) = \mu_{\beta\mathrm{b}}\left(n_\beta, m_{\beta\mathrm{a}}, \theta\right)$$

where $\theta_\beta = \theta$ (the common temperature) has been used. Further, by Lemma 3.1 and the constitutive equation $(3.29)_3$, it follows that at local equilibrium states

$$\frac{\partial\widetilde{\Psi}}{\partial m_{\alpha\mathrm{b}}}\left(E_{IJ}, n_\alpha\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right), m_{\alpha\mathrm{a}}\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right), \theta, \xi\right) = \frac{\partial\Psi}{\partial m_\mathrm{b}}\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right) = \mu_\mathrm{b}\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right)$$

Combination of the two last results yields that at local equilibrium states the chemical potentials $\mu_{\beta\mathrm{b}}$ of the β free fluid and the chemical potentials μ_b of the porous material coincide

$$\mu_{\beta\mathrm{b}}\left(n_\beta\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right), m_{\beta\mathrm{a}}\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right), \theta\right) = \mu_\mathrm{b}\left(E_{IJ}, m_\mathrm{a}, \theta, \xi\right)$$

Using $\mu_{\beta\mathrm{a}} = \mu_\mathrm{a}$ and $\theta_\beta = \theta$ in (3.35) yields the pressure p_β of the β free fluid within the porous material as a function of the chemical potentials μ_a and the temperature θ of the porous material

$$p_\beta = p_\beta(\mu_\mathrm{a}, \theta) \tag{3.36}$$

Note that the pressure p_β of the β free fluid within the porous material is defined provided that there is β free fluid in the porous material (i.e., $n_\beta > 0$). In contrast, the chemical potential μ_a of constituent a in the porous material is defined provided that there is constituent a in the porous material (i.e., $m_\mathrm{a} > 0$).

Remarks

- As already mentioned, averaging of the microscale distribution of an intensive variable requires a weighting function, such that for uniform distributions averaging yields the uniform value of the distribution. At the considered local equilibrium (neglecting gravity forces), a fluid subjected to interaction forces has a non-uniform distribution of pressure but has uniform distributions of chemical potentials. Thus, whereas the definition of a macroscale pressure is questionable, the definition of a macroscale chemical potential is natural.

- In unsaturated soil mechanics, matric suction is defined as the gas pressure minus the liquid pressure. This definition requires that the gas pressure and the liquid pressure can be defined at the macroscale. For fine-grained soils, such as clays, in which the area of the particle surfaces per unit volume is very large, strong short-range interaction forces bind liquid water to the soil skeleton. For low water content, there is no free liquid water, so that the liquid water pressure cannot be defined. In contrast, the chemical potential of water can be defined.

3.3.3 Effective stresses

If there is only one fluid phase φ whose behaviour is assumed to be the same as if it were outside of the porous material and interfaces can be neglected, then the free energy of the porous material per unit reference volume is (cf. (3.32))

$$\tilde{\Psi}\left(E_{IJ}, n_{\varphi}, m_{\sigma\mathrm{a}}, m_{\varphi\mathrm{a}}, \theta, \xi\right) = \tilde{\Psi}_{\mathrm{sk}}\left(E_{IJ}, n_{\sigma}, m_{\sigma\mathrm{a}}, \theta, \xi\right) + \tilde{\Psi}_{\varphi}(n_{\varphi}, m_{\varphi\mathrm{a}}, \theta) \tag{3.37}$$

where $n_{\sigma} = J - n_{\varphi}$. If the solid skeleton is incompressible and there is no mass exchange between the solid skeleton and the fluid, then n_{σ} and $m_{\sigma\mathrm{a}}$ are constant $n_{\sigma} = (n_{\sigma})_0$ and $m_{\sigma\mathrm{a}} = (m_{\sigma\mathrm{a}})_0$. Since

$$J = \left(\det\left(2E_{IJ} + \delta_{IJ}\right)\right)^{1/2} = J(E_{IJ})$$

it follows that $n_{\varphi} = J - n_{\sigma} = J(E_{IJ}) - (n_{\sigma})_0 = n_{\varphi}(E_{IJ})$. As a result, the total free energy of the porous material per unit reference volume becomes

$$\Psi\left(E_{IJ}, m_{\varphi a}, \theta, \xi\right) = \Psi_{\mathrm{sk}}\left(E_{IJ}, \theta, \xi\right) + \Psi_{\varphi}\left(n_{\varphi}\left(E_{IJ}\right), m_{\varphi\mathrm{a}}, \theta\right) \tag{3.38}$$

where we have set

$$\begin{aligned} \Psi\left(E_{IJ}, m_{\varphi a}, \theta, \xi\right) &= \tilde{\Psi}(E_{IJ}, n_{\varphi}(E_{IJ}), (m_{\sigma\mathrm{a}})_0, m_{\varphi\mathrm{a}}, \theta, \xi) \\ \Psi_{\mathrm{sk}}\left(E_{IJ}, \theta, \xi\right) &= \tilde{\Psi}_{\mathrm{sk}}\left(E_{IJ}, (n_{\sigma})_0, (m_{\sigma\mathrm{a}})_0, \theta, \xi\right) \end{aligned}$$

Derivation of (3.38) with respect to E_{IJ} yields

$$\frac{\partial \Psi}{\partial E_{IJ}}\left(E_{IJ}, m_{\varphi a}, \theta, \xi\right) = \frac{\partial \Psi_{\mathrm{sk}}}{\partial E_{IJ}}\left(E_{IJ}, \theta, \xi\right) + \frac{\partial \Psi_{\varphi}}{\partial n_{\varphi}}\left(n_{\varphi}\left(E_{IJ}\right), m_{\varphi a}, \theta\right)\frac{\partial n_{\varphi}}{\partial E_{IJ}}(E_{IJ})$$

and, using the relations

$$\begin{aligned} \frac{\partial \Psi_{\varphi}}{\partial n_{\varphi}}\left(n_{\varphi}, m_{\varphi a}, \theta\right) &= -p_{\varphi}\left(n_{\varphi}, m_{\varphi a}, \theta\right) \\ \frac{\partial J}{\partial E_{IJ}} &= J\delta^{ij}(F^{-1})^{I}_{\ i}(F^{-1})^{J}_{\ j} \end{aligned}$$

it follows

$$\frac{\partial \Psi_{\mathrm{sk}}}{\partial E_{IJ}}\left(E_{IJ}, \theta, \xi\right) = \frac{\partial \Psi}{\partial E_{IJ}}\left(E_{IJ}, m_{\varphi a}, \theta, \xi\right) + p_{\varphi}\left(n_{\varphi}\left(E_{IJ}\right), m_{\varphi a}, \theta\right)J(E_{IJ})\delta^{ij}(F^{-1})^{I}_{\ i}(F^{-1})^{J}_{\ j} \tag{3.39}$$

where $p_{\varphi}J\delta^{ij}(F^{-1})^{I}_{\ i}(F^{-1})^{J}_{\ j}$ is the 2nd Piola-Kirchhoff tensor that corresponds to the Cauchy tensor $p_{\varphi}\delta^{ij}$. If we identify $\partial\Psi/\partial E_{IJ}$ with the 2nd Piola-Kirchhoff stress tensor that corresponds to the Cauchy stress tensor of the porous material σ^{ij}, then the tensor $\partial\Psi_{\mathrm{sk}}/\partial E_{IJ}$ is the 2nd Piola-Kirchhoff stress tensor that corresponds to Terzaghi's effective Cauchy stress tensor $\sigma^{ij} + p_{\varphi}\delta^{ij}$ (Coussy 2004, p. 53).

More generally, if n_{σ} depends on E_{IJ}, then $n_{\varphi}\left(E_{IJ}\right) = J\left(E_{IJ}\right) - n_{\sigma}\left(E_{IJ}\right)$ and it follows

$$\frac{\partial \Psi_{\mathrm{sk}}}{\partial E_{IJ}}\left(E_{IJ}, \theta, \xi\right) = \frac{\partial \Psi}{\partial E_{IJ}}\left(E_{IJ}, m_{\varphi a}, \theta, \xi\right) \tag{3.40}$$

$$+p^{\varphi}\big(n^{\varphi}(E_{IJ}), m^{\varphi}, \theta\big) J(E_{IJ}) (F^{-1})^{I}{}_{i} \left(\delta^{ij} - \frac{1}{J(E_{IJ})} F^{i}{}_{K} \frac{\partial n_{\sigma}}{\partial E_{KL}} (E_{IJ}) F^{j}{}_{L} \right) (F^{-1})^{J}{}_{j}$$

If we identify $\partial\Psi/\partial E_{IJ}$ with the 2nd Piola-Kirchhoff stress tensor that corresponds to the Cauchy stress tensor of the porous material σ^{ij}, then the tensor $\partial\Psi_{\mathrm{sk}}/\partial E_{IJ}$ is the 2nd Piola-Kirchhoff stress tensor that corresponds to a generalization of Terzaghi's effective Cauchy stress tensor, of the form $\sigma^{ij} + p_{\varphi}\big(\delta^{ij} + m^{ij}\big)$ (In Coussy 2004, for non-linear thermoporoelasticty with infinitesimal transformations, in Eq. (4.13a) $d\sigma_{ij} = C_{ijkl} d\varepsilon_{kl} - b_{ij} dp - C_{ijkl} \alpha_{kl} dT$, the tensor $b_{ij} = -\partial^2 G_s / \partial\varepsilon_{ij}\partial p$ is a tangent thermoporoelastic property denoted Biot's tangent tensor. In the case of linear isotropic thermoporoelasticity $b_{ij} = b\delta_{ij}$ is constant and in Eq. (4.26) Biot's effective stress is defined by $\sigma''_{ij} = \sigma_{ij} + bp\delta_{ij}$).

Note that in expressions (3.39) and (3.40), the stress tensor $\partial\Psi_{\mathrm{sk}}/\partial E_{IJ}$ depends only on $\big(E_{IJ}, \theta, \xi\big)$, so that (assuming invertibility) $E_{IJ} = E_{IJ}(\partial\Psi_{\mathrm{sk}}/\partial E_{IJ}, \theta, \xi)$, which justifies to qualify the stress tensor $\partial\Psi_{\mathrm{sk}}/\partial E_{IJ}$ as effective. The previous developments demonstrate that the existence of an effective stress tensor of a porous material with only one free fluid is a consequence of the elimination of n_{σ} as an independent variable.

4 UNSATURATED SOILS

4.1 PRELIMINARIES

4.1.1 Basic assumptions

The thermodynamic framework for porous materials will be applied to unsaturated soils. We will consider the following restrictions

- **Infinitesimal transformations**. The current configuration is approximated by the reference configuration, the Green-Lagrange strain tensor E_{IJ} is approximated by the linearized strain tensor ε_{ij}, the 2nd. Piola-Kirchhoff stress tensor S^{IJ} is approximated by the Cauchy stress tensor σ^{ij}.

- **Constituents**. We assume that in the porous material there are three species: solid mineral, water (liquid, vapor) and air (gas or dissolved). The gas phase is a mixture of water vapor and gas, which behave as ideal gases and as if it were outside the porous material. The liquid phase is a mixture of water and dissolved air, but the effect of the dissolved gas in the mechanical behavior of the porous material will be neglected. Liquid water can be subject to interaction forces with the solid skeleton (vicinal water) or can be free from these interactions (free water). The soil skeleton is made of the solid mineral and the vicinal water.

- **Environmental conditions**. We assume that the temperature θ and the free gas pressure p_G are constant, corresponding to atmospheric conditions. Since at ambient atmospheric conditions the saturation water vapor pressure is a small fraction of the atmospheric pressure (for instance, at $p_G = 1\,\text{atm} = 1013\,\text{mbar}$ as $\theta = 10 - 40°\text{C}$ the saturation water vapor pressure is $p_{Gw} = 12.271 - 73.75\,\text{mbar}$), it follows that $p_G = p_{Ga} + p_{Gw} \cong p_{Ga}$. Since $\mu_{Ga} = \mu_{Ga}(p_{Ga}, \theta)$, it follows that if θ and μ_{Ga} are constant, then μ_{Ga} is constant. Thus we will assume that both θ and μ_a are constant.

- **Material behavior**. The solid skeleton is assumed to behave as a hardening elastoplastic material, with an additive decomposition of the small strains tensor ε_{ij} as the sum of an elastic component ε_{ij}^e and a plastic component ε_{ij}^p. The variation water mass per unit reference volume m_w with respect to water mass in the reference configuration m_{w0} decomposes as the sum of an elastic water content m_w^e and a plastic water component m_w^p. Consequently

$$\begin{aligned} \varepsilon_{ij} &= \varepsilon_{ij}^e + \varepsilon_{ij}^p \\ m_w &= m_{w0} + m_w^e + m_w^p \end{aligned}$$

- **Legendre transform of the free energy**. The Legendre transform of the free energy per unit reference volume $\Psi(\varepsilon_{ij}, m_s, m_w, m_a, \theta, \varepsilon_{ij}^p, m_w^p)$ with respect to the mass of air m_a is a potential $\Pi(\varepsilon_{ij}, m_s, m_w, \mu_a, \theta, \varepsilon_{ij}^p, m_w^p)$, which is convenient for conditions with $m_s = m_{s0}$ (the mass of solid per unit reference volume remains constant) $\mu_a = \mu_{a0}$ and $\theta = \theta_0$. For simplicity, in what follows the potential $\Pi(\varepsilon_{ij}, m_{s0}, m_w, \mu_{\ a0}\ , \theta_0, \varepsilon_{ij}^p, m_w^p)$ will be denoted by $\Psi\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ (an abuse of the already used function symbol Ψ) and will be referred to as the free energy (an abuse of the already used denomination "free energy").

4.1.2 Brief summary of convex analysis results

We give a brief summary of convex analysis results, which has been adapted from Eve et al. (1990). A thorough exposition of convex analysis with proofs of the quoted results can be found in Rockafellar (1970).

4.1.2.1 *Some definitions used in convex analysis*

We denote by E a finite-dimensional vector space and by E^* the dual vector space of E. For $x^* \in E^*$ and $x \in E$, the action of x^* on x is denoted by $x^* \cdot x$.

Let S be a subset of E. The interior and boundary of S are denoted by $\operatorname{int} S$ and $\operatorname{bd} S$, respectively. S is convex if, for any $x, y \in S$ and $0 < \lambda < 1$, $\lambda x + (1-\lambda)y \in S$. The normal cone to a convex set at x, denoted by $N_S(x)$, is defined by

$$N_S(x) = \{x^* \in E^*: x^* \cdot (y - x) \leq 0 \text{ for all } y \in S\}$$

Note that if $x \in \operatorname{int} S$ then $N_S(x) = \{0\}$, and if $x \in \operatorname{bd} S$ then $N_S(x)$ is the cone of outer normals at x.

Let f be a function whose domain is E and whose values are real or $\pm\infty$. The effective domain of f is defined by

$$\operatorname{dom} f = \{x \in E: f(x) < \infty\}$$

The function f is convex if

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y) \quad \text{for all} \quad x, y \in E, 0 < \lambda < 1$$

positively homogeneous if

$$f(\lambda x) = \lambda f(x) \quad \text{for all } x \in E, 0 < \lambda \in \mathbb{R}$$

and lower semicontinuous (lsc) if

$$\liminf_{n\to\infty} f(x_n) \geq f(x)$$

for any sequence $\{x_n\}$ converging to x.

A convex function is proper if $f(x) < +\infty$ for at least one x and $f(x) > -\infty$ for every x.

4.1.2.2 *Legendre-Fenchel transforms and subdifferentials*

Let f be a proper lsc convex function on E. The Legendre-Fenchel conjugate function of f is the function on E^* defined by

$$f^*(x^*) = \sup\{x^* \cdot x - f(x), x \in E\}$$

If f is proper, convex and lsc then so is f^*, and

$$(f^*)^* = f$$

Given a convex function f on E, for any $x \in E$ the subdifferential of f at x is the subset of E^* defined by

$$\partial f(x) = \{x^* \in E^*: f(y) \geq f(x) + x^* \cdot (y - x), \forall y \in E\}$$

Note that $\partial f(x) = \emptyset$ if $x \notin \operatorname{dom} f$. If f is differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$.

A proper lsc convex function f and its dual f^* satisfy Fenchel's inequality

$$x^* \cdot x \leq f(x) + f^*(x^*) \quad \forall x \in E, \forall x^* \in E^*$$

Moreover, the following equivalences hold

$$x^* \cdot x = f(x) + f^*(x^*) \quad \Leftrightarrow \quad x^* \in \partial f(x) \quad \Leftrightarrow \quad x \in \partial f^*(x^*)$$

4.1.2.3 Some functions used in convex analysis

For any set $S \subset E$, the indicator function I_S of S is defined on E by

$$I_S(0) = \begin{cases} 0 & x \in S \\ +\infty & x \notin S \end{cases}$$

and the support function σ_S of S is defined on E^* by

$$\sigma_S(x^*) = \sup\{x^* \cdot x: x \in S\}$$

A function f on E is a gauge if $f(x) \geq 0$ for all $x \in E$, $f(0) = 0$ and is convex, positively homogeneous and lsc.

4.1.2.4 Some results from convex analysis

Lemma 4.1. Let f be a gauge on E and define the closed convex set $K \subset E^*$ by

$$K = \{x^* \in E^*: x^* \cdot x \leq f(x), \forall x \in E\}$$

Then (a) f is the support function of K, $f = \sigma_K$; (b) the function f^* conjugate to f is the indicator function of K, $f^* = I_K$; (c) the set K is the subdifferential of f at the origin $K = \partial f(0)$; (d) $x^* \in \partial f(x) \Leftrightarrow x \in \partial f^*(x^*) = N_K(x^*)$, where $N_K(x^*)$ is the normal cone to K at x^*.

Lemma 4.2. Let g be nonnegative and convex, with $g(0) = 0$ and x a point in the interior of $\operatorname{dom} g$ such that $g(x) > 0$. Set $C = \{z: g(z) \leq g(x)\}$. Then $x^* \in N_C(x)$ if and only if there exists $\lambda \geq 0$ such that $x^* \in \lambda \partial g(x)$.

4.2 ELASTOPLASTIC FRAMEWORK

Throughout this section reference is made to works on convex analysis (Rockafellar 1970) and on application to thermodynamics with internal variables (Halphen and Nguyen 1973; Ziegler 1983; Maugin 1999; Eve et al. 1990; Houlsby and Puzrin 2006).

4.2.1 Free energy function

We assume that the free energy per unit reference volume is a smooth convex function

$$\Psi = \Psi(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p) \tag{4.1}$$

We define the elastic strain tensor ε_{ij}^e and the elastic water content $m_w^e$by

$$\begin{aligned} \varepsilon_{ij}^e &= \varepsilon_{ij} - \varepsilon_{ij}^p \\ m_w^e &= (m_w - m_{w0}) - m_w^p \end{aligned} \tag{4.2}$$

where m_{w0} is the water mass per unit reference volume in the reference configuration. By the state equations, the stress tensor σ_{ij} and the water chemical potential μ_w are given by

$$\begin{aligned} \sigma_{ij} &= \frac{\partial \Psi}{\partial \varepsilon_{ij}}(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p) \\ \mu_w &= \frac{\partial \Psi}{\partial m_w}(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p) \end{aligned} \tag{4.3}$$

Note that, since Ψ is a smooth convex function in ε_{ij} and m_w, relations (4.3) can be solved for ε_{ij} and m_w, so that

$$\begin{aligned} \varepsilon_{ij} &= \varepsilon_{ij}(\sigma_{ij}, \mu_w, \varepsilon_{ij}^p, m_w^p) \\ m_w &= m_w(\sigma_{ij}, \mu_w, \varepsilon_{ij}^p, m_w^p) \end{aligned} \tag{4.4}$$

We define the generalized stress tensor $\bar{\sigma}_{ij}$ and the generalized water chemical potential $\bar{\mu}_w$ by

$$\begin{aligned} \bar{\sigma}_{ij} &= -\frac{\partial \Psi}{\partial \varepsilon_{ij}^p}(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p) \\ \bar{\mu}_w &= -\frac{\partial \Psi}{\partial m_w^p}(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p) \end{aligned} \tag{4.5}$$

4.2.2 Dissipation function

We assume a dissipation function of the form $\Phi = \Phi\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}, \varepsilon_{ij}^{e}, \varepsilon_{ij}^{p}, m_w^e, m_w^p\right)$. Considering $\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right)$ as variables and $\left(\varepsilon_{ij}^{e}, \varepsilon_{ij}^{p}, m_w^e, m_w^p\right)$ as parameters, the dissipation function becomes a function $\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ on the space $E = E_{(\varepsilon^p)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}$, where $E_{(\varepsilon^p)^{\cdot}}$ is the space of plastic strain rates $\left(\varepsilon_{ij}^{p}\right)^{\cdot}$ and $E_{\left(m_w^p\right)^{\cdot}}$ is the space of plastic water mass rates $\left(m_w^p\right)^{\cdot}$. We will assume that this function on $E = E_{(\varepsilon^p)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}$ is convex, positively homogeneous, lower semicontinuous and satisfies

$$\begin{aligned} &\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) \geq 0 \;\text{ for all }\; \left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) \in E_{(\varepsilon^p)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}} \\ &\Phi\left((0,0); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) = 0 \end{aligned} \tag{4.6}$$

Thus, $\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ is a gauge on $E = E_{(\varepsilon^p)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}$.

We define the closed convex subset $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ of the space $E^* = E_{\hat{\sigma}} \times E_{\hat{\mu}_w}$, where $E_{\hat{\sigma}} = \left(E_{(\varepsilon^p)^{\cdot}}\right)^*$ is the space of generalized dissipative stresses $\hat{\sigma}_{ij}$ and $E_{\hat{\mu}_w} = \left(E_{\left(m_w^p\right)^{\cdot}}\right)^*$ is the space of generalized dissipative water chemical potentials $\hat{\mu}_w$, by

$$\begin{aligned} \hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) = \Big\{&\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in E_{\hat{\sigma}} \times E_{\hat{\mu}_w} : \hat{\sigma}_{ij} \cdot \left(\varepsilon_{ij}^{p}\right)^{\cdot} + \hat{\mu}_w \cdot \left(m_w^p\right)^{\cdot} \\ &\leq \Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right), \forall \left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) \in E_{(\varepsilon^p)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}\Big\} \end{aligned} \tag{4.7}$$

Then, by Lemma 4.1, it follows

$\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ is the support function of $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$

$\Phi^*\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ is the indicator function of $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$

$$\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) = \partial\Phi\left((0,0); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) \tag{4.8}$$

$$\begin{aligned} &\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \partial\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) \Leftrightarrow \\ &\qquad\qquad \left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) \in N_{\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)}\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right)\right) \end{aligned}$$

Further, for any $\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \partial\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$, we have the relation

$$\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right) = \hat{\sigma}_{ij} \cdot \left(\varepsilon_{ij}^{p}\right)^{\cdot} + \hat{\mu}_w \cdot \left(m_w^p\right)^{\cdot} \tag{4.9}$$

In particular, if $\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^{p}, m_w^p\right)$ is differentiable at $\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right)$, then the subdifferential contains only the gradient, so that

$$\begin{aligned}\Phi\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot},\left(m_{w}^{p}\right)^{\cdot}\right);\varepsilon_{ij},m_{w},\varepsilon_{ij}^{p},m_{w}^{p}\right)=&\frac{\partial\Phi}{\partial\left(\varepsilon_{ij}^{p}\right)^{\cdot}}\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot},\left(m_{w}^{p}\right)^{\cdot}\right);\varepsilon_{ij},m_{w},\varepsilon_{ij}^{p},m_{w}^{p}\right)\cdot\left(\varepsilon_{ij}^{p}\right)^{\cdot}\\&+\frac{\partial\Phi}{\partial\left(m_{w}^{p}\right)^{\cdot}}\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot},\left(m_{w}^{p}\right)^{\cdot}\right);\varepsilon_{ij},m_{w},\varepsilon_{ij}^{p},m_{w}^{p}\right)\cdot\left(m_{w}^{p}\right)^{\cdot}\end{aligned}\tag{4.10}$$

in agreement with Euler's theorem, and

$$\begin{aligned}\hat{\sigma}_{ij}&=\frac{\partial\Phi}{\partial\left(\varepsilon_{ij}^{p}\right)^{\cdot}}\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot},\left(m_{w}^{p}\right)^{\cdot}\right);\varepsilon_{ij},m_{w},\varepsilon_{ij}^{p},m_{w}^{p}\right)\\\hat{\mu}_{w}&=\frac{\partial\Phi}{\partial\left(m_{w}^{p}\right)^{\cdot}}\left(\left(\left(\varepsilon_{ij}^{p}\right)^{\cdot},\left(m_{w}^{p}\right)^{\cdot}\right);\varepsilon_{ij},m_{w},\varepsilon_{ij}^{p},m_{w}^{p}\right)\end{aligned}\tag{4.11}$$

4.2.3 Ziegler's orthogonality principle

We will apply Ziegler's orthogonality principle (Ziegler 1983), with the free energy function $\Psi = \Psi(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p)$ and the dissipation function $\Phi = \Phi\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}; \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$, namely

$$\left(-\frac{\partial\Psi}{\partial\varepsilon_{ij}^p}, -\frac{\partial\Psi}{\partial m_w^p}\right)\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \in \partial\Phi\left(\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \tag{4.12}$$

which, by Lemma 4.1, is equivalent to

$$\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) \in N_{\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)}\left(\left(-\frac{\partial\Psi}{\partial\varepsilon_{ij}^p}, -\frac{\partial\Psi}{\partial m_w^p}\right)\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\right) \tag{4.13}$$

Note that, if $\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \operatorname{int}\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ then $N_{\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)}\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) = \{(0,0)\}$ and if $\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \operatorname{bd}\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ then $N_{\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)}\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \neq \{(0,0)\}$.

Following Eve et al. (1990), given the closed convex subset $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ of $E_{\hat{\sigma}} \times E_{\hat{\mu}_w}$, we define a function on $E_{\hat{\sigma}} \times E_{\hat{\mu}_w}$, called the canonical yield function, by

$$\hat{f}\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = \inf\left\{\mu > 0 : \left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right)\right) \in \mu\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\right\} \tag{4.14}$$

where $\mu\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = \left\{\mu\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) : \left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\right\}$. From its definition, it follows that $\hat{f}\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ is a gauge on $E_{\hat{\sigma}} \times E_{\hat{\mu}_w}$ and its level set at 1 is equal to $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$, i.e.

$$\left\{\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) : \hat{f}\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \leq 1\right\} = \hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$$

Consequently, by Lemma 4.2, relation (4.13) is equivalent to

$$\begin{aligned}
&\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \operatorname{int}\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \Rightarrow \left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) = (0, 0) \\
&\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \operatorname{bd}\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \Rightarrow \left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) = \lambda\partial\hat{f}\left(\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)
\end{aligned} \tag{4.15}$$

where $\lambda \geq 0$.

Remark

- Eve et al. (1990) note that the canonical yield function and the dissipation function are polars of each other. The canonical yield function minus 1 is 0 on the boundary of the elastic region, as is usually assumed in the theory of plasticity.

We complete the formulation with the consistency condition, which states that at $\left(\hat{\sigma}_{ij}, \hat{\mu}_w\right) \in \operatorname{bd}\left(\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\right)$

$$\lambda(\hat{f})^{\cdot} = 0 \tag{4.16}$$

where $(\hat{f})^{\cdot}$ is the change in $\hat{f}\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ associated with the change in $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ accompanying $\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right)$, so that either $\lambda > 0$ and$(\hat{f})^{\cdot} = 0$ or $\lambda = 0$ and $(\hat{f})^{\cdot} < 0$. Note that $(\hat{f})^{\cdot} > 0$ is excluded because $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ must remain in $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$.

We transform the yield function $\hat{f}\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ on $E_{\hat{\sigma}} \times E_{\hat{\mu}_w}$, where $E_{\hat{\sigma}}$ is the space of generalized dissipative stresses and $E_{\hat{\mu}_w}$ is the space of generalized dissipative water chemical potentials $\hat{\mu}_w$, to the yield function f on $E_\sigma \times E_{\mu_w}$, were E_σ is the space of stresses and E_{μ_w} is the space of water chemical potentials, as follows

$$\begin{aligned} f\left((\sigma_{ij}, \mu_w); \varepsilon_{ij}^p, m_w^p\right) = \hat{f}\Big(\Big(&\bar{\sigma}_{ij}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right), \bar{\mu}_w\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\Big); \\ &\varepsilon_{ij}\left(\sigma_{ij}, \mu_w, \varepsilon_{ij}^p, m_w^p\right), m_w\left(\sigma_{ij}, \mu_w, \varepsilon_{ij}^p, m_w^p\right), \varepsilon_{ij}^p, m_w^p \Big) \end{aligned} \tag{4.17}$$

where, by Ziegler's orthogonality principle (4.12), we have set $(\hat{\sigma}_{ij}, \hat{\mu}_w) = (\bar{\sigma}_{ij}, \bar{\mu}_w)$, and we have used relations (4.4).

Note that the yield function f is defined on $E_\sigma \times E_{\mu_w}$ and depends parametrically on $\left(\varepsilon_{ij}^p, m_w^p\right)$ so that, in general, the boundary of the yield surface depends on stresses σ_{ij}, water chemical potentials μ_w and parametrically on $\left(\varepsilon_{ij}^p, m_w^p\right)$. In this respect, it should be mentioned that the LC (for loading-collapse) curve of the BBM model (Alonso et al. 1990) depends on the net pressure, suction and parametrically on the plastic volumetric strain, a feature that allows to model both swelling upon wetting at low stresses and collapse upon wetting at high stresses, as is experimentally observed.

Remark

- As explained, for instance in Ziegler (1983), Collins and Houlsby (1997) and Houlsby and Puzrin (2006), whereas the elastic region in the space of dissipative stresses is convex and the plastic flow direction is normal to its surface, in the space of true stresses none of these features are in general preserved. This provides more modeling flexibility (Collins and Kelly 2002; Collins and Hilder 2002).

4.2.4 Multisurface plasticity

We will use the framework of multisurface plasticity and we will follow Simo and Hughes (1998).

We will assume that the convex elastic region is defined by

$$\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = \left\{(\hat{\sigma}_{ij}, \hat{\mu}_w): \hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \leq 0 \text{ for all } \alpha \in \{1, \dots m\}\right\} \tag{4.18}$$

where the functions $\hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ are smooth, and define independent constraints $\hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = 0$ at the boundary of the elastic region. Consequently, the boundary of the elastic region is given by

$$\begin{aligned}\text{bd } &\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) \\ &= \left\{(\hat{\sigma}_{ij}, \hat{\mu}_w): \hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = 0 \text{ for some } \alpha \in \{1, \dots m\}\right\}\end{aligned} \tag{4.19}$$

so that it is piecewise smooth.

At a point $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ of the boundary of the elastic region $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ any element of the normal cone $N_{\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)}$ can be expressed as a linear combination of the gradients of the functions $\hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ with coefficients $\lambda^\alpha \geq 0$, so that expression (4.13) becomes

$$\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) = \sum_{\alpha=1}^{m} \lambda^\alpha \left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}}, \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w}\right)\left(\left(-\frac{\partial \Psi}{\partial \varepsilon_{ij}^p}, -\frac{\partial \Psi}{\partial m_w^p}\right); \left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)\right) \tag{4.20}$$

The consistency condition will be applied to each of the constrains, so that at $(\hat{\sigma}_{ij}, \hat{\mu}_w) \in$ bd $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ such that $\hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = 0$ the consistency condition reads

$$\lambda^\alpha \left(\hat{f}_\alpha\right)^{\cdot} = 0 \tag{4.21}$$

where $\left(\hat{f}_\alpha\right)^{\cdot}$ is the change in $\hat{f}_\alpha\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$ associated with the change in $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ accompanying $\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right)$, so that, either $\lambda^\alpha > 0$ and $\left(\hat{f}_\alpha\right)^{\cdot} = 0$ or $\lambda^\alpha = 0$ and $\left(\hat{f}_\alpha\right)^{\cdot} < 0$. Note that $\left(\hat{f}_\alpha\right)^{\cdot} > 0$ is excluded because $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ must remain in $\hat{C}\left(\varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right)$.

For $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ on the boundary of the elastic region, we define the following sets of indices

$$\begin{aligned}\mathbb{J}_{\text{adm}} &= \left\{\beta \in \{1, \dots, m\}: \hat{f}_\beta\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = 0\right\} \\ \mathbb{J}_{\text{act}} &= \left\{\beta \in \mathbb{J}_{\text{adm}}: \left(\hat{f}_\beta\right)^{\cdot}\left((\hat{\sigma}_{ij}, \hat{\mu}_w); \varepsilon_{ij}, m_w, \varepsilon_{ij}^p, m_w^p\right) = 0\right\}\end{aligned} \tag{4.22}$$

Note that if $\alpha \in \mathbb{J}_{\text{adm}}$, then $\left(\hat{f}_\alpha\right)^{\cdot} \leq 0$ because $(\hat{\sigma}_{ij}, \hat{\mu}_w)$ must remain in the elastic region.
By (4.20), which we rewrite in the form

$$\left(\left(\varepsilon_{ij}^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) = \sum_{\alpha=1}^{m} \lambda^\alpha \left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}}, \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w}\right) \tag{4.23}$$

we need to compute the multipliers $\lambda^{\alpha} \geq 0 \ \ \alpha = 1, \dots, m$. The multipliers of the constraints not contained in the set $\mathbb{J}_{\text{act}}$ will be set to zero, because those constraints are not active. The multipliers of the constraints contained in the set $\mathbb{J}_{\text{act}}$, will be computed using the corresponding consistency conditions (4.21).

If $\hat{f}_{\alpha} = 0$, then we proceed to compute $\left(\hat{f}_{\alpha}\right)^{\cdot}$. First we apply the chain rule

$$\left(\hat{f}_{\alpha}\right)^{\cdot} = \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \left(\bar{\sigma}_{ij}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \left(\bar{\mu}_{w}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{ij}} \left(\varepsilon_{ij}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{ij}^{p}} \left(\varepsilon_{ij}^{p}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot}$$

use the relations

$$\begin{aligned}
\left(\bar{\sigma}_{ij}\right)^{\cdot} &= \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}} \left(\varepsilon_{kl}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}^{p}} \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot} \\
\left(\bar{\mu}_{w}\right)^{\cdot} &= \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} \left(\varepsilon_{kl}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}^{p}} \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot}
\end{aligned}$$

and get

$$\begin{aligned}
&\left(\hat{f}_{\alpha}\right)^{\cdot} = \\
&= \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \left(\frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}} \left(\varepsilon_{kl}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}^{p}} \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot} \right) \\
&\quad + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \left(\frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} \left(\varepsilon_{kl}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}^{p}} \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \frac{\partial \bar{\mu}_{w}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot} \right) \\
&\quad + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}} \left(\varepsilon_{kl}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}} \left(m_{w}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}^{p}} \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}^{p}} \left(m_{w}^{p}\right)^{\cdot} \\
&= \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}} \right) \left(\varepsilon_{kl}\right)^{\cdot} + \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}} \right) \left(m_{w}\right)^{\cdot} \\
&\quad \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}^{p}} \right) \left(\varepsilon_{kl}^{p}\right)^{\cdot} + \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial m_{w}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}^{p}} \right) \left(m_{w}^{p}\right)^{\cdot}
\end{aligned}$$

Next we use the expressions

$$\begin{aligned}
\left(\varepsilon_{kl}^{p}\right)^{\cdot} &= \sum_{\beta \in \mathbb{J}_{\text{act}}} \lambda^{\beta} \frac{\partial \hat{f}_{\beta}}{\partial \hat{\sigma}_{kl}} \\
\left(m_{w}^{p}\right)^{\cdot} &= \sum_{\beta \in \mathbb{J}_{\text{act}}} \lambda^{\beta} \frac{\partial \hat{f}_{\beta}}{\partial \hat{\mu}_{w}}
\end{aligned}$$

where we have used $\lambda^{\beta} = 0$ for $\beta \notin \mathbb{J}_{\text{act}}$, and we arrive at

$$\begin{aligned}
&\left(\hat{f}_{\alpha}\right)^{\cdot} = \\
&= \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}} \right) \left(\varepsilon_{kl}\right)^{\cdot} + \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}} \right) \left(m_{w}\right)^{\cdot} \\
&\quad \sum_{\beta \in \mathbb{J}_{\text{act}}} \left(\left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial \varepsilon_{kl}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \varepsilon_{kl}^{p}} \right) \frac{\partial \hat{f}_{\beta}}{\partial \hat{\sigma}_{kl}} + \left(\frac{\partial \hat{f}_{\alpha}}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m_{w}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial \hat{\mu}_{w}} \frac{\partial \bar{\mu}_{w}}{\partial m_{w}^{p}} + \frac{\partial \hat{f}_{\alpha}}{\partial m_{w}^{p}} \right) \frac{\partial \hat{f}_{\beta}}{\partial \hat{\mu}_{w}} \right) \lambda^{\beta}
\end{aligned}$$

Consequently, the consistency condition $\left(\hat{f}_\alpha\right)^{\cdot} = 0$ reads

$$\sum_{\beta \in \mathbb{J}_{\mathrm{act}}} g_{\alpha\beta}\, \lambda^\beta = \ell_\alpha \tag{4.24}$$

where

$$\ell_\alpha = \left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w} \frac{\partial \bar{\mu}_w}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_\alpha}{\partial \varepsilon_{kl}}\right) (\varepsilon_{kl})^{\cdot} + \left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m_w} + \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w} \frac{\partial \bar{\mu}_w}{\partial \varepsilon_{kl}} + \frac{\partial \hat{f}_\alpha}{\partial m_w}\right) (m_w)^{\cdot}$$

$$g_{\alpha\beta} = -\left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial \varepsilon^p_{kl}} + \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w} \frac{\partial \bar{\mu}_w}{\partial \varepsilon^p_{kl}} + \frac{\partial \hat{f}_\alpha}{\partial \varepsilon^p_{kl}}\right) \frac{\partial \hat{f}_\beta}{\partial \hat{\sigma}_{kl}} - \left(\frac{\partial \hat{f}_\alpha}{\partial \hat{\sigma}_{ij}} \frac{\partial \bar{\sigma}_{ij}}{\partial m^p_w} + \frac{\partial \hat{f}_\alpha}{\partial \hat{\mu}_w} \frac{\partial \bar{\mu}_w}{\partial m^p_w} + \frac{\partial \hat{f}_\alpha}{\partial m^p_w}\right) \frac{\partial \hat{f}_\beta}{\partial \hat{\mu}_w}$$

Thus, in order to compute the multipliers λ^β of the constraints contained in the set $\mathbb{J}_{\mathrm{act}}$, we must solve the system of equations (4.24). However, in order for the solution to be valid, all the multipliers must be nonnegative.

To proceed further, in Simo and Hughes (1988) it is assumed that the matrix $\left[g_{\alpha\beta}\right]\ \alpha, \beta \in \mathbb{J}_{\mathrm{adm}}$ is positive definite. With this assumption, they conclude the following loading/unloading conditions: (1) if $\ell_\alpha \leq 0$ for all $\alpha \in \mathbb{J}_{\mathrm{adm}}$ then all $\lambda^\alpha = 0$ (i.e. elastic response); and (2) if $\ell_\alpha < 0$ for at least one $\alpha \in \mathbb{J}_{\mathrm{adm}}$ then not all $\lambda^\alpha = 0$ (i.e. elastoplastic response). They also make special note that, if several constraints are active, the condition $\ell_\alpha > 0$ does not guarantee that $\hat{f}_\alpha$ is ultimately active.

4.3 SOIL REGIMES

The structure at the microscale of a soil determines the behavior at the macroscale. In the first place, there is a solid skeleton, which is made of solid particles and eventually of vicinal liquid, which is tightly bonded to them by short-range interaction forces. Additionally, the soil can contain liquid or gas not subjected to short-range interaction forces with the solid particles, but whose presence or absence have an influence on the soil behavior.

There are several mechanisms that bond the water to the soil skeleton (Lu and Likos 2004). At relative low water content, water is mainly in thin films on the particle surfaces, due to short-range interaction forces. At relative high water content, water is mainly contained in the pores left by the particles due to capillary forces. The relation between the water content and the water chemical potential is the soil-water characteristic curve (SWCC), and its shape depends on the type of soil. In fine-graded soils, such as clays, with a large particle surface, much water is in thin films, while in coarser soils, such as sands, very little water is in thin films.

McQueen and Miller (1974) proposed a conceptual model for describing the general shape of a SWCC, which was defined by 3 straight-line segments on a semi-log plot of suction versus moisture content ranging from zero to saturation: (1) tightly adsorbed segment $s = 10^6 - 10^4$kPa (water retention by molecular bonding); (2) adsorbed film segment $s = 10^4 - 100$kPa (water retention by short-range liquid-solid interaction); and (3) capillary segment $s = 100 - 0$kPa (water retention by capillary).

For modeling purposes, we will distinguish 3 soil regimes:

- **Saturated regime** (free liquid, no free gas). In this regime the pressure of the free liquid is defined. If the soil skeleton (solid particles and vicinal liquid) is incompressible and there are no phase exchanges, Terzaghi's effective stress principle holds. If the quotient of the bulk modulus of the soil skeleton and the bulk modulus of the skeleton matrix is not negligible, Biot's effective stress may conveniently replace Terzaghi's effective stress (Coussy 2004).

- **Capillary regime** (free liquid, free gas). In this regime the pressure of the free liquid and of the free gas are defined. The SWCC exhibits an hysteretic behavior. The presence of the liquid-gas interface increases the stress between the particles, which stiffens and hardens the soil, so that upon wetting at low loads the soil swells elastically and at high loads the soil collapses plastically (Alonso et al. 1987).

- **Dry regime** (no free liquid, free gas). In this regime the pressure of the gas phase is defined, but the liquid pressure is not defined. The SWCC does not exhibit an hysteretic behavior. Vicinal fluid is progressive lost. The soil properties depend on the water chemical potential.

In all these regimes the basic state variables, namely, the deformation of the skeleton, the masses of species and the temperature are the same. However, the different features of the soil behavior in these regimes seem difficult to include in a general constitutive model. We propose therefore to use a different constitutive model for each of these regimes. Further, at the change of regime, the corresponding constitutive models will be linked by the condition of continuity of the basic variables and of the total stress tensor and of chemical potentials.

In order to establish the conditions of change of regime, we propose to use two values of the water chemical potential: μ_{w0} that marks the transition between the saturated and the capillary regimes and μ_{w1} that marks the transition between the capillary and the dry regimes. Setting to 0 the water chemical potential at atmospheric conditions, the value $\mu_{w0} < 0$ corresponds to the air entry value and the value $\mu_{w1} < \mu_{w0}$ corresponds to the vaporization of free liquid water.

Remarks

- If we plot the elastic region in the space (total) pressure p - water pressure p_w (recall that $d\mu_w = (1/\rho_w)dp_w$) near the water saturation limit, we can see that (1) the compression yield pressure increases with increasing water pressure in the saturated zone (Terzaghi's effective principle) but decreases with increasing water pressure in the unsaturated zone; and (2) the extent of the elastic region is constant in the saturated zone (Terzaghi's effective principle) but increases in the unsaturated zone. Indeed, in the unsaturated state the liquid-gas interfaces tends to stabilize the contacts of the soil grains (Gens 2010), and these interfaces disappear when saturation is reached.

- Groenevelt and Parlange (1974) present experimental data on a swelling soil at zero load pressure, and note that the curve $e = e(\theta)$ is not tangent to $e = \theta$ at the air entry point, where $\theta = V_w/V_s$ is the moisture ratio and $e = V/V_s - 1$ is the void ratio. They show that this discontinuity can be associated with a second order phase transition in the sense of Ehrenfest (i.e. continuous molar Gibbs function with continuous first order derivatives and discontinuous second order derivatives (Callen 1960, Sect. 9.9)). They say that this phase transition is linked to the appearance and disappearance of the gas phase due to a small change in the chemical potential of water.

In what follows we will show examples of free energy and dissipation functions for each of the soil regimes. The corresponding constitutive models will follow by use of the state laws and Ziegler's orthogonality principle.

4.3.1 Preliminaries

For simplicity, we will consider isothermal conditions, no chemical reactions, small strains and volumetric deformations of the solid skeleton. The free energy function per unit reference volume Ψ is assumed to be of the form

$$\Psi = \Psi(\varepsilon_v, m_s, m_w, m_a, \theta, \varepsilon_v^p, m_w^p)$$

where ε_v is the volumetric deformation of the solid skeleton, m_s is the mass of mineral per unit reference volume, m_w is the mass of water per unit reference volume, m_a is the mass of air per unit reference volume, θ is the temperature, ε_w^p is the plastic volumetric deformation and m_w^p is the plastic water mass per unit reference volume.

As already mentioned, we will assume that the temperature θ and the air chemical potential μ_a are constant, corresponding to usual atmospheric conditions. This is approximately equivalent to constant gas pressure (i.e. the partial water vapor pressure is neglected). It was also mentioned that, for constant air chemical potential μ_a, it is convenient to perform the Legendre transform of the free energy $\Psi(\varepsilon_v, m_s, m_w, m_a, \theta, \varepsilon_v^p, m_w^p)$ with respect to the mass of air per unit reference volume m_a to get an equivalent thermodynamic potential $\Pi(\varepsilon_v, m_s, m_w, \mu_a, \theta, \varepsilon_v^p, m_w^p)$ per unit reference volume. For notational convenience, since $\theta = \theta_0$ (isothermal conditions), $m_s = m_{s0}$ (no chemical reactions) and $\mu_a = \mu_{a0}$ (air chemical potential is assumed constant), we define a new function

$$\Psi\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \Pi(\varepsilon_v, m_{s0}, m_w, \mu_{a0}, \theta_0, \varepsilon_v^p, m_w^p)$$

for which, for simplicity, we use the symbol Ψ (an abuse of an already defined symbol) and we denominate it the "free energy per unit reference volume" (an abuse of an already defined denomination).

For each of the considered regimes, the constitutive model follows from the free energy function Ψ and the dissipation function Φ by use of Ziegler's orthogonality principle:

$$\begin{aligned} \Psi &= \Psi(\varepsilon_v, m_w, \varepsilon_w^p, m_w^p) \\ \Phi &= \Phi\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}; \varepsilon_v, m_w, \varepsilon_w^p, m_w^p\right) \end{aligned} \tag{4.25}$$

where Ψ is a smooth convex function of ε_v, m_w, ε_w^p and m_w^p, and Φ is a proper, convex, lower semicontinuous positively homogeneous nonnegative function (i.e. a gauge function) of $\left(\varepsilon_v^p\right)^{\cdot}$ and $\left(m_w^p\right)^{\cdot}$, which depends also on ε_v, m_w, ε_w^p and m_w^p.

From the free energy Ψ follow the constitutive laws of the (total) pressure p and of the water chemical potential μ_w

$$\begin{aligned} -p &= \frac{\partial \Psi}{\partial \varepsilon_v}(\varepsilon_v, m_w, \varepsilon_w^p, m_w^p) \\ \mu_w &= \frac{\partial \Psi}{\partial m_w}(\varepsilon_v, m_w, \varepsilon_w^p, m_w^p) \end{aligned} \tag{4.26}$$

and from Ziegler's orthogonality principle follow the constitutive laws of the rate of plastic volumetric strain $\left(\varepsilon_v^p\right)^{\cdot}$ and of the rate of the plastic water mass $\left(m_w^p\right)^{\cdot}$

$$\left(-\frac{\partial \Psi}{\partial \varepsilon_v^p}, -\frac{\partial \Psi}{\partial m_w^p}\right) \in \partial \Phi \tag{4.27}$$

where $\partial\Phi$ denotes the subdifferential of Φ with respect to $\left(\varepsilon_v^p\right)^{\cdot}$ and $\left(m_w^p\right)^{\cdot}$.

We will make the following simplifying assumptions:

- **Vicinal water**. It is subjected to interaction forces with the skeleton, so that it is tightly bond to the soil skeleton, and it is only mobilized in the dry regime. In the saturated and capillary regimes it is constant $m_w^V = m_{w0}^V > 0$; in the dry regime it is variable and $0 < m_w^V < m_{w0}^V$.

- **Free water**. It is not subjected to interaction forces with the skeleton. The mass of free water m_w^F is the sum of the initial (reference) free water m_{w0}^F, the elastic component m_w^e and the plastic component m_w^p, i.e. $m_w^F = m_{w0}^F + m_w^p + m_w^e$. In the saturated and capillary regimes it is variable $m_w^F > 0$; in the dry regime it is zero $m_w^F = 0$.

- **Saturated regime**. The mass of vicinal water is constant $m_w^V = m_{w0}^V > 0$; the mass of free water is variable m_w^F>0.

- **Transition between the saturated and the capillary regimes**. Occurs at $\mu_w = \mu_{w0}$; the mass of vicinal water is constant $m_w^V = m_{w0}^V > 0$; the mass of free water is variable $m_w^F > 0$.

- **Capillary regime.** The mass of vicinal water is constant $m_w^V = m_{w0}^V > 0$; the mass of free water is variable $m_w^F > 0$.

- **Transition between the capillary and the dry regimes**. Occurs at $\mu_w = \mu_{w1}$, with $\mu_{w1} < \mu_{w0}$; the mass of vicinal water is constant $m_w^V = m_{w0}^V > 0$; the mass of free water is zero $m_w^F = 0$.

- **Dry regime**. The mass of vicinal water is variable $0 < m_w^V < m_{w0}^V$; the mass of free water is zero $m_w^F = 0$.

Remarks

- If the mass of vicinal water can be neglected, then the dry regime disappears. This would be the case of sands and gravels.

- The transition between regimes involves a change of model, but the variables ε_v, m_w and ε_v^p are common to all regimes and the variable m_w^p is common to the saturated and capillary regimes but disappears in the dry regime. In the saturated regime m_w^p is linked to ε_v^p

- At the transition between regimes, the free energy and its first derivatives with respect to ε_v and m_w (i.e. $-p$ and μ_w) are required to be continuous.

4.3.2 Saturated regime

The reference configuration will be assumed to be at the water chemical potential μ_{w0} corresponding to the transition between the saturated regime and the capillary regime. We will assume that the solid skeleton, which is made of solid mineral and vicinal water, is incompressible and there is no mass exchange between the vicinal water and the free water, both of which will be assumed to have only the species water. In these conditions, Terzaghi's effective stress principle holds. Recall that we have also assumed small strains.

From these assumptions, it follows

$$\begin{aligned} J &= 1 + \varepsilon_v \quad \text{(small strains)} \\ J - n_w^F &= 1 - n_{w0}^F \quad \text{(incomp. solid skeleton, no mass exchange)} \end{aligned} \tag{4.28}$$

where J and ε_v is the Jacobian and the volumetric deformation of the skeleton motion, n_w^F is the volume of free water per unit reference volume and n_{w0}^F is the corresponding value at the reference configuration. Consequently

$$\varepsilon_v = n_w^F - n_{w0}^F \tag{4.29}$$

and the density of free water is

$$\rho_w^F = \frac{m_w^F}{n_w^F} = \frac{m_w^F}{\varepsilon_v + n_{w0}^F} \tag{4.30}$$

where m_w^F is the mass of free water per unit reference volume.

The volumetric strain of the soil skeleton ε_v and the mass of water per unit reference volume m_w are assumed to decompose as follows

$$\begin{aligned} \varepsilon_v &= \varepsilon_v^e + \varepsilon_v^p \\ m_w &= m_{w0}^V + m_w^F = m_{w0}^V + m_{w0}^F + m_w^e + m_w^p \end{aligned} \tag{4.31}$$

were ε_v^e and ε_v^p are the elastic and plastic volumetric strains, m_{w0}^V and m_{w0}^F are the mass of vicinal water and the mass of free water at the reference configuration per unit reference volume, and m_w^e and m_w^p are the elastic and plastic variations of the mass of water per unit reference volume with respect to the reference configuration (Coussy 1995).

The plastic volumetric strain ε_v^p is the volumetric strain ε_v after (virtual) unloading from the actual state $(-p, \mu_w)$ to the reference state $(-p_0, \mu_{w0})$. The plastic water mass per unit reference volume m_w^p is the variation of the total water mass per unit reference volume m_w with respect to the reference water mass per unit reference volume $m_{w0} = m_{w0}^V + m_{w0}^F$ after (virtual) unloading from the actual state $(-p, \mu_w)$ to the reference state $(-p_0, \mu_{w0})$. Since it is assumed that the solid skeleton (solid mineral and vicinal water) is incompressible and no mass exchange with the free water occurs, it follows that the variation of the total water mass $m_w - m_{w0}$ is equal to the variation of free water mass $m_w^F - m_{w0}^F$. Since the free water density is a function only of the water chemical potential, it follows that after (virtual) unloading the free water density ρ_{w0} is fixed by the water chemical potential at the reference configuration μ_{w0}. Consequently, on (virtual) unloading (i.e. $m_w^e = 0$ and $\varepsilon_v^e = 0$), from relations (4.8) it follows

$$m_w^p = m_w - m_{w0} = m_w^F - m_{w0}^F = \rho_{w0}(n_w^F - n_{w0}^F) = \rho_{w0}\varepsilon_v = \rho_{w0}\varepsilon_v^p$$

so that $\left(m_w^p\right)^{\cdot}$ and $\left(\varepsilon_v^p\right)^{\cdot}$ are related by (Coussy 1995)

$$(m_w^p)^{\cdot} = \rho_{w0}(\varepsilon_v^p)^{\cdot} \tag{4.32}$$

At $\mu_w = \mu_{w0}$, let $p_C(\varepsilon_v^p) > 0$ be the yield pressure in compression and let $p_E(\varepsilon_v^p) < 0$ be the yield pressure in extension. For notational convenience, we define

$$\begin{aligned} \tan\theta &= \rho_{w0} \\ k(\varepsilon_v^p) &= \frac{1}{2}\left(p_C(\varepsilon_v^p) - p_E(\varepsilon_v^p)\right)\cos\theta > 0 \\ \ell(\varepsilon_v^p) &= \frac{1}{2}\left(p_C(\varepsilon_v^p) + p_E(\varepsilon_v^p)\right) \end{aligned} \tag{4.33}$$

4.3.2.1 Free energy function

We assume that the free energy has the following form

$$\Psi(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p) = \Psi_1(\varepsilon_v - \varepsilon_v^p\ ) - \int_0^{\varepsilon_v^p} \ell(s)ds + (m_w - m_{w0}^V)\psi_w^F\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) \tag{4.34}$$

where $\psi_w^F(1/\rho_w^F)$ is the specific (per unit mass) free energy function of free water and ρ_w^F is the density of free water (cf. (4.30) and (4.31)$_2$).

The pressure p and the water chemical potential μ_w are given by

$$\begin{aligned} -p &= \frac{\partial\Psi}{\partial\varepsilon_v} = \frac{\partial\Psi_1}{\partial\varepsilon_v^e}(\varepsilon_v - \varepsilon_v^p) + (\psi_w^F)'\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) = -p'(\varepsilon_v - \varepsilon_v^p) - p_w^F\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) \\ \mu_w &= \frac{\partial\Psi}{\partial m_w} = \psi_w^F\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) - \frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}(\psi_w^F)'\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) = \mu_w^F\left(\frac{\varepsilon_v + n_{w0}^F}{m_w - m_{w0}^V}\right) \end{aligned} \tag{4.35}$$

where p' is (Terzaghi's) effective pressure, $p_w^F(1/\rho_w^F)$ is the pressure function of free water and $\mu_w^F(1/\rho_w^F)$ is the water chemical potential function of free water. Note that (Callen 1985)

$$\begin{aligned} p_w^F\left(\frac{1}{\rho_w^F}\right) &= -(\psi_w^F)'\left(\frac{1}{\rho_w^F}\right) \\ \mu_w^F\left(\frac{1}{\rho_w^F}\right) &= \psi_w^F\left(\frac{1}{\rho_w^F}\right) - \frac{1}{\rho_w^F}(\psi_w^F)'\left(\frac{1}{\rho_w^F}\right) \end{aligned} \tag{4.36}$$

Thus the water chemical potential of the soil μ_w and the chemical potential of free water are equal. From the expressions of $\mu_w^F(1/\rho_w^F)$ and $p_w^F(1/\rho_w^F)$, it follows a relation $p_w^F = p_w^F(\mu_w^F)$ (an abuse of the already used function symbol p_w^F), using which (4.35)$_1$ can be written in the form

$$-p = \frac{\partial\Psi_1}{\partial\varepsilon_v^e}(\varepsilon_v - \varepsilon_v^p) - p_w^F(\mu_w) \tag{4.37}$$

The generalized pressure and water chemical potential are given by

$$\begin{aligned} -\bar{p} &= -\frac{\partial\Psi}{\partial\varepsilon_v^p} = \frac{\partial\Psi_1}{\partial\varepsilon_v^e}(\varepsilon_v - \varepsilon_v^p) + \ell(\varepsilon_v^p) = -p + p_w^F(\mu_w) + \ell(\varepsilon_v^p) \\ \bar{\mu}_w &= -\frac{\partial\Psi}{\partial m_w^p} = 0 \end{aligned} \tag{4.38}$$

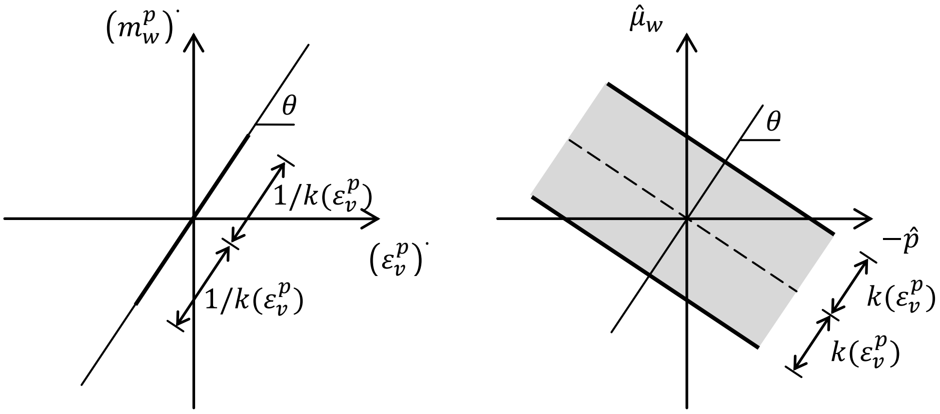
where (4.37) has been used.

4.3.2.2 Dissipation function

We assume that the dissipation function has the following form

$$\begin{gathered}\operatorname{dom}\Phi=\left\{\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right):\left(m_w^p\right)^{\cdot}=\rho_{w0}\left(\varepsilon_v^p\right)^{\cdot}\right\}\\ \Phi\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot};\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\frac{1}{\cos\theta}k\left(\varepsilon_v^p\right)\left|\left(\varepsilon_v^p\right)^{\cdot}\right|\end{gathered}\tag{4.39}$$

Note that $\operatorname{dom}\Phi$ is a closed convex one-dimensional subset of the space $E_{(\varepsilon_v^p)^{\cdot}}\times E_{(m_w^p)^{\cdot}}$. Figure 4.1a shows the effective domain $\operatorname{dom}\Phi$ and the level set $\Phi\le 1$ of the dissipation function. Recall that, by the convention used in convex analysis (Rockafellar 1970), outside the effective domain the value of the proper lower semi-continuous convex function Φ is $+\infty$.



a) b)

Figure 4.1. Saturated regime. a) The thin line that passes through the origin and forms an angle θ with the horizontal axis is the effective domain $\operatorname{dom}\Phi$ of the dissipation function and the thick segment is the level set $\Phi\le 1$ of the dissipation function; b) The gray strip that has a width of $2k(\varepsilon_v^p)$ and its axis passes through the origin and forms an angle of $-(\pi/2-\theta)$ with the horizontal axis is the effective domain $\operatorname{dom}\Phi^*$ of the dual of the dissipation function. The two sets $\Phi\le 1$ and $\operatorname{dom}\Phi^*$ are polars of each other (the length of the segment and the width of the strip are reciprocal to each other).

Since $p_C(\varepsilon_v^P)>0$ and $p_E\left(\varepsilon_v^p\right)<0$, it follows that

$$\frac{1}{\cos\theta}k\left(\varepsilon_v^p\right)=\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)>0$$

so that Φ is a non-negative function.

Note that Φ is not differentiable at any point of $\operatorname{dom}\Phi$. The subdifferential of Φ is

If $\left(\varepsilon_v^p\right)^{\cdot}>0$, $\left(m_w^p\right)^{\cdot}>0$ (yield in extension)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\left\{(\hat{p},\hat{\mu}_w):-\hat{p}\cos\theta+\hat{\mu}_w\sin\theta=k(\varepsilon_v^p)\right\}\\ &\quad=\left\{\left(k\left(\varepsilon_v^p\right)\cos\theta-u\sin\theta,k\left(\varepsilon_v^p\right)\sin\theta+u\cos\theta\right),u\in\mathbb{R}\right\}\end{aligned}\tag{4.40}$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0$, $\left(m_w^p\right)^{\cdot} = 0$ (elasticity)

$$\begin{aligned}
&\partial\Phi\left((0,0);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\left\{(\hat{p},\hat{\mu}_w):-k\left(\varepsilon_v^p\right)\le -\hat{p}\cos\theta+\hat{\mu}_w\sin\theta\le k(\varepsilon_v^p)\right\}\\
&\quad=\left\{(v\cos\theta-u\sin\theta\,,v\sin\theta+u\cos\theta),u\in\mathbb{R},-k\left(\varepsilon_v^p\right)\le v\le k\left(\varepsilon_v^p\right)\right\}
\end{aligned}$$

If $\left(\varepsilon_v^p\right)^{\cdot} < 0$, $\left(m_w^p\right)^{\cdot} < 0$ (yield in compression)

$$\begin{aligned}
&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\left\{(\hat{p},\hat{\mu}_w):-\hat{p}\cos\theta+\hat{\mu}_w\sin\theta=-k(\varepsilon_v^p)\right\}\\
&\quad=\left\{\left(-k\left(\varepsilon_v^p\right)\cos\theta-u\sin\theta\,,-k\left(\varepsilon_v^p\right)\sin\theta+u\cos\theta\right),u\in\mathbb{R}\right\}
\end{aligned}$$

The Legendre-Fenchel dual Φ^* of Φ is the indicator function of the subdifferential of Φ at the origin $\partial\Phi\left(\left(0,0;\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)\right)$, namely

$$\begin{gathered}
\operatorname{dom}\Phi^*=\left\{(-\hat{p},\hat{\mu}_w):\left|-\hat{p}\cos\theta+\hat{\mu}_w\sin\theta\right|\le k\left(\varepsilon_v^p\right)\right\}\\
\Phi^*\left((-\hat{p},\hat{\mu}_w);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=0
\end{gathered}\tag{4.41}$$

Figure 4.1b shows the effective domain $\operatorname{dom}\Phi^*$ of this function, which is a closed convex two-dimensional strip of the dual space $E_{-\hat{p}}\times E_{\hat{\mu}_w}$ of the space $E_{\left(\varepsilon_v^p\right)^{\cdot}}\times E_{\left(m_w^p\right)^{\cdot}}$. By the convention used in convex analysis (Rockafellar 1970), outside the effective domain the value of the proper lower semi-continuous convex function Φ^* is $+\infty$. Thus, the elastic region in the space $E_{-\hat{p}}\times E_{\hat{\mu}_w}$ is

$$\hat{C}\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\left\{(-\hat{p},\hat{\mu}_w):\left|-\hat{p}\cos\theta+\hat{\mu}_w\sin\theta\right|\le k\left(\varepsilon_v^p\right)\right\}$$

or

$$\hat{C}\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\left\{(-\hat{p},\hat{\mu}_w):\left|-\hat{p}+\hat{\mu}_w\rho_{w0}\right|\le\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)\right\}\tag{4.42}$$

The boundary in extension is

$$-\hat{p}+\hat{\mu}_w\rho_{w0}=\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)$$

or

$$\hat{p}=\hat{\mu}_w\rho_{w0}-\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)\tag{4.43}$$

and, at any of its points, the cone of outer normals is

$$N_{\hat{C}\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)}=\{\lambda(1,\rho_{w0})\,,\lambda\ge 0\}\tag{4.44}$$

The boundary in compression is

$$-\hat{p}+\hat{\mu}_w\rho_{w0}=-\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)$$

or

$$\hat{p}=\hat{\mu}_w\rho_{w0}+\frac{1}{2}\left(p_C\left(\varepsilon_v^p\right)-p_E\left(\varepsilon_v^p\right)\right)\tag{4.45}$$

and, at any of its points, the cone of outer normals is

$$N_{\hat{C}\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)}=\{\lambda(-1,-\rho_{w0})\,,\lambda\ge 0\}\tag{4.46}$$

4.3.2.3 *Ziegler's orthogonality principle*

Ziegler's orthogonality principle reads

$$\left(-\frac{\partial\Psi}{\partial\varepsilon_v^p},-\frac{\partial\Psi}{\partial m_w^p}\right)\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)\in\partial\Phi\left(\left((\varepsilon_v^p)^{\cdot},(m_w^p)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)$$

where the left hand side is given by (4.38) and the right hand side by (4.40). Replacing $-\hat{p}$ and $\hat{\mu}_w$ in (4.40) by the expressions of $-\bar{p}$ and $\bar{\mu}_w$ in (4.38), we get

If $(\varepsilon_v^p)^{\cdot}>0$, $(m_w^p)^{\cdot}>0$ (yield in extension)

$$\begin{aligned}-p+p_w^F(\mu_w)+\ell(\varepsilon_v^p)&=k(\varepsilon_v^p)\cos\theta-u\sin\theta\\ 0&=k(\varepsilon_v^p)\sin\theta+u\cos\theta\quad\rightarrow\quad u=-k(\varepsilon_v^p)\tan\theta\end{aligned}$$

$$-p=-p_w^F(\mu_w)-\ell(\varepsilon_v^p)+\frac{1}{\cos\theta}k(\varepsilon_v^p)$$

If $(\varepsilon_v^p)^{\cdot}=0$, $(m_w^p)^{\cdot}=0$ (elasticity)

$$\begin{aligned}-p+p_w^F(\mu_w)+\ell(\varepsilon_v^p)&=v\cos\theta-u\sin\theta\quad\rightarrow\quad v=\left(-p+p_w(\mu_w)+\ell(\varepsilon_v^p)\right)\cos\theta\\ 0&=v\sin\theta+u\cos\theta\quad\rightarrow\quad u=-v\tan\theta\end{aligned}$$

$$-k(\varepsilon_v^p)\le v\le k(\varepsilon_v^p)\tag{4.47}$$

$$-p_w^F(\mu_w)-\ell(\varepsilon_v^p)-\frac{1}{\cos\theta}k(\varepsilon_v^p)\le -p\le -p_w^F(\mu_w)-\ell(\varepsilon_v^p)+\frac{1}{\cos\theta}k(\varepsilon_v^p)$$

If $(\varepsilon_v^p)^{\cdot}<0$, $(m_w^p)^{\cdot}<0$ (yield in compression)

$$\begin{aligned}-p+p_w^F(\mu_w)+\ell(\varepsilon_v^p)&=-k(\varepsilon_v^p)\cos\theta-u\sin\theta\\ 0&=-k(\varepsilon_v^p)\sin\theta+u\cos\theta\quad\rightarrow\quad u=k(\varepsilon_v^p)\tan\theta\end{aligned}$$

$$-p=-p_w^F(\mu_w)-\ell(\varepsilon_v^p)-\frac{1}{\cos\theta}k(\varepsilon_v^p)$$

The transform of the elastic region in the space $E_{-p}\times E_{\mu_w}$ is

$$C(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)=\left\{(-p,\mu_w):\left|-p+p_w^F(\mu_w)+\ell(\varepsilon_v^p)\right|\le\frac{1}{\cos\theta}k(\varepsilon_v^p)\right\}$$

or

$$\begin{aligned}&C(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)\\ &\qquad=\left\{(-p,\mu_w):\left|-p+p_w^F(\mu_w)+\frac{1}{2}\left(p_C(\varepsilon_v^p)+p_E(\varepsilon_v^p)\right)\right|\le\frac{1}{2}\left(p_C(\varepsilon_v^p)-p_E(\varepsilon_v^p)\right)\right\}\end{aligned}\tag{4.48}$$

Figure 4.2 shows the portion of the elastic region in the space $E_{-p}\times E_{\mu_w}$ above the reference μ_{w0} (here taken to be zero by simplicity), which corresponds to the saturated regime. Note that the transformation of the elastic region form the space $E_{-\hat{p}}\times E_{\hat{\mu}_w}$ to the space $E_{-p}\times E_{\mu_w}$ involves a shift due to the term $\ell(\varepsilon_v^p)$ and a deformation due to the term $p_w^F(\mu_w)$, which causes that the flow directions are not orthogonal to the boundary of the elastic region.

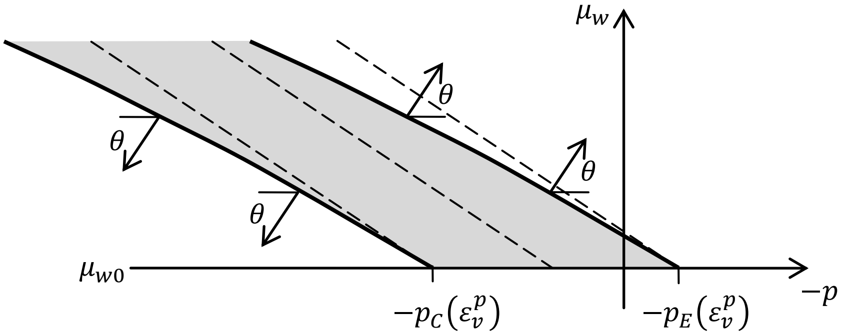


Figure 4.2. Saturated regime. Elastic region in the space $E_{-p} \times E_{\mu_w}$ (here μ_{w0} has been taken to be zero by simplicity). At the transition of regime, $p_C(\varepsilon_v^p)$ is the yield pressure in compression and $p_E(\varepsilon_v^p)$ is the yield pressure in extension. Arrows indicate flow directions, which are not normal to the boundary (they are normal to the boundary of the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$).

The boundary in extension is

$$-p + p_w(\mu_w) + \frac{1}{2}\left(p_C(\varepsilon_v^p) + p_E(\varepsilon_v^p)\right) = \frac{1}{2}\left(p_C(\varepsilon_v^p) - p_E(\varepsilon_v^p)\right)$$

or

$$p = p_E(\varepsilon_v^p) + p_w^F(\mu_w) \tag{4.49}$$

and, at any point on it, the flow rule is given by the cone of outer normals at the corresponding point in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$, namely

$$\left((\varepsilon_v^p)^{\cdot}, (m_w^p)^{\cdot}\right) = \lambda(1, \rho_{w0}) \quad \lambda \geq 0 \tag{4.50}$$

The boundary in compression is

$$-p + p_w(\mu_w) + \frac{1}{2}\left(p_C(\varepsilon_v^p) + p_E(\varepsilon_v^p)\right) = -\frac{1}{2}\left(p_C(\varepsilon_v^p) - p_E(\varepsilon_v^p)\right)$$

or

$$p = p_C(\varepsilon_v^p) + p_w(\mu_w) \tag{4.51}$$

and, at any point on it, the flow rule is given by the cone of outer normals at the corresponding point in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$, namely

$$\left((\varepsilon_v^p)^{\cdot}, (m_w^p)^{\cdot}\right) = \lambda(-1, -\rho_{w0}) \quad \lambda \geq 0 \tag{4.52}$$

Remarks

- In the expression (4.34) of the free energy Ψ, the first two terms can be attributed to the free energy of the solid skeleton and the last one to the free energy of free water.
- The effective domain of the dissipation function Φ is one-dimensional because of the constraint $(m_w^p)^{\cdot} = \rho_{w0}(\varepsilon_v^p)^{\cdot}$. As a result, Φ is not differentiable at any point of its effective domain. For

instance, the subdifferential $\partial\Phi$ at points of the effective domain $\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right) \neq (0,0)$ contains more elements than just the gradient of Φ along the one-dimensional effective domain (i.e. $(-\hat{p}, \hat{\mu}_w) = k\left(\varepsilon_v^p\right)(\cos\theta\,, \sin\theta)$ in extension, $(-\hat{p}, \hat{\mu}_w) = -k\left(\varepsilon_v^p\right)(\cos\theta\,, \sin\theta)$ in compression).

- The flow rule is associated in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ but it is not associated in the space $E_{-p} \times E_{\mu_w}$. This is due to the expressions (4.38) of $-\bar{p}$ and $\bar{\mu}_w$.

4.3.3 Capillary regime

The transition from the saturated regime to the capillary regime occurs at $\mu_w = \mu_{w0}$, and the transition from the capillary regime to the dry regime occurs at $\mu_w = \mu_{w1} < \mu_{w0}$. It will be assumed that in the capillary regime the vicinal water mass is equal to its initial value in the reference configuration m_{w0}^V and the free water mass m_w^F varies.

Let the soil be virtually unloaded to the reference load $(-p_0, \mu_{w0})$. By definition, the elastic volumetric deformation ε_v^e and the elastic water mass m_w^e are zero. The water mass m_{w0} and the plastic water mass m_{w0}^p depend on the plastic volumetric deformation

$$\begin{aligned} m_{w0}\left(\varepsilon_v^p\right) &= m_{w0}^V + m_{w0}^F + \rho_{w0}\varepsilon_v^p \\ m_{w0}^p\left(\varepsilon_v^p\right) &= \rho_{w0}\varepsilon_v^p \end{aligned} \tag{4.53}$$

Let us fix the soil skeleton and assume that the main wetting curve W and the main drying curve D are given by the following expressions ($I = W, D$)

$$\mu_{wI}\left(m_w, \varepsilon_v^p\right) = \mu_{w0} + (\mu_{w0} - \mu_{w1}) f_I\left(\frac{m_w - m_{w1}}{m_{w0}\left(\varepsilon_v^p\right) - m_{w1}}\right) \quad \left(m_{w1} \le m_w \le m_{w0}(\varepsilon_v^p)\right) \tag{4.54}$$

and that the scanning line determined by m_w^p is given by

$$\mu_{wS}(m_w - m_w^p) = \mu_{w0} + K\left(m_w - \left(m_{w0}^V + m_{w0}^F + m_w^p\right)\right) \tag{4.55}$$

where $m_{w0}\left(\varepsilon_v^p\right)$ is the water mass at $\mu_w = \mu_{w0}$, $m_{w1} = m_{w0}^V$ is the water mass at $\mu_w = \mu_{w1}$ (i.e. the soil has only the vicinal water mass of the reference configuration), m_w^p is the plastic water mass that determines the considered scanning line and the constant K, the normalized main wetting curve $f_W(s)$ and the normalized main drying curve $f_D(s)$ are such that

$$K > 0$$

for $I = W, D$

$$f_I \colon [0,1] \to [-1, 0]$$

$$\begin{aligned} f_I(0) &= -1 \\ f_I(1) &= 0 \\ \frac{df_I}{ds}(s) &> 0 \end{aligned} \tag{4.56}$$

and

$$f_D(s) < f_W(s) \quad (0 < s < 1)$$

Figure 4.3a shows the main wetting curve $\mu_{wW}(m_w, \varepsilon_v^p)$ and the main drying curve $\mu_{wW}(m_w, \varepsilon_v^p)$. The main wetting curve and the main drying curve are strictly increasing functions. The main wetting curve is above the main drying curve at all m_w except at $m_w = m_{w0}(\varepsilon_v^p)$ and at $m_w = m_{w1}$, where they coincide. Figure 4.3b shows the normalized main wetting curve $f_W(s)$ and the normalized main drying curve $f_D(s)$, which, respectively, have the same properties.

Figure 4.3a shows also the scanning line $\mu_{wS}(m_w - m_w^p)$ determined by m_w^p. The scanning line has only one intersection point with the main wetting curve and has only one intersection point with the main drying curve. This property follows if the slope K of the scanning line is strictly greater than the slopes of the main wetting and drying curves at all m_w.

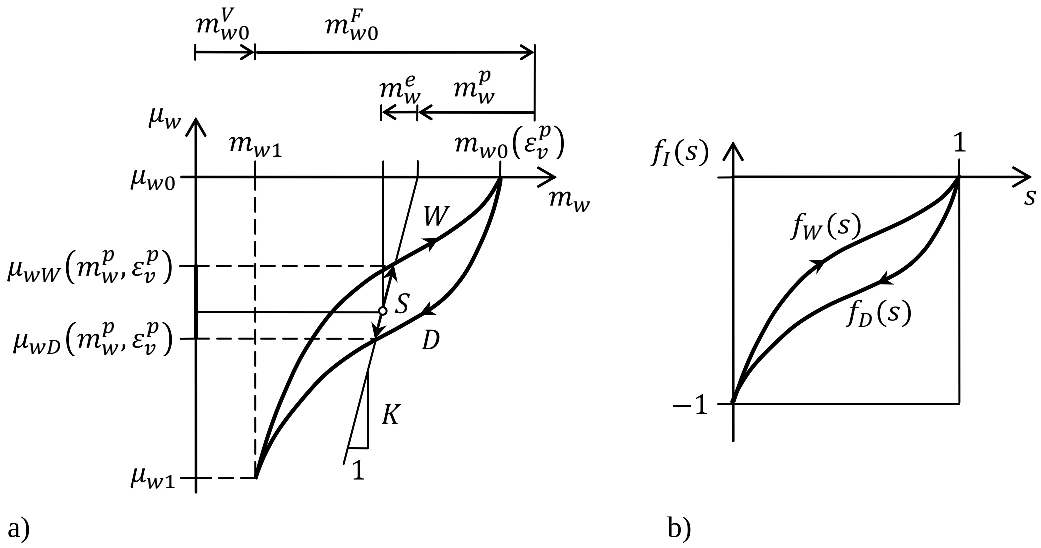


Figure 4.3. Capillary regime. a) The small circle is the current state, W is the main wetting curve, D is the main drying curve and S is the current scanning line; the thick segment on the vertical axis is the projection of the current elastic region, which at $\mu_w = \mu_{w0}$ (transition to the saturated regime) and at $\mu_w = \mu_{w1}$(transition to the dry regime) reduces to a point; The scanning line, which has slope K, intersects the main wetting curve at only one point and intersects the main drying curve at only one point; also shown are the vicinal water mass at the reference configuration m_{w0}^V, the free water mass at the reference configuration m_{w0}^F, the current plastic water mass m_w^p (here it is negative), the current elastic water mass m_w^e (here it is negative), the water mass $m_{w0}(\varepsilon_v)$ at $\mu_w = \mu_{w0}$ and the water mass m_{w1} at $\mu_w = \mu_{w1}$; b) normalized main wetting curve $f_W(s)$ and normalized main drying curve $f_D(s)$.

Since the scanning line $\mu_{wS}(m_w - m_w^p)$ determined by m_w^p intersects at only one point any of the main curves $\mu_{wI}(m_w, \varepsilon_v^p)$, it is possible to express these curves in the form $\mu_{wI}(m_w^p, \varepsilon_v^p)$. In order to find the expressions of the derivatives of $\mu_{wI}(m_w^p, \varepsilon_v^p)$, let us introduce the variable

$$s = \frac{m_w - m_{w1}}{m_{w0}(\varepsilon_v^p) - m_{w1}} = \frac{m_w - m_{w0}^V}{m_{w0}^F + \rho_{w0}\varepsilon_v^p} \quad (0 \le s \le 1) \tag{4.57}$$

where $m_{w1} = m_{w0}^V$ and (4.53) have been used. Consequently

$$m_w(s, \varepsilon_v^p) = m_{w0}^V + (m_{w0}^V + \rho_{w0}\varepsilon_v^p)s \tag{4.58}$$

Expression (4.54) becomes

$$\mu_{wI}(s) = \mu_{w0} + (\mu_{w0} - \mu_{w1})f_I(s) \tag{4.59}$$

and by (4.55) the value of m_w^p that determines the scanning line that intersects the curve I at the point determined by s is such that

$$\mu_{w0} + (\mu_{w0} - \mu_{w1})f_I(s) = \mu_{w0} + K\left(m_w - \left(m_{w0}^V + m_{w0}^F + m_w^p\right)\right)$$

so that

$$m_w^p = -\frac{\mu_{w0} - \mu_{w1}}{K} f_I(s) + (m_w - m_{w0}^V) - m_{w0}^F$$

and using (4.57) it becomes

$$m_w^p\big(s, \varepsilon_v^p\big) = -\frac{\mu_{w0} - \mu_{w1}}{K} f_I(s) + \big(m_{w0}^F + \rho_{w0}\varepsilon_v^p\big)s - m_{w0}^F \tag{4.60}$$

Replacing (4.59) and (4.60) in $\mu_{wI} = \mu_{wI}(m_w^p, \varepsilon_v^p)$ yields

$$\mu_{wI}(s) = \mu_{wI}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big) \tag{4.61}$$

Partial derivation of (4.61) with respect to s yields

$$\frac{\partial \mu_{wI}}{\partial s}(s) = \frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big)\frac{\partial m_w^p}{\partial s}\big(s, \varepsilon_v^p\big) \tag{4.62}$$

and partial derivation of (4.61) with respect to ε_v^p yields

$$0 = \frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big)\frac{\partial m_w^p}{\partial \varepsilon_v^p}\big(s, \varepsilon_v^p\big) + \frac{\partial \mu_{wI}}{\partial \varepsilon_v^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big) \tag{4.63}$$

Using (4.59) and (4.60) in (4.62) yields

$$(\mu_{w0} - \mu_{w1})f_I'(s) = \frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big)\left(-\frac{\mu_{w0} - \mu_{w1}}{K} f_I'(s) + m_{w0}^F + \rho_{w0}\varepsilon_v^p\right) \tag{4.64}$$

and using the expression (4.57) of s yields

$$\frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p, \varepsilon_v^p\big) = \frac{(\mu_{w0} - \mu_{w1})f_I'\left(\dfrac{m_w - m_{w0}^V}{m_{w0}^F + \rho_{w0}\varepsilon_v^p}\right)}{m_{w0}^F + \rho_{w0}\varepsilon_v^p - \dfrac{\mu_{w0} - \mu_{w1}}{K} f_I'\left(\dfrac{m_w - m_{w0}^V}{m_{w0}^F + \rho_{w0}\varepsilon_v^p}\right)} \tag{4.65}$$

Using (4.60) in (4.63) yields

$$0 = \frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big)\rho_{w0}s + \frac{\partial \mu_{wI}}{\partial \varepsilon_v^p}\big(m_w^p\big(s, \varepsilon_v^p\big), \varepsilon_v^p\big) \tag{4.66}$$

and using the expression (4.57) of s yields

$$0 = \rho_{w0}\frac{m_w - m_{w0}^V}{m_{w0}^V + \rho_{w0}\varepsilon_v^p}\frac{\partial \mu_{wI}}{\partial m_w^p}\big(m_w^p, \varepsilon_v^p\big) + \frac{\partial \mu_{wI}}{\partial \varepsilon_v^p}\big(m_w^p, \varepsilon_v^p\big) \tag{4.67}$$

Expressions (4.65) and (4.67) give the partial derivatives of the function $\mu_{wI}(m_w^p, \varepsilon_v^p)$.

The requirement that the slope of the main curve I (i.e. the partial derivative of the function $\mu_{wI}\big(m_w, \varepsilon_v^p\big)$ given by (4.54) with respect to m_w) is less than the slope K of the scanning line yields

$$\frac{\mu_{w0} - \mu_{w1}}{m_{w0}^F + \rho_{w0}\varepsilon_v^p} f_I'\left(\frac{m_w - m_{w1}}{m_{w0}^F + \rho_{w0}\varepsilon_v^p}\right) < K$$

where $m_{w1} = m_{w0}^V$ and (4.53) have been used. Consequently, since $m_{w0}^F + \rho_{w0}\varepsilon_v^p > 0$ (it is the mass of free water at $\mu_w = \mu_{w0}$), the denominator of (4.65) is positive. Furthermore, since $f_I'(s) > 0$ and $\mu_{w0} - \mu_{w1} > 0$, it follows that

$$\frac{\partial \mu_{wI}}{\partial m_w^p}\left(m_w^p, \varepsilon_v^p\right) > 0 \tag{4.68}$$

Since in expression (4.67), ρ_{w0} is positive, by (4.57) the fraction that multiplies the partial derivative of $\mu_{wI}\left(m_w^p, \varepsilon_v^p\right)$ with respect to m_w^p is positive, except at $m_w = m_{w0}^V$ (i.e. at $\mu_{wI} = \mu_{w1}$) where it is zero, and by (4.68) the partial derivative is positive, it follows that

$$\begin{aligned} &\frac{\partial \mu_{wI}}{\partial \varepsilon_v^p}\left(m_w^p, \varepsilon_v^p\right) < 0 \quad \text{if} \quad \mu_{w1} < \mu_{wI} \leq \mu_{w0} \\ &\frac{\partial \mu_{wI}}{\partial \varepsilon_v^p}\left(m_w^p, \varepsilon_v^p\right) = 0 \quad \text{if} \quad \mu_{wI} = \mu_{w1} \end{aligned} \tag{4.69}$$

Note that the function $\mu_{wI}(m_w^p, \varepsilon_v^p)$ exists if and only if any scanning line intersects at only one point the corresponding main curve. As already mentioned, a sufficient condition is that the slope K of the scanning lines is greater than the slope of the corresponding main curve at any of its points. Since the main wetting and drying curves are obtained from the corresponding normalized curves by an affine transformation (see relations (4.54) and Figure 4.3) so that the square of size 1×1 is transformed into a rectangle of size $\left(m_{w0}^V + \rho_{w0}\varepsilon_v^p\right) \times (\mu_{w0} - \mu_{w1})$, the slopes of the transformed curves increase as ε_v^p decreases, so that, for sufficiently low ε_v^p the aforementioned sufficient condition does not hold. Values of ε_v^p such that this condition does not hold will be considered to be outside the model capabilities.

In the previous exposition it has been assumed that the soil is virtually unloaded to the reference load $(-p_0, \mu_{w0})$ so that the volumetric strains ε_v and the plastic volumetric strains ε_v^p coincide and that the soil skeleton was fixed. For simplicity it will be assumed that the effect of the elastic volumetric strains on the main wetting and drying curves is negligible. Consequently in what follows it will be assume that this formulation holds in general.

4.3.3.1 Free energy function

We assume that the free energy has the following form

$$\Psi\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \Psi_1\left(\varepsilon_v - \varepsilon_v^p\right) + \Psi_2\left(m_w - m_w^p\right) + \Psi_3\left(\varepsilon_v^p, m_w^p\right)$$

where

$$\begin{aligned} \Psi_2\left(m_w - m_w^p\right) &= \mu_{w0}\left(m_w - m_w^p\right) + \frac{1}{2}K\left(m_w - (m_{w0}^V + m_{w0}^F + m_w^p)\right)^2 \\ \Psi_3\left(\varepsilon_v^p, m_w^p\right) &= \int_{\rho_{w0}\varepsilon_v^p}^{m_w^p} \frac{1}{2}\left(\mu_{wW}(\varepsilon_v^p, s) + \mu_{wD}(\varepsilon_v^p, s)\right) ds \end{aligned} \tag{4.70}$$

The pressure p and the water chemical potential μ_w are given by

$$\begin{aligned} -p &= \frac{\partial \Psi}{\partial \varepsilon_v} = \frac{\partial \Psi_1}{\partial \varepsilon_v^e}\left(\varepsilon_v - \varepsilon_v^p\right) \\ \mu_w &= \frac{\partial \Psi}{\partial m_w} = \mu_{w0} + K\left(m_w - \left(m_{w0}^V + m_{w0}^F + m_w^p\right)\right) \end{aligned} \tag{4.71}$$

Note that (4.71) coincides with the expression (4.55) of the scanning line determined by m_w^p.

The generalized pressure and water chemical potential are given by

$$\begin{aligned}
-\bar{p} &= -\frac{\partial\Psi}{\partial\varepsilon_v^p}\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \frac{\partial\Psi_1}{\partial\varepsilon_v^e}\left(\varepsilon_v - \varepsilon_v^p\right) - \frac{\partial\Psi_3}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \\
&= -p - \frac{\partial\Psi_3}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \\
\bar{\mu}_w &= -\frac{\partial\Psi}{\partial m_w^p}\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \frac{\partial\Psi_2}{\partial m_w^e}\left(m_w - m_w^p\right) - \frac{\partial\Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) \\
&= \mu_w - \frac{\partial\Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right)
\end{aligned} \tag{4.72}$$

The partial derivative of $\Psi_3\left(\varepsilon_v^p, m_w^p\right)$ with respect to m_w^p is

$$\begin{aligned}
\frac{\partial\Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) &= \frac{\partial}{\partial m_w^p}\left(\int_{\rho_{w0}\varepsilon_v^p}^{m_w^p} \frac{1}{2}\left(\mu_{wW}(\varepsilon_v^p, s) + \mu_{wD}(\varepsilon_v^p, s)\right) ds\right) \\
&= \frac{1}{2}\left(\mu_{wW}(\varepsilon_v^p, m_w^p) + \mu_{wD}(\varepsilon_v^p, m_w^p)\right)
\end{aligned}$$

thus

$$\frac{\partial\Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) = \frac{1}{2}\left(\mu_{wW}(\varepsilon_v^p, m_w^p) + \mu_{wD}(\varepsilon_v^p, m_w^p)\right) \tag{4.73}$$

The partial derivative of $\Psi_3\left(\varepsilon_v^p, m_w^p\right)$ with respect to ε_v^p is

$$\begin{aligned}
\frac{\partial\Psi_3}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) &= \frac{\partial}{\partial\varepsilon_v^p}\left(\int_{\rho_{w0}\varepsilon_v^p}^{m_w^p} \frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, s\right) + \mu_{wD}\left(\varepsilon_v^p, s\right)\right) ds\right) \\
&= -\frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right)\left(1 \times \frac{\partial\left(\rho_{w0}\varepsilon_v^p\right)}{\partial\varepsilon_v^p}\right) \\
&\quad -\frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) + \mu_{wD}\left(\varepsilon_v^p, m_w^p\right)\right)\left(-1 \times \frac{\partial\left(m_w^p\right)}{\partial\varepsilon_v^p}\right) \\
&\quad -\int_{m_w^p}^{\rho_{w0}\varepsilon_v^p} \frac{1}{2}\left(\frac{\partial\mu_{wW}}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, s\right) + \frac{\partial\mu_{wD}}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, s\right)\right) ds \\
&= -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right) \\
&\quad +\rho_{w0}\frac{1}{2}\int_{m_w^p}^{\rho_{w0}\varepsilon_v^p}\left(\frac{m_{w0}^F + s}{m_{w0}^F + \rho_{w0}\varepsilon_v^p}\right)\left(\frac{\partial\mu_{wW}}{\partial m_w^p}\left(\varepsilon_v^p, s\right) + \frac{\partial\mu_{wD}}{\partial m_w^p}\left(\varepsilon_v^p, s\right)\right) ds
\end{aligned}$$

where the Reynolds transport theorem has been used to compute the derivative of the integral. Thus

$$\begin{aligned}
\frac{\partial\Psi_3}{\partial\varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) &= -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right) \\
&\quad +\rho_{w0}\frac{1}{2}\int_{m_w^p}^{\rho_{w0}\varepsilon_v^p}\left(\frac{m_{w0}^F + s}{m_{w0}^F + \rho_{w0}\varepsilon_v^p}\right)\left(\frac{\partial\mu_{wW}}{\partial m_w^p}\left(\varepsilon_v^p, s\right) + \frac{\partial\mu_{wD}}{\partial m_w^p}\left(\varepsilon_v^p, s\right)\right) ds
\end{aligned} \tag{4.74}$$

We now evaluate bounds of this integral.

Since $-m_{w0}^F < s \leq \rho_{w0}\varepsilon_v^p$ so that $m_{w0}^F + \rho_{w0}\varepsilon_v^p > 0$, it follows

$$0 = \frac{m_{w0}^F - m_{w0}^F}{m_{w0}^F + \rho_{w0}\varepsilon_v^p} < \frac{m_{w0}^F + s}{m_{w0}^F + \rho_{w0}\varepsilon_v^p} \leq \frac{m_{w0}^F + \rho_{w0}\varepsilon_v^p}{m_{w0}^F + \rho_{w0}\varepsilon_v^p} = 1$$

Using these bounds and the relation (4.68)

$$\frac{\partial \mu_{wI}}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) > 0$$

in expression (4.74) yields

$$\begin{aligned}
&\frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) > -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right)\\
&\frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \leq -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right)\\
&\quad + \rho_{w0}\frac{1}{2}\int_{m_w^p}^{\rho_{w0}\varepsilon_v^p}\left(\frac{\partial \mu_{wW}}{\partial m_w^p}\left(\varepsilon_v^p, s\right) + \frac{\partial \mu_{wD}}{\partial m_w^p}\left(\varepsilon_v^p, s\right)\right)ds\\
&= -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right)\\
&\quad + \rho_{w0}\frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right) - \rho_{w0}\frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) + \mu_{wD}\left(\varepsilon_v^p, m_w^p\right)\right)\\
&= -\frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) + \mu_{wD}\left(\varepsilon_v^p, m_w^p\right)\right)
\end{aligned}$$

since

$$\begin{gathered}
\mu_{w1} \leq \mu_{wD}\left(\varepsilon_v^p, m_w^p\right) \leq \mu_{w0}\\
\mu_{w1} \leq \mu_{wW}\left(\varepsilon_v^p, m_w^p\right) \leq \mu_{w0}\\
\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) = \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) = \mu_{w0}
\end{gathered}$$

it follows

$$\begin{aligned}
&-\frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) < \frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right) + \mu_{wD}\left(\varepsilon_v^p, \rho_{w0}\varepsilon_v^p\right)\right) = \rho_{w0}\mu_{w0}\\
&-\frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \geq \frac{1}{2}\rho_{w0}\left(\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) + \mu_{wD}\left(\varepsilon_v^p, m_w^p\right)\right) \geq \rho_{w0}\mu_{w1}
\end{aligned}$$

so that we have the bounds

$$\rho_{w0}\mu_{w1} \leq -\frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) < \rho_{w0}\mu_{w0} \tag{4.75}$$

4.3.3.2 Dissipation function

We assume that the dissipation function has the following form

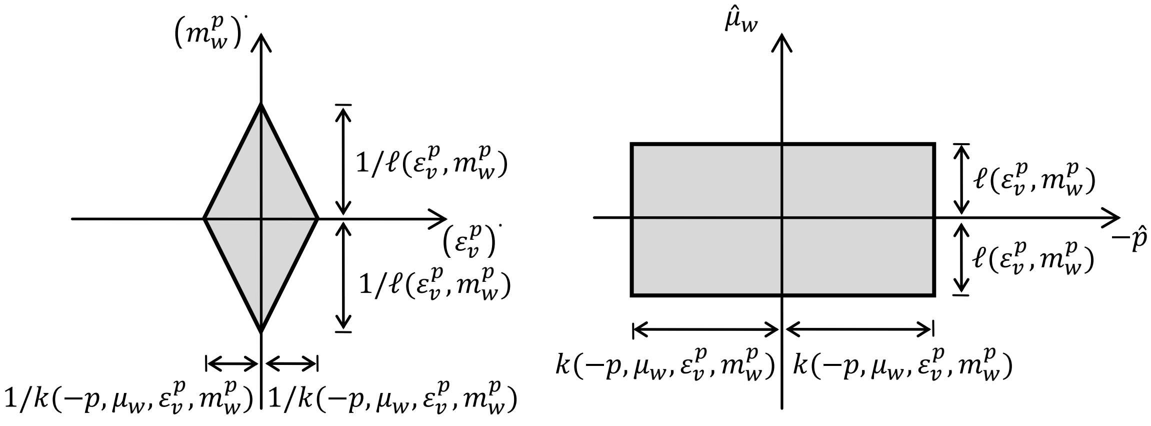
$$\begin{gathered}
\operatorname{dom}\Phi = \left\{\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right): \left(\varepsilon_v^p\right)^{\cdot} \in \mathbb{R}, \left(m_w^p\right)^{\cdot} \in \mathbb{R}\right\}\\
\Phi\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}; \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \left(\alpha(\cdot)(-p) + \beta(\cdot)\right)\left|\left(\varepsilon_v^p\right)^{\cdot}\right| + \ell(\cdot)\left|\left(m_w^p\right)^{\cdot}\right|
\end{gathered} \tag{4.76}$$

where $\alpha(\cdot)$, $\beta(\cdot)$ and $\ell(\cdot)$ are functions of the state $(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)$. The dissipation function must be non-negative. Consequently, for the range of admissible pressure p, water chemical potential μ_w, plastic volumetric deformation ε_v^p and plastic water mass m_w^p, the functions of state $\alpha(\cdot)$, $\beta(\cdot)$ and $\ell(\cdot)$ must be such that

$$\begin{aligned}&\alpha(\cdot)(-p) + \beta(\cdot) \geq 0\\ &\ell(\cdot) \geq 0\end{aligned}$$

We will determine these functions in terms of the yield pressure in extension $p_E\left(\mu_w, \varepsilon_v^p\right)$, the yield pressure in compression $p_C\left(\mu_w, \varepsilon_v^p\right)$, the yield water chemical potential in wetting $\mu_{wW}\left(m_w^p, \varepsilon_v^p\right)$ and the yield water chemical potential in drying $\mu_{wD}\left(m_w^p, \varepsilon_v^p\right)$. In the following developments we will assume that $k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot) \geq 0$ and $\ell(\cdot) \geq 0$.

Figure 4.4a shows the level set $\Phi \leq 1$ of the dissipation function. Note that Φ is not differentiable on the axes $\left(m_w^p\right)^{\cdot} = 0$ and $\left(\varepsilon_v^p\right)^{\cdot} = 0$.



a) b)

Figure 4.4. Capillary regime. a) The effective domain $\operatorname{dom}\Phi$ of the dissipation function is the whole plane and the gray rhombus centered at the origin is the level set $\Phi \leq 1$ of the dissipation function; b) the effective domain $\operatorname{dom}\Phi^*$ of the dual of the dissipation function is the gray rectangle centered at the origin. The two sets $\Phi \leq 1$ and $\operatorname{dom}\Phi^*$ are polars of each other (the lengths of the diagonals of the rhombus and the lengths of the respectively orthogonal sides of the rectangle are reciprocal to each other).

The subdifferential of Φ is

If $\left(\varepsilon_v^p\right)^{\cdot} \neq 0$ and $\left(m_v^p\right)^{\cdot} \neq 0$ (at these points Φ is differentiable)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right)\\ &\quad = \left\{(\hat{p}, \hat{\mu}_w) : -\hat{p} = k(-p,\cdot)\operatorname{sgn}\left(\left(\varepsilon_v^p\right)^{\cdot}\right), \hat{\mu}_w = \ell(\cdot)\operatorname{sgn}\left(\left(m_w^p\right)^{\cdot}\right)\right\}\end{aligned}$$

If $\left(\varepsilon_v^p\right)^{\cdot} > 0$, $\left(m_w^p\right)^{\cdot} = 0$ (4.77)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right)\\ &\quad = \left\{(\hat{p}, \hat{\mu}_w) : -\hat{p} = k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\right\}\end{aligned}$$

If $\left(\varepsilon_v^p\right)^{\cdot} < 0, \left(m_w^p\right)^{\cdot} = 0$

$$\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \\ = \{(\hat{p}, \hat{\mu}_w): -\hat{p} = -k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\}$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0, \left(m_w^p\right)^{\cdot} > 0$

$$\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \\ = \{(\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), \hat{\mu}_w = \ell(\cdot)\}$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0, \left(m_w^p\right)^{\cdot} < 0$

$$\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \\ = \{(\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), \hat{\mu}_w = -\ell(\cdot)\}$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0, \left(m_w^p\right)^{\cdot} = 0$

$$\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \\ = \{(\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\}$$

The Legendre-Fenchel dual Φ^* of Φ is the indicator function of the subdifferential of Φ at the origin $\partial\Phi\left(\left(0, 0; \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right)\right)$, namely

$$\begin{gathered} \operatorname{dom}\Phi^* = \{(-\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\} \\ \Phi^*\left((-\hat{p}, \hat{\mu}_w); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = 0 \end{gathered} \tag{4.78}$$

Figure 4.4b shows the effective domain $\operatorname{dom}\Phi^*$ of this function, which is a rectangle centered at the origin of the dual space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ of the space $E_{\left(\varepsilon_v^p\right)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}$. By the convention used in convex analysis (Rockafellar 1970), outside the effective domain the value of the proper lower semi-continuous convex function Φ^* is $+\infty$. Thus, the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ is

$$\hat{C}\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \{(-\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\} \tag{4.79}$$

The sides of the boundary of the elastic region and the respective cones of outer normals are

$$\begin{gathered} S_E = \{(-\hat{p}, \hat{\mu}_w): -\hat{p} = k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\} \quad \text{(extension)} \\ N_{\hat{C}(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)}(-\hat{p}, \hat{\mu}_w) = \{\lambda(1, 0)\,, \lambda \geq 0\} \\ S_C = \{(-\hat{p}, \hat{\mu}_w): -\hat{p} = -k(-p,\cdot), |\hat{\mu}_w| \leq \ell(\cdot)\} \quad \text{(compression)} \\ N_{\hat{C}(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)}(-\hat{p}, \hat{\mu}_w) = \{\lambda(-1, 0)\,, \lambda \geq 0\} \\ S_W = \{(-\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), \hat{\mu}_w = \ell(\cdot)\} \quad \text{(wetting)} \\ N_{\hat{C}(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)}(-\hat{p}, \hat{\mu}_w) = \{\lambda(0, 1)\,, \lambda \geq 0\} \\ S_D = \{(-\hat{p}, \hat{\mu}_w): |-\hat{p}| \leq k(-p,\cdot), \hat{\mu}_w = -\ell(\cdot)\} \quad \text{(drying)} \end{gathered} \tag{4.80}$$

$$N_{\hat{C}(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)}(-\hat{p},\hat{\mu}_w) = \{\lambda(0,-1)\,,\lambda \geq 0\}$$

The corners of the boundary of the elastic region and the respective cones of outer normals are

$$\begin{aligned}
&C_{EW} = \{(-\hat{p},\hat{\mu}_w): -\hat{p} = k(-p,\cdot), \hat{\mu}_w = \ell(\cdot)\} \quad \text{(extension-wetting)}\\
&\quad N_{\hat{C}(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)}(-\hat{p},\hat{\mu}_w) = \{\lambda_1(1,0) + \lambda_2(0,1)\,,\lambda_1 \geq 0, \lambda_2 \geq 0\}\\
&C_{CW} = \{(-\hat{p},\hat{\mu}_w): -\hat{p} = -k(-p,\cdot), \hat{\mu}_w = \ell(\cdot)\} \quad \text{(compression-wetting)}\\
&\quad N_{\hat{C}(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)}(-\hat{p},\hat{\mu}_w) = \{\lambda_1(-1,0) + \lambda_2(0,1)\,,\lambda_1 \geq 0, \lambda_2 \geq 0\}\\
&C_{ED} = \{(-\hat{p},\hat{\mu}_w): -\hat{p} = k(-p,\cdot), \hat{\mu}_w = -\ell(\cdot)\} \quad \text{(extension-drying)}\\
&\quad N_{\hat{C}(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)}(-\hat{p},\hat{\mu}_w) = \{\lambda_1(1,0) + \lambda_2(0,-1)\,,\lambda_1 \geq 0, \lambda_2 \geq 0\}\\
&C_{CD} = \{(-\hat{p},\hat{\mu}_w): -\hat{p} = -k(-p,\cdot), \hat{\mu}_w = -\ell(\cdot)\} \quad \text{(compression-drying)}\\
&\quad N_{\hat{C}(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p)}(-\hat{p},\hat{\mu}_w) = \{\lambda_1(-1,0) + \lambda_2(0,-1)\,,\lambda_1 \geq 0, \lambda_2 \geq 0\}
\end{aligned} \tag{4.81}$$

4.3.3.3 Ziegler's orthogonality principle

Ziegler's orthogonality principle reads

$$\left(-\frac{\partial\Psi}{\partial\varepsilon_v^p}, -\frac{\partial\Psi}{\partial m_w^p}\right)(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p) \in \partial\Phi\left(\left((\varepsilon_v^p)^{\cdot},(m_w^p)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)$$

where the left hand side is given by (4.72) and the right hand side by (4.77). Replacing $-\hat{p}$ and $\hat{\mu}_w$ in (4.77) by the expressions of $-\bar{p}$ and $\bar{\mu}_w$ in (4.72), we get

$$\begin{aligned}
&\text{If } (\varepsilon_v^p)^{\cdot} \neq 0, (m_w^p)^{\cdot} \neq 0\\
&-p - \frac{\partial\Psi_3}{\partial\varepsilon_v^p}(\varepsilon_v^p, m_w^p) = k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot)\\
&\mu_w - \frac{\partial\Psi_3}{\partial m_w^p}(\varepsilon_v^p, m_w^p) = \ell(\cdot)\\
&\text{If } (\varepsilon_v^p)^{\cdot} > 0, (m_w^p)^{\cdot} = 0 \text{ (yield in extension)}\\
&-p - \frac{\partial\Psi_3}{\partial\varepsilon_v^p}(\varepsilon_v^p, m_w^p) = k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot)\\
&\left|\mu_w - \frac{\partial\Psi_3}{\partial m_w^p}(\varepsilon_v^p, m_w^p)\right| \leq \ell(\cdot)\\
&\text{If } (\varepsilon_v^p)^{\cdot} < 0, (m_w^p)^{\cdot} = 0 \text{ (yield in compression)}\\
&-p - \frac{\partial\Psi_3}{\partial\varepsilon_v^p}(\varepsilon_v^p, m_w^p) = -k(-p,\cdot) = -\big(\alpha(\cdot)(-p) + \beta(\cdot)\big)
\end{aligned} \tag{4.82}$$

$$\left|\mu_w - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right)\right| \leq \ell(\cdot)$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0$, $\left(m_w^p\right)^{\cdot} > 0$ (yield in wetting)

$$\left|-p - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)\right| \leq k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot)$$
$$\mu_w - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) = \ell(\cdot)$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0$, $\left(m_w^p\right)^{\cdot} > 0$ (yield in drying)

$$\left|-p - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)\right| \leq k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot)$$
$$\mu_w - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) = -\ell(\cdot)$$

The transform of the elastic region in the space $E_{-p} \times E_{\mu_w}$ is

$$\begin{aligned} &C\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \\ &\quad = \left\{(-p, \mu_w): \left|-p - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)\right| \leq \alpha(\cdot)(-p) + \beta(\cdot), \left|\mu_w - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right)\right| \leq \ell(\cdot)\right\} \end{aligned} \tag{4.83}$$

We proceed to determine the functions $\alpha(\cdot)$, $\beta(\cdot)$ and $\ell(\cdot)$.

- For yield in wetting

$$\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) = \ell\left(m_w^p, \varepsilon_v^p\right)$$

- For yield in drying

$$\mu_{wD}\left(\varepsilon_v^p, m_w^p\right) - \frac{\partial \Psi_3}{\partial m_w^p}\left(\varepsilon_v^p, m_w^p\right) = -\ell\left(m_w^p, \varepsilon_v^p\right)$$

Consequently

$$\ell\left(m_w^p, \varepsilon_v^p\right) = \frac{1}{2}\left(\mu_{wW}\left(\varepsilon_v^p, m_w^p\right) - \mu_{wD}\left(\varepsilon_v^p, m_w^p\right)\right) \tag{4.84}$$

and, since (4.54) and (4.56) imply $\mu_{wW}\left(m_w, \varepsilon_v^p\right) - \mu_{wD}\left(m_w, \varepsilon_v^p\right) \geq 0$, it follows

$$\ell\left(m_w^p, \varepsilon_v^p\right) \geq 0 \tag{4.85}$$

- For yield in extension

$$-p_E\left(\mu_w, \varepsilon_v^p\right) - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) = \alpha\left(-p_E\left(\mu_w, \varepsilon_v^p\right)\right) + \beta$$

- For yield in compression

$$-p_C\left(\mu_w, \varepsilon_v^p\right) - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) = -\left(\alpha\left(-p_C\left(\mu_w, \varepsilon_v^p\right)\right) + \beta\right)$$

Consequently

$$\begin{aligned}
\alpha(\mu_w, \varepsilon_v^p, m_w^p) &= -\frac{p_C\left(\mu_w, \varepsilon_v^p\right) + p_E\left(\mu_w, \varepsilon_v^p\right) + 2\dfrac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)}{p_C\left(\mu_w, \varepsilon_v^p\right) - p_E\left(\mu_w, \varepsilon_v^p\right)} \\
\beta(\mu_w, \varepsilon_v^p, m_w^p) &= -\frac{2p_C\left(\mu_w, \varepsilon_v^p\right)p_E\left(\mu_w, \varepsilon_v^p\right) + \left(p_C\left(\mu_w, \varepsilon_v^p\right) + p_E\left(\mu_w, \varepsilon_v^p\right)\right)\dfrac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)}{p_C\left(\mu_w, \varepsilon_v^p\right) - p_E\left(\mu_w, \varepsilon_v^p\right)}
\end{aligned} \tag{4.86}$$

The expressions

$$\begin{aligned}
\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)\left(-p_E\left(\mu_w, \varepsilon_v^p\right)\right) + \beta\left(\mu_w, \varepsilon_v^p, m_w^p\right) &= -p_E\left(\mu_w, \varepsilon_v^p\right) - \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \\
\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)\left(-p_C\left(\mu_w, \varepsilon_v^p\right)\right) + \beta\left(\mu_w, \varepsilon_v^p, m_w^p\right) &= p_C\left(\mu_w, \varepsilon_v^p\right) + \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right)
\end{aligned}$$

are positive if and only if

$$-p_C\left(\mu_w, \varepsilon_v^p\right) < \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) < -p_E\left(\mu_w, \varepsilon_v^p\right) \tag{4.87}$$

and in this case, since $\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)(-p) + \beta\left(\mu_w, \varepsilon_v^p, m_w^p\right)$ is linear in $-p$, it follows

$$\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)(-p) + \beta\left(\mu_w, \varepsilon_v^p, m_w^p\right) > 0 \quad -p_C\left(\mu_w, \varepsilon_v^p\right) \leq -p \leq -p_E(\mu_w, \varepsilon_v^p) \tag{4.88}$$

Since by (4.75) we have the bounds

$$-\rho_{w0}\mu_{w0} < \frac{\partial \Psi_3}{\partial \varepsilon_v^p}\left(\varepsilon_v^p, m_w^p\right) \leq -\rho_{w0}\mu_{w1}$$

it follows that the conditions

$$\begin{gathered}
-p_C\left(\mu_w, \varepsilon_v^p\right) \leq -\rho_{w0}\mu_{w0} \\
-\rho_{w0}\mu_{w1} \leq -p_E(\mu_w, \varepsilon_v^p)
\end{gathered}$$

imply the conditions (4.87). Consequently, we have

$$\begin{gathered}
-p_C\left(\mu_w, \varepsilon_v^p\right) \leq -\rho_{w0}\mu_{w0} \text{ and } -\rho_{w0}\mu_{w1} \leq -p_E(\mu_w, \varepsilon_v^p) \\
\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)(-p) + \beta\left(\mu_w, \varepsilon_v^p, m_w^p\right) > 0 \quad \text{for} \quad -p_C\left(\mu_w, \varepsilon_v^p\right) \leq -p \leq -p_E\left(\mu_w, \varepsilon_v^p\right)
\end{gathered} \tag{4.89}$$

This condition restricts the range of applicability of the model, although with the values of μ_{w0} and μ_{w1} (the zero of water chemical potential is taken for free water at 1atm and 20°C), which correspond, respectively, to the air entry value and to the total evaporation of free water, this condition is not too restrictive. Note that it is necessary that $p_C\left(\mu_w, \varepsilon_v^p\right) - p_E\left(\mu_w, \varepsilon_v^p\right) > 0$ for the expressions (4.86) of $\alpha\left(\mu_w, \varepsilon_v^p, m_w^p\right)$ and $\beta\left(\mu_w, \varepsilon_v^p, m_w^p\right)$ to be defined.

Figure 4.5 shows the elastic region in the space $E_{-p} \times E_{\mu_w}$, with a shape similar to the elastic region proposed in the BBM model (Alonso et al. 1990), but restricted to a variable horizontal strip $\mu_{wW}\left(m_w^p, \varepsilon_v^p\right) \leq \mu_w \leq \mu_{wD}\left(m_w^p, \varepsilon_v^p\right)$, whose projection on the vertical axis is the thick segment shown in Figure 4.3a. This strip reduces to a horizontal line at the transition from the saturated regime to the capillary regime $\mu_w = \mu_{w0}$ and at the transition between the capillary regime and the dry regime $\mu_w = \mu_{w1}$. The flow directions are not normal to the boundary of the elastic region (they are normal to the boundary of the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$).

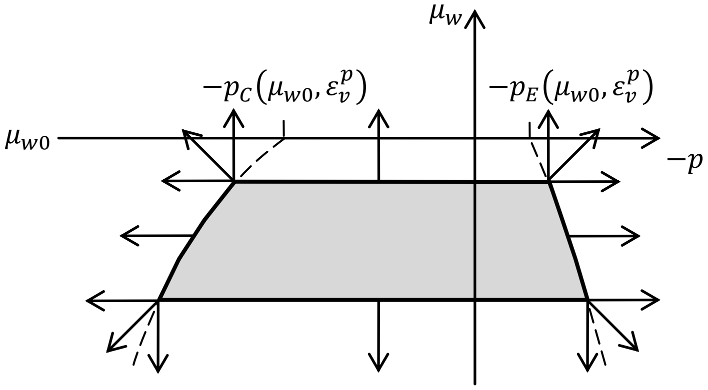


Figure 4.5. Capillary regime. Elastic region in the space $E_{-p} \times E_{\mu_w}$. At the transition from the saturated regime to the capillary regime $\mu_w = \mu_{w0}$ (here μ_{w0} has been taken to be zero by simplicity), $p_C(\mu_{w0}, \varepsilon_v^p)$ is the yield pressure in compression and $p_E\left(\mu_{w0}, \varepsilon_v^p\right)$ is the yield pressure in extension. Arrows indicate flow directions, which, except at the horizontal boundaries (yield in drying and yield in wetting), are not normal to the boundary (they are normal to the boundary of the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$). At each corner there is a fan of flow directions.

Remarks

- The interior of the elastic region in the space $E_{-p} \times E_{\mu_w}$ vanishes at $\mu_w = \mu_{w0}$, the transition from the saturated regime to the capillary regime, and at $\mu_w = \mu_{w1}$ the transition from the capillary regime to the dry regime.

- The elastic region can have a shape similar to the elastic region proposed in the BBM model (Alonso et al. 1990), which allows to reproduce reversible shrinking and hardening upon drying or irreversible collapse upon wetting.

- In the space $E_{-p} \times E_{\mu_w}$ the flow rule is associated in wetting and in drying, but it is not associated extension and in compression. In the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ the flow rule is associated.

4.3.4 Dry regime

The transition from the capillary regime to the dry regime occurs at $\mu_w = \mu_{w1}$. It will be assumed that in the dry regime there is no free water $m_w^F = 0$ and the vicinal water varies m_w^V.

4.3.4.1 *Free energy function*

We assume that the free energy has the following form

$$\Psi(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p) = \Psi_1(\varepsilon_v - \varepsilon_v^p, m_w) + \Psi_2(\varepsilon_v^p) \tag{4.90}$$

The pressure p and the water chemical potential μ_w are given by

$$\begin{aligned} -p &= \frac{\partial \Psi}{\partial \varepsilon_v} = \frac{\partial \Psi_1}{\partial \varepsilon_v^e}(\varepsilon_v - \varepsilon_v^p, m_w) \\ \mu_w &= \frac{\partial \Psi}{\partial m_w} = \frac{\partial \Psi_1}{\partial m_w}(\varepsilon_v - \varepsilon_v^p, m_w) \end{aligned} \tag{4.91}$$

The generalized pressure and water chemical potential are given by

$$\begin{aligned} -\bar{p} &= -\frac{\partial \Psi}{\partial \varepsilon_v^p} = \frac{\partial \Psi_1}{\partial \varepsilon_v^e}(\varepsilon_v - \varepsilon_v^p, m_w) - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) = -p - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) \\ \bar{\mu}_w &= -\frac{\partial \Psi}{\partial m_w^p} = 0 \end{aligned} \tag{4.92}$$

4.3.4.2 *Dissipation function*

We assume that the dissipation function has the following form

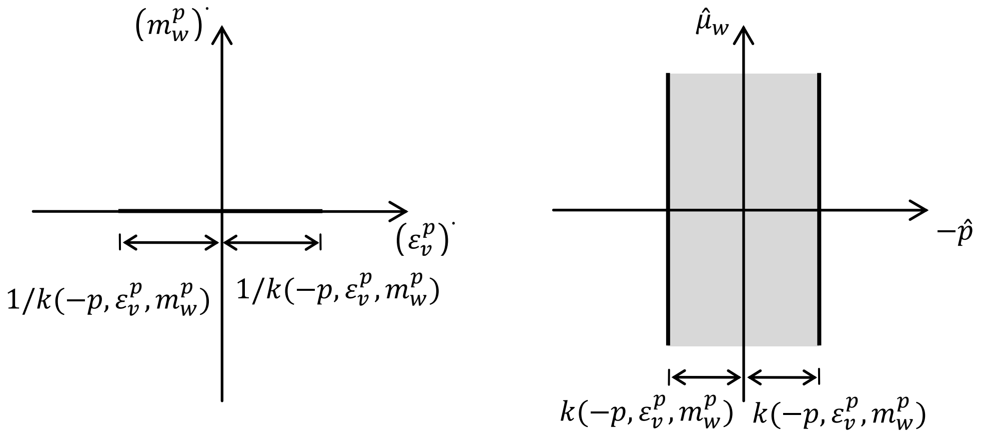
$$\begin{aligned} \operatorname{dom} \Phi &= \left\{ \left((\varepsilon_v^p)^{\cdot}, (m_w^p)^{\cdot} \right) : (m_w^p)^{\cdot} = 0 \right\} \\ \Phi\left((\varepsilon_v^p)^{\cdot}, (m_w^p)^{\cdot}; \varepsilon_v, m_w, \varepsilon_v^p, m_w^p \right) &= \left(\alpha(\cdot)(-p) + \beta(\cdot) \right) \left| (\varepsilon_v^p)^{\cdot} \right| \end{aligned} \tag{4.93}$$

where $\alpha(\cdot)$ and $\beta(\cdot)$ are functions of state. Note that $\operatorname{dom}\Phi$ is a closed convex one-dimensional subset of the space $E_{(\varepsilon_v^p)^{\cdot}} \times E_{(m_w^p)^{\cdot}}$. The dissipation function must be non-negative. Consequently, for the range of admissible pressure p, water chemical potential μ_w, plastic volumetric deformation ε_v^p and plastic water mass m_w^p, the functions of state $\alpha(\cdot)$, $\beta(\cdot)$ and $\ell(\cdot)$ must be such that

$$\alpha(\cdot)(-p) + \beta(\cdot) \geq 0$$

We will determine these functions by prescribing the pressure in extension yield $p_E(\mu_w, \varepsilon_v^p)$ and the pressure in compression yield $p_C(\mu_w, \varepsilon_v^p)$. In the following developments we will assume that $k(-p,\cdot) = \alpha(\cdot)(-p) + \beta(\cdot) \geq 0$.

Figure 4.6a shows the effective domain $\operatorname{dom}\Phi$ and the level set $\Phi \leq 1$ of the dissipation function. Recall that, by the convention used in convex analysis (Rockafellar 1970), outside the effective domain the value of the proper lower semi-continuous convex function Φ is $+\infty$.



a) b)

Figure 4.6. Dry regime. a) The horizontal axis is the effective domain $\operatorname{dom}\Phi$ of the dissipation function and the thick segment is the level set $\Phi \le 1$ of the dissipation function; b) The gray strip that has a width of $2k(\varepsilon_v^p)$ and its axis is the vertical axis is the effective domain $\operatorname{dom}\Phi^*$ of the dual of the dissipation function. The two sets $\Phi \le 1$ and $\operatorname{dom}\Phi^*$ are polars of each other (the length of the segment and the width of the strip are reciprocal to each other).

The subdifferential of Φ is

If $\left(\varepsilon_v^p\right)^{\cdot} > 0$, $\left(m_w^p\right)^{\cdot} = 0$ (yield in compression)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\{(\hat{p},\hat{\mu}_w):-\hat{p}=k(-p,\cdot)\}\\&=\{(k(-p,\cdot),u),u\in\mathbb{R}\}\end{aligned}$$

If $\left(\varepsilon_v^p\right)^{\cdot} < 0$, $\left(m_w^p\right)^{\cdot} = 0$ (yield in extension)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\{(\hat{p},\hat{\mu}_w):-\hat{p}=-k(-p,\cdot)\}\\&=\{(-k(-p,\cdot),u),u\in\mathbb{R}\}\end{aligned} \tag{4.94}$$

If $\left(\varepsilon_v^p\right)^{\cdot} = 0$, $\left(m_w^p\right)^{\cdot} = 0$ (elasticity)

$$\begin{aligned}&\partial\Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot},\left(m_w^p\right)^{\cdot}\right);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\{(\hat{p},\hat{\mu}_w):|-\hat{p}|\le k(-p,\cdot)\}\\&=\{(v,u),u\in\mathbb{R},-k(-p,\cdot)\le v\le k(-p,\cdot)\}\end{aligned}$$

The Legendre-Fenchel dual Φ^* of Φ is the indicator function of the subdifferential of Φ at the origin $\partial\Phi\left(\left(0,0;\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)\right)$, namely

$$\begin{aligned}\operatorname{dom}\Phi^*&=\{(-\hat{p},\hat{\mu}_w):|-\hat{p}|\le k(-p,\cdot)\}\\ \Phi^*\left((-\hat{p},\hat{\mu}_w);\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)&=0\end{aligned} \tag{4.95}$$

Figure 4.6b shows the effective domain $\operatorname{dom}\Phi^*$ of this function, which is stripe whose axis is the vertical axis of the dual space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ of the space $E_{\left(\varepsilon_v^p\right)^{\cdot}} \times E_{\left(m_w^p\right)^{\cdot}}$. By the convention used in convex analysis (Rockafellar 1970), outside the effective domain the value of the proper lower semi-continuous convex function Φ^* is $+\infty$. Thus, the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ is

$$\hat{C}\left(\varepsilon_v,m_w,\varepsilon_v^p,m_w^p\right)=\{(-\hat{p},\hat{\mu}_w):|-\hat{p}|\le k(-p,\cdot)\} \tag{4.96}$$

The sides of the boundary of the elastic region and the respective cones of outer normals are

$$
\begin{aligned}
&S_E = \{(-\hat{p}, \hat{\mu}_w) : -\hat{p} = k(-p, \cdot)\} \quad \text{(extension)} \\
&\quad N_{\hat{C}(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)}(-\hat{p}, \hat{\mu}_w) = \{\lambda(1, 0)\,, \lambda \geq 0\} \\
&S_C = \{(-\hat{p}, \hat{\mu}_w) : -\hat{p} = -k(-p, \cdot)\} \quad \text{(compression)} \\
&\quad N_{\hat{C}(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p)}(-\hat{p}, \hat{\mu}_w) = \{\lambda(-1, 0)\,, \lambda \geq 0\}
\end{aligned}
\tag{4.97}
$$

4.3.4.3 Ziegler's orthogonality principle

Ziegler's orthogonality principle reads

$$\left(-\frac{\partial \Psi}{\partial \varepsilon_v^p}, -\frac{\partial \Psi}{\partial m_w^p}\right)\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) \in \partial \Phi\left(\left(\left(\varepsilon_v^p\right)^{\cdot}, \left(m_w^p\right)^{\cdot}\right); \varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right)$$

where the left hand side is given by (4.92) and the right hand side by (4.94). Replacing $-\hat{p}$ and $\hat{\mu}_w$ in (4.94) by the expressions of $-\bar{p}$ and $\bar{\mu}_w$ in (4.92), we get

If $\left(\varepsilon_v^p\right)^{\cdot} > 0$, $\left(m_w^p\right)^{\cdot} = 0$ (yield in extension)

$$
\begin{gathered}
-p - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right) = k(-p, \cdot) \\
0 = u \\
-p = \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right) + k(-p, \cdot)
\end{gathered}
$$

If $\left(\varepsilon_v^p\right)^{\cdot} < 0$, $\left(m_w^p\right)^{\cdot} = 0$ (yield in compression)

$$
\begin{gathered}
-p - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right) = -k(-p, \cdot) \\
0 = u \\
-p = \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right) - k(-p, \cdot)
\end{gathered}
\tag{4.98}
$$

The transform of the elastic region in the space $E_{-p} \times E_{\mu_w}$ is

$$C\left(\varepsilon_v, m_w, \varepsilon_v^p, m_w^p\right) = \left\{(-p, \mu_w) : \left|-p - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right)\right| \leq \alpha(\cdot)(-p) + \beta(\cdot)\right\} \tag{4.99}$$

We proceed to determine the functions $\alpha(\cdot)$ and $\beta(\cdot)$.

- For yield in extension

$$-p_E\left(\mu_w, \varepsilon_v^p\right) - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}\left(\varepsilon_v^p\right) = \alpha\left(-p_E\left(\mu_w, \varepsilon_v^p\right)\right) + \beta$$

- For yield in compression

$$-p_C(\mu_w, \varepsilon_v^p) - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) = -\left(\alpha\left(-p_C(\mu_w, \varepsilon_v^p)\right) + \beta\right)$$

Consequently

$$\begin{aligned} \alpha(\mu_w, \varepsilon_v^p) &= -\frac{p_C(\mu_w, \varepsilon_v^p) + p_E(\mu_w, \varepsilon_v^p)}{p_C(\mu_w, \varepsilon_v^p) - p_E(\mu_w, \varepsilon_v^p)} \\ \beta(\mu_w, \varepsilon_v^p) &= -\frac{2p_C(\mu_w, \varepsilon_v^p)p_E(\mu_w, \varepsilon_v^p)}{p_C(\mu_w, \varepsilon_v^p) - p_E(\mu_w, \varepsilon_v^p)} \end{aligned} \tag{4.100}$$

The expressions

$$\begin{aligned} \alpha(\mu_w, \varepsilon_v^p)\left(-p_E(\mu_w, \varepsilon_v^p)\right) + \beta(\mu_w, \varepsilon_v^p) &= -p_E(\mu_w, \varepsilon_v^p) - \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) \\ \alpha(\mu_w, \varepsilon_v^p)\left(-p_C(\mu_w, \varepsilon_v^p)\right) + \beta(\mu_w, \varepsilon_v^p) &= p_C(\mu_w, \varepsilon_v^p) + \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) \end{aligned}$$

are positive if and only if

$$-p_C(\mu_w, \varepsilon_v^p) < \frac{\partial \Psi_2}{\partial \varepsilon_v^p}(\varepsilon_v^p) < -p_E(\mu_w, \varepsilon_v^p) \tag{4.101}$$

and in this case, since $\alpha(\mu_w, \varepsilon_v^p, m_w^p)(-p) + \beta(\mu_w, \varepsilon_v^p, m_w^p)$ is linear in $-p$, it follows

$$\alpha(\mu_w, \varepsilon_v^p)(-p) + \beta(\mu_w, \varepsilon_v^p) > 0 \quad -p_C(\mu_w, \varepsilon_v^p) \le -p \le -p_E(\mu_w, \varepsilon_v^p) \tag{4.102}$$

This condition is satisfied if $p_C(\mu_w, \varepsilon_v^p) > 0$ and $p_E(\mu_w, \varepsilon_v^p) \le 0$. Note that it is necessary that $p_C(\mu_w, \varepsilon_v^p) - p_E(\mu_w, \varepsilon_v^p) > 0$ for the expressions (4.100) of $\alpha(\mu_w, \varepsilon_v^p)$ and $\beta(\mu_w, \varepsilon_v^p)$ to be defined.

Figure 4.7 shows the elastic region in the space $E_{-p} \times E_{\mu_w}$,

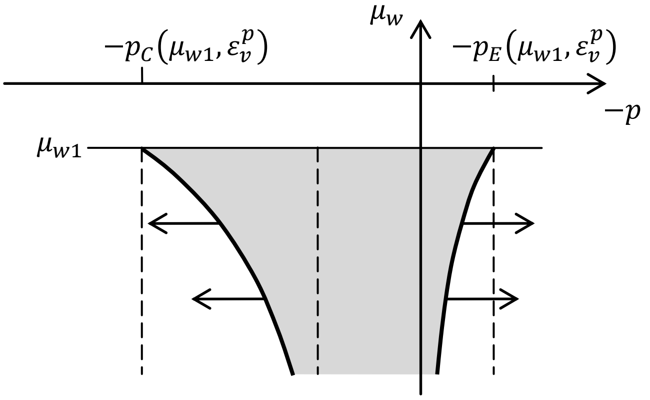


Figure 4.7. Dry regime. Elastic region in the space $E_{-p} \times E_{\mu_w}$. At the transition $\mu_w = \mu_{w1}$ from the capillary regime to the dry regime, $p_C(\mu_{w1}, \varepsilon_v^p)$ is the yield pressure in compression and $p_E(\mu_{w1}, \varepsilon_v^p)$ is the yield pressure in extension. Arrows indicate flow directions, which are not normal to the boundary (they are normal to the boundary of the elastic region in the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$).

Remarks

- Since water mass is fully recoverable, there is no plastic water mass component m_w^p.

- As the water mass decreases with the water chemical potential, the stabilizing effect of the liquid-gas interfaces tends to decrease, so that the increase of the compression yield pressure and the decrease of the extension yield pressure acquired during the capillary regime tend to vanish.

- In the space $E_{-p} \times E_{\mu_w}$ the flow rule is not associated extension and in compression. In the space $E_{-\hat{p}} \times E_{\hat{\mu}_w}$ the flow rule is associated.

- Since there is no free water, all water in the soil is vicinal water. In the scientific literature exceedingly high negative pressures are usual. However, if water is tightly bonded to the soil skeleton, water pressures at the microscale are expected to be highly positive. In the proposed formulation for the dry regime water pressures are not used.

4.4 SOME ADDITIONAL TOPICS

4.4.1 Work input, matric suction and negative pore water pressures

Houlsby (1997) considers the power input to an unsaturated soil made of a solid phase, a water phase, an air phase and an air-water interface. The total stress tensor is the sum of contributions from the solid, water and air phases and from the air-water interface, but it is assumed that the solid phase and the air-water interface move with the same velocity. He derives two alternative expressions of the power input to an unsaturated soil, one with Bishop's stress (with $\chi = S_r$) and suction as stress variables and another with net stress and suction as stress variables. From these work input expressions follow in each case the identification of the corresponding work-conjugated variables.

Coussy (2004) considers the power input to an unsaturated soil made of a solid phase, a water phase, an air phase and the corresponding interfaces. The total stress tensor is the sum of contributions from the solid, water and air phases. Gray et al. (2010) consider the power input to unsaturated elastic porous media made of a solid phase, a wetting fluid phase, a non-wetting fluid phase, the interfaces between these phases and the common curve along the solid surface where the two fluid phases meet. The total stress tensor is the sum of contributions from all phases, all interfaces and the common curve. In these works, the liquid and gas pressures multiplied by their respective volume fractions correspond to the (smeared) spherical stress tensors of the liquid and gas phases.

The expressions of the power input to an unsaturated soil obtained in Houlsby (1997) are often referred in the unsaturated soil mechanics literature. However they have been applied even when liquid pressures have exceedingly large negative values. Gray and Hassanizadeh (1991) consider that negative absolute water pressures are unrealistic and in their work they introduce wetting potentials to account for the attraction forces between the solid and fluid phases. In fact, short-range interaction forces bonding water to the solid skeleton should give rise to microscale positive (compressive) pressures (Nitao and Bear 1996), so that averaging of microscale distributions of those pressures would yield positive (compressive) macroscale pressures. But, in this case, the expression of the work input used in those developments should include also a contribution from the short-range interaction forces. In this regard Alcoverro (2003) noted that, if at a microscale point x an incompressible fluid with pressure $p(x)$ is subjected to a potential body force field $-\varphi_{,i}(x)$, then the terms of the balance of momentum of the fluid at the microscale $\left(-p\delta_{ij}\right)_{,j} - \varphi_{,i}$ can be written in the form $\left(-\tilde{p}\delta_{ij}\right)_{,j}$ with $\tilde{p}(x) = p(x) + \varphi(x)$. If $\varphi(x)$ is the potential of an attraction force field (i.e. bonds the fluid to the solid skeleton) that vanishes at infinity, then it follows that $\varphi(x) < 0$. Consequently, although the (absolute) pressure $p(x)$ is positive, the modified pressure $\tilde{p}(x)$ can be negative. Note that, at local equilibrium states, the microscale distribution of $\tilde{p}(x)$ is uniform (neglecting gravity forces).

In thermodynamics the work input is used in the balance of energy, which, when combined with the balance of entropy, yields the entropy inequality. In the present formulation the entropy inequality (3.18) is written in terms of the power of the total stress tensor on the solid skeleton deformation, the working of the chemical potentials of the species on the corresponding mass variations and the heating. For free water, which is not subjected to interaction forces with the solid skeleton, microscale distributions of pressure are uniform (neglecting gravity forces), giving rise to macroscale water pressures with the same value as the microscale water pressures. Since free water behaves as if it were outside the unsaturated soil, large absolute negative water pressures should not be expected.

In unsaturated soil mechanics, matric suction s is defined by the relation

$$s = p_G - p_L \qquad (4.103)$$

where p_G is the pressure of the gas phase and p_L is the pressure of the liquid phase. As already mentioned, high matric suction values (i.e. several MPa), which at atmospheric gas pressure imply large negative liquid pressures, are acknowledged to in fact represent bonding energies per unit volume. In the proposed framework, matric suction $s = p_G - p_L$ can be defined only in the capillary regime, in which both free liquid and free gas are present in the soil, so that the gas pressure and the liquid pressure can be defined. It is therefore of interest to state the matric suction in terms of chemical potentials.

In an unsaturated soil with a free liquid phase and a free gas phase, the respective pressures can be defined as functions of the chemical potentials of the constituents and temperature using their respective state equations, as in (3.36). In an unsaturated soil, we assume that the constituents of the free liquid and the free gas are water and air. Using the definition of matric suction s yields

$$s(\mu_w, \mu_a, \theta) = p_G(\mu_w, \mu_a, \theta) - p_L(\mu_w, \mu_a, \theta) \tag{4.104}$$

where p_G is the pressure of the free gas and p_L is the pressure of the free liquid. Thus matric suction s is a function of the chemical potentials of water μ_w and air μ_a and of the temperature θ. We assume that the free gas is a mixture of air and water vapor, which behave as ideal gases. Since at ambient atmospheric conditions the saturation water vapor pressure is a small fraction of the atmospheric pressure (for instance, at $p_G = 1\ \text{atm} = 1013\ \text{mbar}$ and $\theta = 10 - 40°\text{C}$ the saturation water vapor pressure is $p_{Gw} = 12.271 - 73.75\ \text{mbar}$), it follows that $p_G = p_{Ga} + p_{Gw} \cong p_{Ga}$. Since $\mu_{Ga} = \mu_{Ga}(p_{Ga}, \theta)$, it follows that the matric suction s is a function of the chemical potential of water μ_w, the gas pressure p_G and the temperature θ, namely

$$\bar{s}(\mu_w, p_G, \theta) = p_G - p_L(\mu_w, \mu_{Ga}(p_G, \theta), \theta) \tag{4.105}$$

If the air dissolved in the liquid can be neglected, this relation reduces to

$$\bar{s}(\mu_w, p_G, \theta) = p_G - p_L(\mu_w, \theta) \tag{4.106}$$

Consequently, at constant ambient atmospheric pressure p_G and temperature θ, the matric suction s is a function of the water chemical potential μ_w. This conclusion holds only if there is free liquid and free gas in the unsaturated soil (i.e. in the capillary regime).

4.4.2 Local equilibrium states and Coussy's formulation

We will show that Coussy's formulation (Coussy 2004) for a porous material saturated by a fluid can be interpreted by considering local equilibrium states. This formulation can be summarized as follows

- The free energy of the porous material per unit reference volume Ψ of a porous material saturated by a fluid is assumed to be of the form (Coussy 2004, Eq. (3.68))

  $$\Psi = \Psi(\Delta_{ij}, m_f, T; \chi_J)$$

  where Δ_{ij} is the Green-Lagrange strain tensor of the porous material, m_f is the fluid mass content per unit reference volume, T is the temperature and χ_J is a set of internal variables. Considering evolutions where the internal variables do not vary, the following state equations are derived from the vanishing of the internal dissipation (Coussy 2004, Eq. (3.69))

  $$\pi_{ij} = \frac{\partial \Psi}{\partial \Delta_{ij}} \qquad g_f = \frac{\partial \Psi}{\partial m_f} \qquad S = -\frac{\partial \Psi}{\partial T}$$

  where π_{ij} is the total second Piola-Kirchhoff stress tensor and g_f is the fluid-specific free enthalpy.

- The free energy and entropy of the porous material per unit reference volume are given by (Coussy 2004, Eq. (3.62))

  $$\Psi = \Psi_S + m_f \psi_f \qquad S = S_S + m_f s_f$$

  where Ψ_S and S_S are the free energy and entropy of the solid skeleton per unit reference volume and ψ_f and s_f are the fluid-specific Helmholtz free energy and the fluid-specific entropy.

- The fluid state equations are (Coussy 2004, Eq. (3.8))

  $$\psi_f = \psi_f\left(\frac{1}{\rho_f}, T\right) \qquad p = -\frac{\partial \psi_f}{\partial\left(\frac{1}{\rho_f}\right)} \qquad s_f = -\frac{\partial \psi_f}{\partial T}$$

  where p is the fluid pressure and ρ_f is the fluid density.

- The free energy of the skeleton per unit reference volume is assumed to be of the form (Coussy 2004, Eq. (3.62))

  $$\Psi_S = \Psi_S(\Delta_{ij}, \phi, T; \chi_J)$$

  where ϕ is the pore volume per unit reference volume. Considering evolutions where the internal variables do not vary, the following state equations are derived from the vanishing of the internal dissipation (Coussy 2004, Eq. (3.65))

  $$\pi_{ij} = \frac{\partial \Psi_S}{\partial \Delta_{ij}} \qquad p = \frac{\partial \Psi_S}{\partial \phi} \qquad S_S = -\frac{\partial \Psi_S}{\partial T}$$

Taking into account that (Coussy 2004, Eq. (1.64))

$$m_f = \rho_f \phi$$

it follows that

$$\Psi\left(\Delta_{ij}, m_f, T; \chi_J\right) = \Psi_S\left(\Delta_{ij}, \phi, T; \chi_J\right) + m_f \psi_f\left(\frac{\phi}{m_f}, T\right)$$

but, since $\Psi_S\left(\Delta_{ij}, \phi, T; \chi_J\right)$ and $\psi_f(\phi/m_f, T)$ are a priori unrelated functions, it follows that the variables Δ_{ij}, ϕ, m_f, T and χ_J cannot be independent. However such a dependency is not mentioned in Coussy's formulation.

In the proposed formulation, $\widetilde{\Psi} = \tilde{\Psi}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right)$ and $\widetilde{\Psi}_S = \widetilde{\Psi}_S\left(\Delta_{ij}, \phi, T; \chi_J\right)$, so that

$$\tilde{\Psi}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) = \widetilde{\Psi}_S\left(\Delta_{ij}, \phi, T; \chi_J\right) + m_f \psi_f\left(\frac{\phi}{m_f}, T\right)$$

Consequently

$$\begin{aligned}
\frac{\partial \widetilde{\Psi}}{\partial \Delta_{ij}}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \frac{\partial \widetilde{\Psi}_S}{\partial \Delta_{ij}}\left(\Delta_{ij}, \phi, T; \chi_J\right) \\
\frac{\partial \widetilde{\Psi}}{\partial \phi}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \frac{\partial \widetilde{\Psi}_S}{\partial \phi}\left(\Delta_{ij}, \phi, T; \chi_J\right) + \frac{\partial \psi_f}{\partial\left(\frac{1}{\rho_f}\right)}\left(\frac{\phi}{m_f}, T\right) \\
\frac{\partial \widetilde{\Psi}}{\partial m_f}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \psi_f\left(\frac{\phi}{m_f}, T\right) - \frac{\phi}{m_f} \frac{\partial \psi_f}{\partial\left(\frac{1}{\rho_f}\right)}\left(\frac{\phi}{m_f}, T\right) \\
\frac{\partial \widetilde{\Psi}}{\partial T}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \frac{\partial \widetilde{\Psi}_S}{\partial T}\left(\Delta_{ij}, \phi, T; \chi_J\right) + m_f \frac{\partial \psi_f}{\partial T}\left(\frac{\phi}{m_f}, T\right)
\end{aligned}$$

The last 3 relations can be rewritten as

$$\begin{aligned}
\frac{\partial \widetilde{\Psi}}{\partial \phi}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \frac{\partial \widetilde{\Psi}_S}{\partial \phi}\left(\Delta_{ij}, \phi, T; \chi_J\right) - p\left(\frac{\phi}{m_f}, T\right) \\
\frac{\partial \widetilde{\Psi}}{\partial m_f}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= g_f\left(\frac{\phi}{m_f}, T\right) \\
\frac{\partial \widetilde{\Psi}}{\partial T}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) &= \frac{\partial \widetilde{\Psi}_S}{\partial T}\left(\Delta_{ij}, \phi, T; \chi_J\right) - m_f s_f\left(\frac{\phi}{m_f}, T\right)
\end{aligned}$$

Solving for ϕ in the minimization condition

$$\frac{\partial \widetilde{\Psi}}{\partial \phi}\left(\Delta_{ij}, \phi, m_f, T; \chi_J\right) = 0$$

yields the relation $\phi = \phi(\Delta_{ij}, m_f, T; \chi_J)$, so that, at local equilibrium states

$$\frac{\partial \widetilde{\Psi}_S}{\partial \phi}\left(\Delta_{ij}, \phi(\Delta_{ij}, m_f, T; \chi_J), T; \chi_J\right) = p\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right)$$

If we interpret that Coussy's functions $\Psi(\Delta_{ij}, m_f, T; \chi_J)$ and $\Psi_S\left(\Delta_{ij}, \phi, T; \chi_J\right)$ are given by the relations

$$
\begin{aligned}
\Psi\big(\Delta_{ij}, m_f, T; \chi_J\big) &= \widetilde{\Psi}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), m_f, T; \chi_J\big) \\
&= \widetilde{\Psi}_S\big(\Delta_{ij}, \phi(\Delta_{ij}, m_f, T; \chi_J), T; \chi_J\big) + m_f \psi_f\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right) \\
\Psi_S\big(\Delta_{ij}, \phi, T; \chi_J\big) &= \widetilde{\Psi}_S\big(\Delta_{ij}, \phi, T; \chi_J\big)
\end{aligned}
$$

then, using Lemma 3.1 and the previous results, we get Coussy's results quoted above

$$
\begin{aligned}
\frac{\partial \Psi}{\partial \Delta_{ij}}\big(\Delta_{ij}, m_f, T; \chi_J\big) &= \frac{\partial \widetilde{\Psi}}{\partial \Delta_{ij}}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), m_f, T; \chi_J\big) \\
&= \frac{\partial \widetilde{\Psi}_S}{\partial \Delta_{ij}}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), T; \chi_J\big) \\
&= \frac{\partial \Psi_S}{\partial \Delta_{ij}}\big(\Delta_{ij}, \phi(\Delta_{ij}, m_f, T; \chi_J), T; \chi_J\big)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \Psi}{\partial T}\big(\Delta_{ij}, m_f, T; \chi_J\big) &= \frac{\partial \widetilde{\Psi}}{\partial T}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), m_f, T; \chi_J\big) \\
&= \frac{\partial \widetilde{\Psi}_S}{\partial T}\big(\Delta_{ij}, \phi(\Delta_{ij}, m_f, T; \chi_J), T; \chi_J\big) - m_f s_f\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right) \\
&= \frac{\partial \Psi_S}{\partial T}\big(\Delta_{ij}, \phi(\Delta_{ij}, m_f, T; \chi_J), T; \chi_J\big) - m_f s_f\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \Psi}{\partial m_f}\big(\Delta_{ij}, m_f, T; \chi_J\big) &= \frac{\partial \widetilde{\Psi}}{\partial m_f}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), m_f, T; \chi_J\big) \\
&= g_f\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \Psi_S}{\partial \phi}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), T; \chi_J\big) &= \frac{\partial \widetilde{\Psi}_S}{\partial \phi}\big(\Delta_{ij}, \phi\big(\Delta_{ij}, m_f, T; \chi_J\big), T; \chi_J\big) \\
&= p\left(\frac{\phi(\Delta_{ij}, m_f, T; \chi_J)}{m_f}, T\right)
\end{aligned}
$$

We believe that these results, which are based on the minimization condition, can shed light on the issues raised in Schreyer (2016) concerning Coussy's thermodynamical definition of fluid pressure.

5 CONCLUSIONS

5.1 GENERAL MODELING APPROACH

The unsaturated soil is modeled as a porous material using the framework of thermodynamics with internal variables. Porous materials are characterized by the presence of a solid skeleton and a number of fluids, which can flow through the solid skeleton. The solid skeleton provides a natural reference for the evolution of the porous material, which can be used in a Lagrangian description. The approach followed is summarized below.

- **Microscale continua**. It is assumed that the porous material is made of a number of microscale regions of various dimensions (3D, 2D, 1D, 0D) containing several species. Each microscale region is assumed to be modeled as a mixture of microscale interacting continua $c_{\alpha \mathrm{a}}$, corresponding to the species a in the microscale region α.

- **Macroscale continua**. It is assumed that, by an averaging process, to each microscale continuum $c_{\alpha \mathrm{a}}$ corresponds a macroscale continuum $\mathcal{C}_{\alpha a}$, which is defined on macroscale 3D regions, and the porous material is considered to be the mixture of these interacting macroscale continua. Grouping all these macroscopic continua containing species a yields macroscale continua $\mathcal{C}_{\mathrm{a}}$, and the porous material is considered to be the mixture of these macroscale interacting continua.

- **State variables**. During the averaging process microscale information is lost. Part of this information can be recovered by macroscale geometric variables n_{α}, defined as the measure of microscale region α (volume, area, length, number of points) per unit (reference) volume (e.g. volume fractions in geomechanics) and by mass distribution variables $m_{\alpha \mathrm{a}}$, defined as the mass of species a in microscale region α per unit (reference) volume. Additional geometric variables can be defined from the geometry of the microscale regions, giving rise to structural tensors. The state of the porous material is assumed to be given by $\left(E_{IJ}, n_{\mathrm{\alpha}}, m_{\mathrm{\alpha a}}, \theta, \xi\right)$, where E_{IJ} is the Green-Lagrange strain tensor of the solid skeleton, θ is the temperature and ξ is a set of internal variables.

- **Local equilibrium states**. The number of state variables can be significantly reduced by considering local equilibrium states. Let m_{a} be the total mass of species a per unit reference volume, so that $m_{\mathrm{a}} = \sum_{\mathrm{\alpha}} m_{\mathrm{\alpha a}}$. It will be assumed that, for prescribed values of E_{IJ}, m_{a}, θ and ξ, the variables $n_{\mathrm{\alpha}}$ and $m_{\mathrm{\alpha a}}$ take unique values $n_{\mathrm{\alpha}} = n_{\mathrm{\alpha}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ and $m_{\mathrm{\alpha a}} = m_{\mathrm{\alpha a}}(E_{IJ}, m_{\mathrm{a}}, \theta, \xi)$ such that the total free energy per unit reference volume reaches a minimum. The state $\left(E_{IJ}, n_{\mathrm{\alpha}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), m_{\mathrm{\alpha a}}\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right), \theta, \xi\right)$ will be called the local equilibrium state defined by $\left(E_{IJ}, m_{\mathrm{a}}, \theta, \xi\right)$. This minimization assumption is in line with the postulates of equilibrium thermodynamics, and similar approaches have been used by a number of authors, in an explicit or an implicit way.

- **Constitutive equations**. The behavior of the porous material will be assumed to be rate independent. The laws of state will be derived from the free energy and the evolution equations of the internal variables from the dissipation function, applying Ziegler's orthogonality principle separately to the dissipation due to changes in the local equilibrium state, to the dissipation due to mass flow of constituents through the solid skeleton, and to the dissipation due to heat flow. The dissipation due to changes in the local equilibrium state has been treated in more detail, with the outcome of a generalized elastoplastic behavior, in which the small strain tensor and the variation with respect to the reference configuration of mass per unit reference volume of constituents are considered to be the sum of an elastic and a plastic part. The dissipations due to mass and heat flow have only been treated in a simplified manner, with the outcome of equations analogous to Darcy's and Fourier's laws.

5.2 SOIL REGIMES

For unsaturated soils, additional simplifying assumptions are made: (1) small strains of the solid skeleton; (2) isothermal atmospheric conditions; (3) three species: solid mineral, water and gas; and (4) elastoplastic response of the deformation of the solid skeleton and of the water mass content.

The behavior of a soil depends on its structure at the microscale (e.g. phases and interfaces). In this regard, three soil regimes can be distinguished.

5.2.1 Saturated regime

The saturated regime is defined by the presence of fixed vicinal water, variable free water and no gas phase. It corresponds to water chemical potential values higher that the air entry value. If the solid skeleton (solid particles, water) can be assumed to be incompressible and there is no mass exchange with the free liquid, Terzaghi's effective principle holds.

5.2.2 Capillary regime

The capillary regime is defined by the presence of fixed vicinal water, variable free water and gas phase. It corresponds to water chemical potential values between the air entry value and the evaporation of free water value. The free water-air interfacial tension increase the intergranular stresses, which decreases the soil volume, increases its stiffness and increases its resistance. Due to the geometry of the pore space, water content hysteresis in drying-wetting cycles is observed. As a result, in the total stress - water chemical potential space, the elastic region is bounded above and below by the values of the water chemical potential corresponding to the main drying and wetting curves. This feature is unique to this regime.

5.2.3 Dry regime

The dry regime is defined by the presence of variable vicinal water, no free water and gas phase. It corresponds to water chemical potential values lower than the evaporation of free water. The vicinal water progressively disappears, so that the interaction forces between the solid particles and the vicinal water and the water-air interface progressively disappear.

Because of the different features of these soil regimes, we propose to use a different constitutive model for each of them. A generic example of constitutive model for each soil regime has been presented, including the corresponding free energy and dissipation functions.

5.3 FEATURES OF THE PROPOSED FORMULATION

We discuss aspects of some features of the proposed formulation, that have interest for the modeling of unsaturated soils.

- **Thermodynamic consistency**. In the proposed formulation, the constitutive equations are derived from the free energy using the state equations and from the dissipation function using Ziegler's orthogonality principle. The resulting models for unstaturated soils are thermodynamically consistent. Although there are models for unsaturated soils developed without a thermodynamic basis that are able to reproduce many salient features of the behavior of unsaturated sois (e.g. Alonso et al. 1990), thermodynamic consistency is recognized to be a convenient feature of a physical model.

- **Chemical potentials and temperature**. At local equilibrium states, the microscale distributions of chemical potentials and temperature are uniform (neglecting gravity forces). As a result, the values of the corresponding macroscale variables are the same as the uniform values of the distributions of their microscale counterparts. The proposed formulation uses these macroscale variables. In this regard, Bear and Nitao (1995) considered these variables to be the degrees of freedom of a porous medium with surface effects in complete equilibrium. Measuring the values of these macroscale variables can be done by bringing the measuring device in contact with the soil until equilibrium is established.

- **Pore water pressure**. Eventually, short-range interaction forces bond water to the soil skeleton. The microscale distributions of water bond to the skeleton (vicinal water) are not uniform, so that the relationship with a macroscale pressure is questionable. In contrast, the microscale distributions of water not bond to the soil skeleton (free water) are uniform (neglecting gravity forces), so that a macroscale pressure with the same value as the uniform microscale distributions is appropriate. Absolute negative pore water pressures are considered to be unrealistic (Gray and Hassanizadeh 1991). They are the result of applying the relationship between water chemical potential, water pressure and temperature obtained for water outside the soil to the water chemical potential of water in the soil. In fact, short-range attractive interaction forces between the soil skeleton and water give rise to microscale distributions of water pressure which are increasingly positive as the surface of solid is approached (Niao and Bear 1995). The proposed formulation does not use water pressures. However, macroscale free water pressures can be determined using the chemical potentials and temperature, because free water behaves as if it were outside the soil.

- **Local equilibrium states**. Macroscale geometric variables, such as porosity, degree of saturation and area of air-water interface per unit volume are macroscale variables that are used to recover part of the geometric information that is lost during averaging. These variables are usually estimated from measures of weights and volumes (e.g. in natural conditions and after oven drying) assuming constant density of solids and water or by use of special laboratory techniques. In some cases the results are not reliable. For instance, the determination of the degree of saturation from measurement of weights and volumes in clays with a large specific surface area often leads to degrees of saturation larger than 100%. The proposed formulation does not use macroscale geometric variables, because the evolution of these variables is implicit in the considered evolutions along local equilibrium states. A similar approach was used by Bowen (1976).

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