UNIVERSITÀ
DEGLI STUDI
DI PADOVA

Sede Amministrativa: Università degli Studi di Padova

DIPARTIMENTO DI INGEGNERIA CIVILE, EDILE ED AMBIENTALE

SCUOLA DI DOTTORATO DI RICERCA IN SCIENZE DELL'INGEGNERIA CIVILE, EDILE ED AMBIENTALE

CICLO XXIV°

DEVELOPMENT OF A MODEL FOR THE THERMO-HYDRO-MECHANICAL ANALYSIS OF MULTIPHASE POROUS MEDIA IN DYNAMICS

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SUMMARY

Nowadays an increasing interest on thermo-hydro-mechanical analysis of multiphase porous media is observed because of a wide spectrum of application in civil and environmental engineering. The onset of landslides caused by rainfall or earthquake, the onset of catastrophic landslides, the seismic behaviour of deep radioactive waste disposal and concrete or earth dams are just few and challenging examples.

As novel aspect, this work presents the development of a mathematical and numerical model for the analysis of the thermo-hydro-mechanical behaviour of multiphase porous materials in dynamics.

The fully coupled multiphase model for non isothermal deformable porous media is developed within the hybrid mixture theory.

In order to analyse the thermo-hydro-mechanical behaviour of a soil structure in the low frequency domain, e.g. under earthquake excitation, the **u**-p(-T) formulation is advocated for the finite element discretization, neglecting the relative fluids acceleration and their convective terms. As a consequence, the number of the independent variables is reduced to four: gas pressure, capillary pressure, temperature and solid skeleton displacements. Moreover, the dynamic seepage forcing terms in the mass and enthalpy balance equations and the compressibility of the solid grain at the microscopic level are neglected.

The standard Bubnov-Galerkin method is applied to the governing equations for the spatial discretization, whereas the generalized Newmark scheme is used for the time domain discretization. The final algebraic, non linear and coupled system of equations is solved by the Newton method with a monolithic approach.

The formulation and the implemented solution procedure are validated through the comparison with literature benchmarks, finite element solutions or analytical solutions when available.

SOMMARIO

Al giorno d’oggi è evidente un crescente interesse nell’analisi termo-idro-meccanica dei mezzi porosi multifase e ciò è dovuto all’ampio spettro di applicazioni in ingegneria civile ed ambientale. L'innesco di frane dovuto a eventi sismici o forti eventi piovosi, l'innesco di frane catastrofiche, il comportamento sismico di depositi profondi di scorie radioattive o di dighe in terra o calcestruzzo sono solo alcuni esempi.

Come aspetto innovativo, questo lavoro presenta lo sviluppo di un modello matematico e numerico per l'analisi del comportamento termo-idro-meccanico di materiali porosi multifase in dinamica.

Il modello multifase per mezzi porosi deformabili in condizioni non isoterme, completamente accoppiato, è stato sviluppato nell’ambito della teoria ibrida delle miscele.

Per analizzare il comportamento termo-idro-meccanico di una struttura in materiale granulare nel dominio delle basse frequenze, ad esempio in caso di sollecitazione sismica, viene ricavata la formulazione **u**-p(-T), trascurando le accelerazioni relative dei fluidi e i loro termini convettivi. Come conseguenza, il numero delle variabili indipendenti è ridotto a quattro: la pressione del gas, la pressione capillare, la temperatura e le componenti di spostamento dello scheletro solido. Inoltre si trascurano le forze di filtrazione dinamica nelle equazioni di bilancio massa e dell’entalpia e la comprimibilità del grano solido a livello microscopico.

Per la discretizzazione nel dominio dello spazio viene utilizzato il metodo di Bubnov-Galerkin, mentre per la discretizzazione nel dominio del tempo viene utilizzato lo schema generalizzato di Newmark. Il sistema finale di equazioni algebriche, non lineari ed accoppiate, viene risolto con il metodo di Newton, con un approccio monolitico.

Il modello implementato è stato validato mediante il confronto con casi di riferimento presenti in letteratura, con soluzioni agli elementi finiti e con soluzioni analitiche quando disponibili.

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INTRODUCTION

The analysis of the dynamic response of multiphase porous media has many applications in civil engineering. Onset of landslide due to earthquake or rainfall and the seismic behaviour of dams are just few examples where inertial forces cannot be neglected because of the mass involved. Moreover, there are situations where it is important to consider the effect of temperature variation that causes a decrease of the solid skeleton strength and an increase of the pore pressures. We could observe these phenomena for example during the onset of catastrophic landslide, as described by Vardoulakis [Va02], where the mechanical energy, dissipated in heat inside the slip zone, may lead to the vaporization of pore water, creating a cushion of zero friction. Another example is the seismic behaviour of deep nuclear waste disposal, because, in case of failure of canisters, an increment of temperature could create localized failure zones, those could act as preferential escape zones for fluids containing radionuclides.

Many authors have developed models for the analysis of the transient behaviour of multiphase porous media. A recent state of art can be found in Zienkiewicz et al. [Z99] and Schanz [SC09]. A fully coupled finite element code based on mixture theory is developed by Zerfa and Loret where a new viscous boundary is implemented to avoid wave reflections towards the structure (This boundary is able to absorb the two dilatational waves and the shear wave) [ZL03]. Nenning and Schanz [NS11] presented an infinite element to treat wave propagation problems in unbounded saturated porous media modelled by Biot's theory. Conventional finite elements are used to model the near field, whereas infinite elements are used to represent the behaviour of the far field. The elements are constructed in such a way that the waves decay with distance and are not reflected at infinity. Heider et al. [He11] analyzed an accurate and stable numerical solution of dynamic wave propagation problems in infinite half spaces. Proceeding from an isothermal, biphasic, linear poroelasticity model with incompressible constituents, finite elements are used to discretize the near field and infinite elements to approximate the far field.

A model based on the theory of porous media describing the dynamic behaviour of a saturated binary porous medium was presented by Diebels including both geometrical and material non-linearities [Die96]. Lòpez-Querol et al. [LQ07] presented the constitutive Pastor–Zienkiewicz model for sands implemented in a dynamic coupled code formulated in terms of displacements for both solid and fluid phases (**u**-**w** formulation). A **u**-p^c-**w** formulation of a fully coupled porous solid-fluid formulation is presented by Jeremic et al. [Je08]. They took into account water acceleration and fluid compressibility. Ravichandran and Muraleetharan [RM09] presented a complete formulation of the fully coupled equations representing the dynamics of unsaturated soils. Two finite element formulations of all the terms in the governing equations are presented and implemented within a finite element framework.

Analytical solutions were developed for the response of saturated and nearly saturated porous media under plane strain condition by Ulker and Rahman (2009) [UR08]. An explicit 3D Laplace transform domain fundamental solution is obtained for governing equations and a closed-form analytical transient 3D fundamental solution is presented in Ashayeri et al. [As10]. Gajo and Denzer [Ga11] provided the finite element implementation for dynamics analyses of saturated porous media at large strains with compressible solid and fluid constituents for both high-frequency and low-frequency dynamic problems. Uzuoka and Borja [UB11] derived the governing equations for the dynamic response of unsaturated poroelastic solids at finite strain. They obtained simplified governing equations from the complete coupled formulation by neglecting the material time derivative of the relative velocities and the advection terms of the pore fluids relative to the solid skeleton, leading to a **u**-p^w-p^a formulation.

This thesis presents as a novel contribution the study and the implementation of a fully coupled model for the analysis of deformable multiphase geomaterials in dynamics including thermal effects. The fully coupled multiphase model for non isothermal deformable porous media is developed following Lewis and Schrefler [LS98]. The **u**-p(-T) formulation is obtained by neglecting the relative fluids acceleration and their convective terms, this is valid for low frequency problems as in earthquake engineering, Zienkiewicz et al [Z99]. In the model devolvement, the dynamic seepage forcing terms in the mass balance equations and in the enthalpy balance equation and the compressibility of the grain at the microscopic level are neglected. The implemented model is validated through the comparison with analytical or finite element quasi-static and dynamics solutions from the literature.

This thesis is organised as follows.

Chapter 2 concerns the derivation of the mathematical model. The generalized form of the governing equations describing the thermo-hydro-mechanical behaviour of porous media in dynamics is presented. The simplifications introduced in the model development are explained and justified.

Chapter 3 describes the discretization of the governing equations. The classical Galerkin Method is used for the space discretization, whereas the generalized Newmark method is used for the time discretization. The linearization of the non-linear algebraic equations system close this chapter. The model has been implemented in the quasi-static finite element code COMES-GEO [GS96], [LS98], [SPS6].

Chapter 4 presents the finite element solutions aiming to validate numerically the implemented model. The single phase solid model is validated by analyzing a monodimensional wave propagation problem in a solid bar [Sl92] and by solving a sand column subjected to a step load [SS98]. The isothermal water saturated model is validated by studying a dynamic consolidation problem of a saturated poroelastic column under harmonic load [Ma10]. The non-isothermal water saturated model is validated by solving a fully saturated non-isothermal mechanical consolidation problem [Ab85]. The isothermal partially saturated model is validated by simulating the Liakopoulos test that is a quasi-static drainage of liquid water from a soil column [L65] and by analyzing a sand column subjected to a step load in an initially unsaturated soil column [SS98].

In Chapter 5 the concluding remarks are presented.

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GOVERNING EQUATIONS FOR DYNAMICS T-H-M BEHAVIOUR OF POROUS MEDIA*

2.1 Introduction

In this chapter the governing equations for the full dynamic behaviour of a partially saturated porous medium are developed following [LS98]. In particular, we consider here the voids filled with water and air. Today the description of multiphase systems made of interpenetrating continuous bodies, such as porous media, is based either on the mixture theory integrated by the concept of volume fractions, or on averaging theories and from a classical point of view on Biot's theory. Since the averaging theories offer the possibilities of a better understanding of the microscopic situation and its relation to the macroscopic one, which is, however, the natural domain of all continuum mechanical models, we use in the following the averaging theory based on spatial averaging operators. Within this theory we make use of macroscopic variables which correspond to real measurable quantities directly linked to laboratory practice, e.g. in soil mechanics. It has to be pointed out that, under appropriate assumptions, the averaging theory yields the same equations as the classical mixture theory, as shown in [deB91]. Care has to be taken, however, in the linear momentum balance equation. For the reader mainly interested in the resulting governing equations and their numerical solution we derive these equations again in section 2.6 using Biot's theory. This also permits us to establish a link between the classical, phenomenological approach and the description of the real microscopic composition of the multiphase system. Furthermore, it shows the essential correctness of Biot's findings.

Tensorial notation is used throughout this chapter.

2.2 Averaging principles

Here a short summary of the principles necessary for the development of the governing equations is given. For a full account of the averaging theories the reader is referred to References [deB91] and [BB84].

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* From Chapter 2: Mechanics of saturated and partially saturated porous media, R.W. Lewis and B.A. Schrefler, *The Finite Element Method in the Static and Dynamic Deformation and Consolidation of Porous Media*, Wiley, Chichester, 1998.

Sections 2.2 and 2.3 follow, in particular, the work by Hassanizadeh and Gray, [H79-1] and [H86-2], and by de Boer et al. [deB91].

We introduce the following definitions:

Microscopic level: we consider the real non-homogeneous structure of the porous medium domain (Figure 2. 1). The scale of inhomogeneity is of the order of magnitude of the dimensions of a pore or a grain, say d. Attention is focussed on what happens at a mathematical point within a single phase and the field variables describing the status of a phase are defined only at the points occupied by that phase. For the practical description of the processes taking place in a porous medium, this level is not useful since microscopic quantities are generally not measurable. Only their average values are measurable.

Macroscopic level: the real multiphase system that occupies the porous medium domain is replaced by a model in which each phase is assumed to fill up the entire domain. This means that at every point all phases are supposed present at the same time (overlapping continua). This is the level of interest of continuum mechanics, where we investigate the continuous distribution of the constituents through a macroscopic control space. At this level, we usually deal with homogeneous media, but non-homogeneities may still be present, e.g. strata. Their scale is of an order of magnitude comparable with the order of magnitude of the entire domain, say L.

Megascopic level: at this level the conditions are similar to those of the previously defined level. The difference depends on the fact that some macroscopic inhomogeneities are eliminated by averaging and/or on the fact that the mathematical model is stated in a domain which has less dimensions than the real domain, e.g. 2D problem with field values averaged over the thickness [BC81], [SS89]. Typical applications of this level are found in the simulation of land subsidence problems on regional scale.

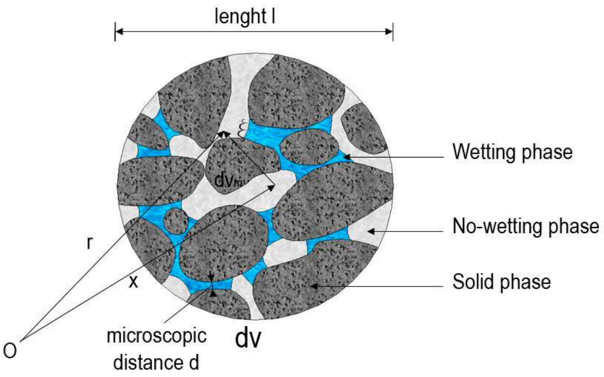

Figure 2. 1 *Typical averaging volume dv of a porous media consisting of three constituents*

2.2.1 Averaging process

We consider here a multiphase system occupying a total volume V, and bounded by surface A. The constituents π, $\pi = 1, 2,\dots k$, have the partial volumes V^{π}. Each point of the total volume V, is considered to be the centroid of a representative elementary volume (REV) or average volume element dv. The position of the centre of a REV in a global coordinate system is described by position vector **x** while **r** indicates the position of a microscopic volume element dv_{m} (Figure 2. **1**). The volume of constituent π within a REV, called average volume element dv^{π}, is obtained by defining a phase distribution function γ^{π}:

$$\gamma^{\pi}(\mathbf{r},t) = \begin{cases} 1 & \text{for } \mathbf{r} \in dv^{\pi} \\ 0 & \text{for } \mathbf{r} \in dv^{\alpha} \quad \pi \neq \alpha \end{cases} \tag{2. 1}$$

$$dv^{\pi}(\mathbf{x},t) = \int_{dv} \gamma^{\pi}(\mathbf{r},t)\, dv_m \tag{2. 2}$$

where $\mathbf{r} = \mathbf{x} + \xi$ and the integration refers to the microscopic local coordinate system ξ with its origin in $\mathbf{x}$ (Figure 2. 1). Similarly we write for the part da^{π} of area da of the REV, occupied by constituent π

$$da^{\pi}(\mathbf{x},t) = \int_{da} \gamma^{\pi}(\mathbf{r},t)\, da_m \tag{2. 3}$$

where da_m is the microscopic area element. The knowledge of dv^{π} enables the introduction of the concept of volume fraction η^{π}, which is of paramount importance in multiphase systems:

$$\eta^{\pi}(\mathbf{x},t) = \frac{dv^{\pi}}{dv} = \frac{1}{dv}\int_{dv} \gamma^{\pi}(\mathbf{r},t)dv_m \qquad [2.\ 4]$$

with

$$\sum_{\pi=1}^{\kappa} \eta^{\pi} = 1 \qquad [2.\ 5]$$

In fact, as indicated under the heading "Macroscopic level" in paragraph 2.2, substitute continua fill the entire domain simultaneously, instead of the real fluids and the solid which each fill only part of it. These substitute continua have a reduced density which is obtained through the volume fractions.

In the following, averaged quantities are obtained by integrating (averaging) a microscopic quantity over the volume *dv* or the area *da* of a REV. A field of macroscopic variables results from this, where the average volume *dv* and the average area *da* are associated with material points.

The size of a REV is an important choice. Average quantities have to be independent from the size of the average volume and continuous in space and time. Thus a REV has to fulfil the following requirements:

- *dv* has to be small enough to be considered as infinitesimal, i.e. the partial derivatives appearing in the governing equations must make sense
- *dv* must be large enough, with respect to the heterogeneities of the material, to give average quantities without fluctuations depending on the size of the REV (Figure 2. 2).

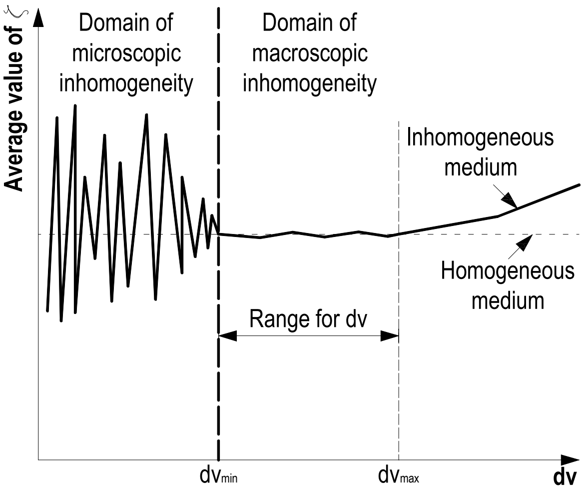

Figure 2. 2: *Averaged value ζ vs size of the average volume dv*

To obtain meaningful average values, the characteristic length l of the average volume must satisfy the inequality

$$d << l << L$$

where l is dependent on the specific material which constitutes the medium. Some typical values of l are given in [LC88]:

Metals	0.5 mm
Plastics	1 mm
Wood	10 mm

Usually there are no boundary conditions associated with a REV, except in the case of the megascopic level. Attention is needed when defining the averaged values for a megascopic level [SS89]. Another exception is the case of a medium with periodic structure, where asymptotic analysis is used [Au91].

The following average operators are now defined and applied to a function $\zeta(\mathbf{r},t)$ which is a microscopic field variable.

Volume average operators:

- phase average

$$\langle\zeta\rangle_{\pi}(\mathbf{x},t)=\frac{1}{dv}\int_{dv}\zeta(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_{m} \qquad [2.\ 6]$$

- intrinsic phase average

$$\langle\zeta\rangle_{\pi}^{\pi}(\mathbf{x},t)=\frac{1}{dv^{\pi}}\int_{dv}\zeta(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_{m} \qquad [2.\ 7]$$

where we have to take into account that

$$\int_{dv^{\pi}}\zeta(\mathbf{r},t)dv_{m}=\int_{dv}\zeta(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_{m} \qquad [2.\ 8]$$

From the definition of volume fraction [2.4] it follows that

$$\langle\zeta\rangle_{\pi}(\mathbf{x},t)=\eta^{\pi}(\mathbf{x},t)\langle\zeta\rangle_{\pi}^{\pi}(\mathbf{x},t) \qquad [2.\ 9]$$

Mass average operator, with $\rho(\mathbf{r},t)$ microscopic mass density as weighting function, is

$$\overline{\zeta}^{\pi}(\mathbf{x},t)=\frac{\int_{dv}\rho(\mathbf{r},t)\zeta(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_{m}}{\int_{dv}\rho(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_{m}} \qquad [2.\ 10]$$

With constant microscopic mass density the following equation holds

$$\frac{1}{\eta^{\pi}(\mathbf{x},t)}\langle\zeta\rangle_{\pi}(\mathbf{x},t)=\overline{\zeta}^{\pi}(\mathbf{x},t) \qquad [2.\ 11]$$

Area average operator

$$\overline{\overline{\zeta}}^{\pi}(\mathbf{x},t)=\frac{1}{da}\int_{da}\zeta(\mathbf{r},t)\cdot\mathbf{n}\,\gamma^{\pi}(\mathbf{r},t)da_{m} \qquad [2.\ 12]$$

with **n** the outward normal unit vector of an area element da_{m} and in [2.12] ζ has a tensorial nature.

In the following, averages of velocity, external body force, internal energy, external supply of heat, internal entropy, external supply of entropy and total production of entropy are obtained through the mass average operator [2.10], [H79-1]. These density functions are only additive in the form $\rho\zeta dv$. Volume averaged quantities, through [2.7], and mass averaged quantities, through [2.10], are the same only for constant microscopic mass density, [2.11]. The area average operator [2.12] will be used to define the average of flux terms such as the stress tensor, heat flux and entropy flux.

For an isotropic distribution of phases, the volume and area average values differ only slightly from each other [H79-1]. This follows from Delesse's law, which states that on each cut surface in an isotropic mixture, the surface ratio of each partial constituent must be equal to its volume ratio.

2.2.2 Microscopic balance equations

We now consider the classical balance equations of continuum mechanics which are used to describe the microscopic situation of any π phase. At the interfaces with other constituents, the material properties and thermodynamic quantities may present step discontinuities.

For a generic conserved variable ψ, the conservation equation within the π phase may be written as

$$\frac{\partial(\rho\psi)}{\partial t}+div(\rho\psi\dot{\mathbf{r}})-div\,\mathbf{i}-\rho b=\rho G \qquad [2.\ 13]$$

where $\dot{\mathbf{r}}$ is the local value of the velocity field of the π phase at a fixed point in space, **i** is the flux vector associated with ψ, b is the external supply of ψ, G is the net production of ψ.

At the interface between two constituents π and α, the jump condition holds

$$\left[\rho\psi(\mathbf{w}-\dot{\mathbf{r}})+\mathbf{i}\right]\Big|_{\pi}.\mathbf{n}^{\pi\alpha}+\left[\rho\psi(\mathbf{w}-\dot{\mathbf{r}})+\mathbf{i}\right]\Big|_{\alpha}.\mathbf{n}^{\alpha\pi}=0 \qquad [2.\ 14]$$

where $\mathbf{w}$ is the velocity of the interface, $\mathbf{n}^{\pi\alpha}$ is the unit normal vector pointing out of the π phase and into the α phase, with

$$\mathbf{n}^{\pi\alpha}=-\mathbf{n}^{\alpha\pi} \qquad [2.\ 15]$$

And $\big|_{\pi}$ indicates that the preceding term [...] must be evaluated with respect to the π phase. No thermomechanical properties are attributed to these interfaces. This assumption does not exclude the possibility of exchange of mass, momentum or energy between the constituents.

Moreover the local thermodynamic equilibrium hypothesis is assumed to hold because the time scale of the modelled phenomenon is substantially larger than the relaxation time required to reach equilibrium locally.

2.2.3 Macroscopic balance equations

Instead of deriving the macroscopic balance equation separately for each quantity to which the conservation law applies, we derive it for the generic quantity ψ as in [deB91] and [BB84] and specialise the law afterwards for specific quantities: mass, linear momentum, angular momentum and energy. Note that the balance equations are written in a material-free manner. The constitutive equations are introduced successively.

A general average macroscopic balance equation is obtained from the microscopic balance equation [2.13] by multiplying it with the distribution function $\gamma^{\pi}(\mathbf{r},t)$ and by integrating this product over the volume element *dv* and over the total volume *V*. In this elaboration of the balance equations, macroscopic quantities are obtained through the previously defined averaging operators.

This averaging procedure yields [deB91],[BB84]

$$\int_V\left[\frac{1}{dv}\int_{dv}\frac{\partial(\rho(\mathbf{r},t)\psi(\mathbf{r},t))}{\partial t}\gamma^{\pi}(\mathbf{r},t)dv_m\right]dV$$

$$+\int_V\left[\frac{1}{dv}\int_{dv}div(\rho(\mathbf{r},t)\dot{\mathbf{r}}(\mathbf{r},t)\psi(\mathbf{r},t))\gamma^{\pi}(\mathbf{r},t)dv_m\right]dV$$

$$-\int_V \left[\frac{1}{dv}\int_{dv} div\, \mathbf{i}(\mathbf{r},t)\,\gamma^{\pi}(\mathbf{r},t)\,dv_m\right]dV \qquad [2.\ 16]$$

$$-\int_V \left[\frac{1}{dv}\int_{dv} \rho(\mathbf{r},t)\,b(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)\right]dV$$

$$=\int_V \left[\frac{1}{dv}\int_{dv} \rho(\mathbf{r},t)G(\mathbf{r},t)\gamma^{\pi}(\mathbf{r},t)dv_m\right]dV$$

As suggested in References [H79-1], [H79-2], [H80-3] and [deB91], it is possible to obtain the following form of the general balance equation for the macroscopic thermodynamic property $\overline{\psi}^{\pi}$ associated with the π phase:

$$\int_V \left\{\frac{\partial}{\partial t}\left[\langle\rho\rangle_{\pi}(\mathbf{x},t)\overline{\psi}^{\pi}(\mathbf{x},t)\right]+div\left[\langle\rho\rangle_{\pi}(\mathbf{x},t)\overline{\mathbf{v}}^{\pi}(\mathbf{x},t)\overline{\psi}^{\pi}(\mathbf{x},t)\right]\right\}dV$$

$$-\int_V \left\{\frac{1}{dv}\sum_{\alpha\neq\pi}^{k}\int_{da^{\pi\alpha}} \rho(\mathbf{r},t)\psi(\mathbf{r},t)\left[\mathbf{w}(\mathbf{r},t)-\dot{\mathbf{r}}(\mathbf{r},t)\right]\cdot\mathbf{n}^{\pi\alpha}(\mathbf{r},t)da_m\right\}dV$$

$$-\int_V \left[\frac{1}{dv}\sum_{\alpha\neq\pi}^{k}\int_{da^{\pi\alpha}} \mathbf{i}(\mathbf{r},t)\cdot\mathbf{n}^{\pi\alpha}(\mathbf{r},t)da_m\right]dV \qquad [2.\ 17]$$

$$-\int_A \left\{\frac{1}{da}\int_{da}\left[\mathbf{i}(\mathbf{r},t)-\rho(\mathbf{r},t)\tilde{\psi}^{\pi}(\mathbf{x},\xi,t)\tilde{\dot{\mathbf{r}}}^{\pi}\right]\cdot\mathbf{n}(\mathbf{r},t)\gamma^{\pi}da_m\right\}dA$$

$$-\int_V \langle\rho\rangle_{\pi}(\mathbf{x},t)\overline{b}^{\pi}(\mathbf{x},t)dV=\int_V \langle\rho\rangle_{\pi}(\mathbf{x},t)\overline{G}^{\pi}(\mathbf{x},t)dV$$

or in more concise form

$$\int_V \left[\frac{\partial}{\partial t}\left(\langle\rho\rangle_{\pi}\overline{\psi}^{\pi}\right)+div\left(\langle\rho\rangle_{\pi}\overline{\psi}^{\pi}\overline{\mathbf{v}}^{\pi}\right)-div\,\mathbf{i}^{\pi}\right.$$

$$\left.-\langle\rho\rangle_{\pi}\left(\overline{b}^{\pi}+e^{\pi}(\rho\psi)+\mathbf{I}^{\pi}\right)\right]dV=\int_V \rho_{\pi}\overline{G}^{\pi}dv \qquad [2.\ 18]$$

where $\mathbf{i}^{\pi}$ is the flux vector associated with $\overline{\psi}^{\pi}$, $\overline{b}^{\pi}$ is the external supply of $\overline{\psi}^{\pi}$, $\langle\rho\rangle_{\pi}$ is the volume average value of mass density.

This last balance equation contains two further interaction terms, which describe chemical and physical exchanges.

Exchange of $\overline{\psi}^{\pi}$ due to mechanical interactions between the constituents is given by

$$\mathbf{I}^{\pi}=\frac{1}{\langle\rho\rangle_{\pi}dv}\sum_{\alpha\neq\pi}\int_{da^{\pi\alpha}}\mathbf{n}^{\pi\alpha}\cdot\mathbf{i}\,da_m \qquad [2.\ 19]$$

Phase change of a constituent or possible mass exchange between the constituent π and the other constituents α is given by

$$\mathrm{e}^{\pi}(\rho\psi) = \frac{1}{\langle\rho\rangle_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} \rho\psi(\mathbf{w} - \dot{\mathbf{r}}) \cdot \mathbf{n}^{\pi\alpha} da_m \qquad [2.\ 20]$$

The fourth term of the left-hand side of [2.17] is the macroscopic non convective flux of $\overline{\psi}^{\pi}$ and an averaged flux density may be defined as

$$\tilde{i}^{\pi} = \frac{1}{da} \int_{da} \left(\mathbf{i} - \rho\tilde{\psi}^{\pi} \tilde{\dot{\mathbf{r}}}^{\pi}\right) \cdot \mathbf{n} \gamma^{\pi} da_m \qquad [2.\ 21]$$

With the averaged macroscopic flux there exists a flux vector $\mathbf{i}^{\pi}$ such that $\tilde{i}^{\pi}$ can be defined as a linear function of the normal unit vector $\mathbf{n}$ of *da* in $\mathbf{x}$ [H79-1]:

$$\tilde{i}^{\pi} = \mathrm{n} \cdot \mathrm{i}^{\pi} \qquad [2.\ 22]$$

and the divergence theorem may be applied to obtain the term $div\, \mathbf{i}^{\pi}$ in [2.18], i.e.

$$\int_{A} \mathbf{n} \cdot \mathbf{i}^{\pi} dA = \int_{V} div\, \mathbf{i}^{\pi}\, dV \qquad [2.\ 23]$$

For the proof of the existence of the average flux vector $\mathbf{i}^{\pi}$, the tetrahedron argument is invoked [H79-1], as in stress analysis for Cauchy stresses.

A condition for all internal exchange processes is obtained by integrating equation [2.14] over all interfaces, $da^{\pi\alpha}$ and $da^{\alpha\pi}$, and over the total volume *V*, then by summation over all constituents π, taking into account [2.19] and [2.20]

$$\int_{V} \sum_{\pi} \langle\rho\rangle_{\pi} \left[\mathrm{e}^{\pi}(\rho\psi) + \mathrm{I}^{\pi}\right] dV = 0 \quad \forall \mathbf{x} \in V \qquad [2.\ 24]$$

The differential form of the balance equation is derived under certain smoothness conditions by localization at macroscopic level:

$\forall \mathbf{x} \in V$

$$\frac{\partial}{\partial t}\left(\langle\rho\rangle_{\pi} \overline{\psi}^{\pi}\right) + div\left(\langle\rho\rangle_{\pi} \overline{\psi}^{\pi}\, \overline{\mathbf{v}}^{\pi}\right) - div\, \mathbf{i}^{\pi} - \langle\rho\rangle_{\pi} \left[\overline{\mathrm{b}}^{\pi} + \mathrm{e}^{\pi}(\rho\psi) + \mathrm{I}^{\pi}\right] = \langle\rho\rangle_{\pi} \overline{\mathrm{G}}^{\pi} \qquad [2.\ 25]$$

subject to

$$\sum_{\pi} \langle\rho\rangle_{\pi} \left[\mathrm{e}^{\pi}(\rho\psi) + I^{\pi}\right] = 0 \quad \forall \mathbf{x} \in V \qquad [2.\ 26]$$

If the body is separated by a discontinuity surface Σ at macroscopic scale, which moves with velocity $\overline{\mathbf{w}}$, the following additional relation must be fulfilled [H79-1], [H79-2]:

$$\left[\langle\rho\rangle_{\pi} \overline{\psi}^{\pi} \left(\overline{\mathbf{v}}^{\pi} - \overline{\mathbf{w}}\right) - \mathbf{i}^{\pi}\right] \cdot \mathbf{N} = 0 \qquad \forall \mathbf{x} \in \Sigma \qquad [2.\ 27]$$

where $\mathbf{N}$ is the normal unit vector of Σ in $\mathbf{x}$.

2.3 Macroscopic balance equations for a non isothermal partially saturated porous material

In this section the macroscopic balance equations for mass, linear momentum, angular momentum and energy (enthalpy) are obtained and then specialised for a deforming porous material where heat transfer and flow of water (liquid and vapour) and dry air are taking place. The starting points are the microscopic balance equations [2.13], where, for each constituent, the generic thermodynamic variable ψ is replaced by appropriate microscopic quantities, suitable for a microscopic non polar material.

For the proper description of the non isothermal unsaturated porous medium, we need to take into account not only heat conduction and vapour diffusion, but also heat convection, liquid water flow due to pressure gradients or capillary effects and latent heat transfer due to water phase change (evaporation and condensation) inside the pores. Furthermore the solid is deformable, resulting in coupling of the fluid, the solid and the thermal fields. All fluid phases are in contact with the solid phase.

The constituents are assumed to be immiscible except for dry air and vapour, and chemically non reacting. Because of the local thermodynamic equilibrium hypothesis, the temperatures of each constituent at a point in the multiphase medium are taken to be equal. This does not mean that the temperature is uniform throughout the medium but only that at each point one temperature is sufficient to characterize the state.

Momentum exchanges due to mechanical interaction are independent of the temperature gradient.

In the following the stress is defined as tension positive for the solid phase, while pore pressure is defined as compressive positive for the fluids.

It should be noticed that in this section the formulation is still material free, i.e. no specific assumptions for the material behaviour have been introduced so far, except for the quite general ones, indicated above. For the development of the macroscopic balance equations in the following sections, we still need to specify the kinematics.

2.3.1 Kinematic Equations

As indicated in section 2.2, a multiphase medium can be described as the superposition of all π phases, whose material points $\mathbf{X}^{\pi}$ can be thought of as occupying simultaneously each spatial point $\mathbf{x}$ in the actual configuration. The state of motion of each phase is, however, described independently. Based on these assumptions, the kinematics of a multiphase medium is dealt with next.

In a Lagrangian or material description of motion, the position of each material point $\mathbf{x}^{\pi}$ at time *t* is function of its placement in a chosen reference configuration, and of the current time *t*:

$$\mathbf{x}^{\pi} = \mathbf{x}^{\pi}\left(\mathbf{X}^{\pi},t\right) = x_i^{\pi}\left(X_1,X_2,X_3,t\right) = f_t\left(\mathbf{X}^{\pi}\right) = f\left(\mathbf{X}^{\pi},t\right) \quad i = 1,2,3 \qquad [2.\ 28]$$

To have this mapping continuous and bijective at all times, the Jacobian *J* of this transformation must be non-zero and strictly positive, since it is equal to the determinant of the deformation gradient tensor, F^{π}:

$$\mathbf{F}^{\pi} = grad\ \mathbf{x}^{\pi} \qquad \left(\mathbf{F}^{\pi}\right)^{-1} = grad\ \mathbf{X}^{\pi} \qquad [2.\ 29]$$

Because of the non-singularity of the Lagrangian relationship [2.28], its inverse can be written and the Eulerian or spatial description of motion follows:

$$\mathbf{X}^{\pi} = \mathbf{X}^{\pi}\left(\mathbf{x}^{\pi},t\right) \qquad [2.\ 30]$$

It is also assumed that functions which describe the motion have continuous derivatives. If the path of the particle of the π phase is known, its velocity and acceleration are, in the material description:

$$\mathbf{V}^{\pi} = \frac{\partial\, \mathbf{x}^{\pi}\left(\mathbf{X}^{\pi},t\right)}{\partial t} \qquad [2.\ 31]$$

$$\mathbf{A}^{\pi} = \frac{\partial^2 \mathbf{x}^{\pi}\left(\mathbf{X}^{\pi},t\right)}{\partial t^2} \qquad [2.\ 32]$$

The corresponding spatial expression can be obtained by introducing equation [2.30] into the above two equations. But, if only the spatial description is given for the velocity field in the form

$$\mathbf{v}^{\pi} = \mathbf{v}^{\pi}(\mathbf{x}^{\pi},t) \qquad [2.\ 33]$$

to evaluate its time derivative with material coordinates held constant, we introduce the description of motion of equation [2.30] into the last equation. By applying the chain rule of differentiation, it follows that

$$\mathbf{a}^{\pi} = \frac{\partial\, \mathbf{v}^{\pi}}{\partial t} + grad\ \ \mathbf{v}^{\pi} \cdot \mathbf{v}^{\pi} \qquad [2.\ 34]$$

The material time derivative of any differentiable function $f^{\pi}\left(\mathbf{x},t\right)$ given in its spatial description and referring to a moving particle of the π phase is

$$\frac{D^{\pi} f^{\pi}}{Dt} = \frac{\partial f^{\pi}}{\partial t} + grad\ f^{\pi} \cdot \mathbf{v}^{\pi} \qquad [2.35]$$

If superscript α is used for the operator $\frac{D}{Dt}$, we obtain

$$\frac{D^{\alpha} f^{\pi}}{Dt} = \frac{\partial f^{\pi}}{\partial t} + grad\ \ f^{\pi} \cdot \mathbf{v}^{\alpha} \qquad [2.36]$$

the time derivative is taken moving with the α phase.

Subtraction of equation [2.35] from equation [2.36] yields the following relation

$$\frac{D^{\pi} f^{\pi}}{Dt} = \frac{D^{\pi} f^{\pi}}{Dt} + grad\ f^{\pi} \cdot \mathbf{v}^{\alpha\pi} \qquad [2.37]$$

where

$$\mathbf{v}^{\alpha\pi} = \mathbf{v}^{\alpha} - \mathbf{v}^{\pi} \qquad [2.38]$$

is the velocity of the α phase with respect to the π phase. This velocity is called the diffusion velocity [H80-3].

The operator $\frac{D}{Dt}$ is a scalar operator and may be applied either to a vector quantity or a scalar quantity. If $\mathbf{f}^{\pi}$ is a vector property per unit volume referring to the π phase, the total time derivative of its integral over a volume *V* is given by

$$\frac{d}{dt}\int_{v} \mathbf{f}^{\pi} dV = \int_{v} \left(\frac{\partial \mathrm{f}^{\pi}}{\partial t} + grad\, \mathbf{f}^{\pi} \cdot \mathbf{v}^{\pi} + \mathbf{f}^{\pi}\ div\ \mathbf{v}^{\pi} \right) d\,V = \int_{v} \left[\frac{\partial \mathrm{f}^{\pi}}{\partial t} + div\left(\mathbf{f}^{\pi} \otimes \mathbf{v}^{\pi} \right) \right] dV \qquad [2.39]$$

For a scalar property f^{π}, we obtain

$$\frac{d}{dt}\int_{v} f^{\pi} dV = \int_{v} \left(\frac{\partial f^{\pi}}{\partial t} + div\left(f^{\pi} \mathbf{v}^{\pi} \right) \right) dV \qquad [2.40]$$

In the above equations, velocities and accelerations of the π phase are considered as mass averaged quantities since they are the quantities usually measured in a field situation or in laboratory practice. In porous media theory it is customary to describe the motion of the fluid phases in terms of mass averaged velocities relative to the moving solid. Their motion is described with reference to the actual configuration assumed by the solid skeleton. The velocities and accelerations of each fluid particle can then be written with reference to the ones of corresponding solid points, once the relative velocities are introduced. We specify the superscripts π now as *s* for soil, *w* for the liquid phase and *g* for the gas phase (dry air plus water vapour) and write for the relative velocities of water and gas phase respectively:

$$\mathbf{v}^{ws} = \mathbf{v}^{w} - \mathbf{v}^{s} \qquad [2.\ 41]$$

$$\mathbf{v}^{gs} = \mathbf{v}^{g} - \mathbf{v}^{s} \qquad [2.\ 42]$$

Water and gas acceleration are given from [2.34], [2.36], [2.41] and [2.42] as

$$\mathbf{a}^{w} = \mathbf{a}^{s} + \frac{D^{s}\mathbf{v}^{ws}}{Dt} + grad\left(\mathbf{v}^{s} + \mathbf{v}^{ws}\right)\cdot \mathbf{v}^{ws} \qquad [2.\ 43]$$

$$\mathbf{a}^{g} = \mathbf{a}^{s} + \frac{D^{s}\mathbf{v}^{gs}}{Dt} + grad\left(\mathbf{v}^{s} + \mathbf{v}^{gs}\right)\cdot \mathbf{v}^{gs} \qquad [2.\ 44]$$

The deformation process of the solid skeleton can be described by the velocity gradient tensor $\mathbf{L}^{s}$, which when referred to spatial coordinates, is given by [CT92] and [Mo86]:

$$\mathbf{L}^{s} \equiv grad\ \mathbf{v}^{s} = \mathbf{D}^{s} + \mathbf{W}^{s} \qquad [2.\ 45]$$

Its symmetric part $\mathbf{D}^{s}$, is called the Eulerian strain rate tensor, being related to pure straining while its skew-symmetric component $\mathbf{W}^{s}$ is the spin tensor.

2.3.2 Mass balance equations

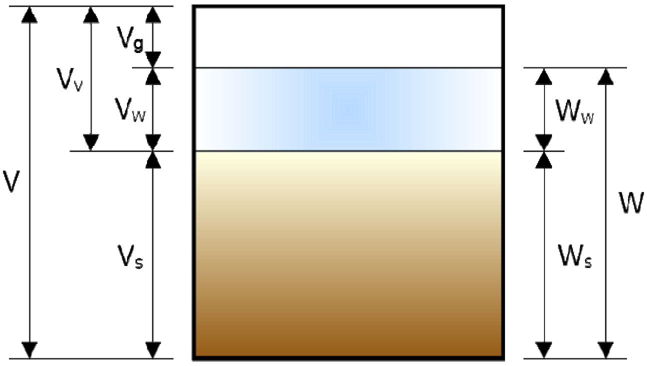

Figure 2. 3: *Schematic composition of soil*

In the following we identify the volume fractions η^{π} of the constituents as:

- solid phase

$$\eta^{s} = 1 - n \qquad [2.\ 46]$$

where $n = \dfrac{dv^{w} + dv^{g}}{dv}$ is the porosity

- water

$$\eta^{w} = nS_{w} \qquad [2.\ 47]$$

where $S_{w} = \dfrac{dv^{w}}{dv^{w} + dv^{g}}$ is the degree water of saturation

- gas

$$\eta^g = nS_g \tag{2. 48}$$

where $S_g = \dfrac{dv^g}{dv^w + dv^g}$ is the degree of gas saturation.

It follows immediately that

$$S_w + S_g = 1 \tag{2. 49}$$

2.3.2.1 Solid phase

In the microscopic situation, the variables for solid in equation [2.13] assume the following values

$$\psi = 1 \qquad \mathbf{i} = \mathbf{0} \qquad b = 0 \qquad G = 0 \tag{2. 50}$$

and the microscopic mass balance equation results in

$$\frac{\partial \rho}{\partial t} + div(\rho\,\dot{\mathbf{r}}) = 0 \tag{2. 51}$$

The averaged macroscopic solid mass balance equation is

$$\frac{\partial \rho_s}{\partial t} + div\left(\rho_s \overline{\mathbf{v}}^s\right) = \rho_s e^s(\rho) \tag{2. 52}$$

where ρ_s stands simply for $\langle \rho \rangle_s$, the phase averaged solid density and $\overline{\mathbf{v}}^s$ is the mass averaged solid velocity. The same simplified notation will be used for the other constituents, once π is accordingly specified.

From [2.35] we have

$$\frac{D^s \rho_s}{Dt} = \frac{\partial \rho_s}{\partial t} + grad\ \rho_s \cdot \overline{\mathbf{v}}^s \tag{2. 53}$$

By introducing [2.53] in [2.52] we obtain

$$\frac{D^s \rho_s}{Dt} + \rho_s div\ \overline{\mathbf{v}}^s = 0 \tag{2. 54}$$

Because the following vector identity holds:

$$div\left(\rho_s \overline{\mathbf{v}}^s\right) = \rho_s div\ \overline{\mathbf{v}}^s + grad\ \rho_s \cdot \overline{\mathbf{v}}^s \tag{2. 55}$$

By introducing intrinsic phase averaged densities through equation [2.9] we have finally

$$\frac{D^s (1-n)\rho^s}{Dt} + \rho^s (1-n) div\, \overline{\mathbf{v}}^s = 0 \qquad [2.\ 56]$$

where the shorthand $\rho_s = \langle \rho \rangle_s^s$ has been introduced for the intrinsic phase averaged density.

2.3.2.2 Liquid phase: water

As for the solid phase we have:

$$\frac{\partial \rho_w}{\partial t} + div\left(\rho_w \overline{\mathbf{v}}^w\right) = \rho_w\, e^w(\rho) \qquad [2.\ 57]$$

$$\frac{D^w \rho_w}{Dt} + \rho_w\, div\, \overline{\mathbf{v}}^w = \rho_w\, e^w(\rho) \qquad [2.\ 58]$$

and finally

$$\rho_w\, e^w(\rho) = -\dot{m} \qquad [2.\ 59]$$

is the quantity of water lost through evaporation per unit time and volume.

2.3.2.3 Gaseous phases: dry air and vapour

The gaseous phase here is a multi-component material, composed of two different species: dry air and vapour. These species are miscible. We first write the mass balance equations for both species.

Their microscopic mass balance equations are again given by equation [2.51] if we neglect net production of mass of each species, due to chemical reactions with the other species [H86-2].

The macroscopic mass balance equation for dry air is given by equation [2.52] with appropriate superscripts and subscripts and with exchange term equal to zero. We introduce intrinsic phase averaged densities and use super/subscript *ga* to indicate dry air. Because the two species, dry air and vapour, are miscible, they have the same volume fraction $n\, S_g$, so

$$\frac{\partial}{\partial t}\left(n\, S_g \rho^{ga}\right) + div\left(n\, S_g \rho^{ga} \overline{\mathbf{v}}^{ga}\right) = 0 \qquad [2.\ 60]$$

Similarly we write for vapour, using super/subscript

$$\frac{\partial}{\partial t}\left(n\,S_g\,\rho^{gw}\right)+div\left(n\,S_g\rho^{gw}\overline{\mathbf{v}}^{gw}\right)=n\,S_g\rho^{gw}e^{gw}(\rho)=\dot{m} \qquad [2.\ 61]$$

We now derive the mass balance equation for the whole gaseous phase. This is obtained by summing the macroscopic balance equations of the two species and using appropriate definitions for bulk properties of the gaseous phase [H86-2].

$$\frac{\partial}{\partial t}\left(n\,S_g\rho^g\right)+div\left(n\,S_g\rho^g\overline{\mathbf{v}}^g\right)=\dot{m} \qquad [2.\ 62]$$

with

$$\rho^g=\rho^{ga}+\rho^{gw} \qquad [2.\ 63]$$

and

$$\overline{\mathbf{v}}^g=\frac{1}{\rho^g}\left(\rho^{ga}\overline{\mathbf{v}}^{ga}+\rho^{gw}\overline{\mathbf{v}}^{gw}\right)=c^{ga}\overline{\mathbf{v}}^{ga}+c^{gw}\overline{\mathbf{v}}^{gw} \qquad [2.\ 64]$$

where $c^\pi=\rho^\pi/\rho^g$ is the mass fraction of component π, subject to

$$\sum_\pi c^\pi=1 \qquad \pi=gw,ga \qquad [2.\ 65]$$

We introduce further the macroscopic diffusive dispersive velocity $\mathbf{u}^\pi,\pi=ga,gw$ defined as [H86-1]

$$\mathbf{u}^\pi=\overline{\mathbf{v}}^{\pi g}=\overline{\mathbf{v}}^\pi-\overline{\mathbf{v}}^g \qquad [2.\ 66]$$

and subject to

$$\rho^{ga}\mathbf{u}^{ga}+\rho^{gw}\mathbf{u}^{gw}=\rho^g\sum_\pi c^\pi\mathbf{u}^\pi=0 \qquad [2.\ 67]$$

Equation [2.62] for the gas phase can be transformed in a similar way to the equation for the solid phase, this yields to

$$\frac{D^g\left(n\,S_g\rho^g\right)}{Dt}+n\,S_g\,\rho^g\,div\,\overline{\mathbf{v}}^g=\dot{m} \qquad [2.\ 68]$$

With a proceedings similar to the earlier we obtained the following form of the mass balance equation for vapour

$$\frac{D^g}{Dt}\left(n\,S_g\rho^{gw}\right)+div\left(n\,S_g\rho^{gw}\mathbf{u}^{gw}\right)+n\,S_g\rho^{gw}div\,\overline{\mathbf{v}}^g=\dot{m} \qquad [2.\ 69]$$

We introduce now the diffusive-dispersive mass flux of component *gw* as [ES64]

$$\mathbf{J}_g^{gw}=n\,S_g\rho^{gw}\mathbf{u}^{gw} \qquad [2.\ 70]$$

and now we can write

$$\frac{D^g}{Dt}\left(n\,S_g\rho^{gw}\right)+div\,\mathbf{J}_g^{gw}+n\,S_g\,\rho^{gw}div\,\overline{\mathbf{v}}^g=\dot{m} \qquad [2.\ 71]$$

2.3.3 Linear momentum balance equation

The microscopic variables for equation [2.13] are as follows:

$$\boldsymbol{\psi}=\dot{\mathbf{r}} \qquad \mathbf{i}=\mathbf{t}_m \qquad \mathbf{b}=\mathbf{g} \qquad \mathbf{G}=\mathbf{0} \tag{2. 72}$$

where $\mathbf{t}_m$ is the microscopic stress tensor and $\boldsymbol{g}$ is the external momentum supply related to gravitational effects. The microscopic linear momentum balance is therefore

$$\frac{\partial}{\partial t}(\rho\dot{\mathbf{r}})+div\,(\rho\dot{\mathbf{r}}\otimes\dot{\mathbf{r}})-div\,\mathbf{t}_m-\rho\mathbf{g}=\mathbf{0} \tag{2. 73}$$

Since

$$div\,(\rho\dot{\mathbf{r}}\otimes\dot{\mathbf{r}})=\dot{\mathbf{r}}\otimes\dot{\mathbf{r}}\cdot grad\;\rho+\rho\;grad\,\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}+\rho\,\dot{\mathbf{r}}\;div\,\dot{\mathbf{r}} \tag{2. 74}$$

and

$$\frac{\partial\dot{\mathbf{r}}}{\partial t}+grad\,\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}=\ddot{\mathbf{r}} \tag{2. 75}$$

Equation [2.73] can be transformed by using the microscopic mass balance equation [2.51] to yield

$$div\,\mathbf{t}_m+\rho(\mathbf{g}-\ddot{\mathbf{r}})=\mathbf{0} \tag{2. 76}$$

which is the usual form of the momentum balance equation for a single phase material. For the averaged linear momentum balance equation obtained from [2.25] we have $\overline{\boldsymbol{\psi}}^{\pi}=\overline{\mathbf{v}}^{\pi}$, the mass averaged velocity of the constituent and

$$\tilde{\mathbf{i}}^{\pi}=\tilde{\mathbf{t}}^{\pi}=\frac{1}{da}\int_{da}\left(\mathbf{t}_m-\rho\,\tilde{\dot{\mathbf{r}}}^{\pi}\otimes\tilde{\dot{\mathbf{r}}}^{\pi}\right)\cdot\mathbf{n}\,\gamma^{\pi}\,da_m \tag{2. 77}$$

According to [2.21] there exists a stress tensor $\mathbf{t}^{\pi}$ such that

$$\tilde{\mathbf{t}}^{\pi}=\mathbf{t}^{\pi}\cdot\mathbf{n} \tag{2. 78}$$

In mixture theories $\mathbf{t}^{\pi}$ is called a partial stress tensor. The stress vector $\tilde{\mathbf{t}}^{\pi}$ is composed of the sum of the averaged microscopic stress tensor in the π phase and an averaged stress influx, produced by the mass fluxes, $\rho\,\tilde{\dot{\mathbf{r}}}^{\pi}$, which occur in the microscopic field relative to the macroscopic velocity of the π phase [deB91].

Note that only terms acting from the π phase on the π phase itself appear here. Hence $\tilde{\mathbf{t}}^{\pi}$ is the surface density of an interaction force within the π phase which is balanced by the body force [2.79] and inertia force [2.90], both additive and volume bounded functions, and by diffusive interactions [2.80] and [2.83] which are also volume bounded and additive. An important constitutive assumption which allows us to define $\mathbf{t}^{\pi}$ as a stress tensor will be discussed below. Furthermore

$$\overline{\mathbf{g}}^{\pi} = \frac{1}{\rho_{\pi} dv} \int_{dv} \rho \, \mathbf{g} \, \gamma^{\pi} dv_m$$

[2. 79]

is the external momentum supply, which we assume to be related to gravitational effects. $\rho_{\pi} \overline{\mathbf{g}}^{\pi}$ is the density of an additive volume bounded function.

$$\mathbf{e}^{\pi}(\rho \, \dot{\mathbf{r}}) = \mathbf{e}^{\pi}(\rho) \overline{\mathbf{v}}^{\pi} + \mathbf{e}^{\pi}\left(\rho \, \tilde{\dot{\mathbf{r}}}^{\pi}\right)$$

[2. 80]

where

$$\rho_{\pi} \mathbf{e}^{\pi}(\rho) = \frac{1}{dv} \sum_{\alpha \neq \pi}^{k} \int_{da^{\pi\alpha}} \rho \left[\overline{\mathbf{v}}^{\pi} \otimes (\mathbf{w} - \dot{\mathbf{r}})\right] \cdot \mathbf{n}^{\pi\alpha} \, da_m$$

[2. 81]

is the momentum exchange due to averaged mass supply, while

$$\rho_{\pi} \mathbf{e}^{\pi}\left(\rho \, \tilde{\dot{\mathbf{r}}}^{\pi}\right) = \frac{1}{dv} \sum_{\alpha \neq \pi}^{k} \int_{da^{\pi\alpha}} \rho \left[\tilde{\dot{\mathbf{r}}}^{\pi} \otimes (\mathbf{w} - \dot{\mathbf{r}})\right] \cdot \mathbf{n}^{\pi\alpha} da_m$$

[2. 82]

is the intrinsic momentum supply, with reference to the deviation $\tilde{\dot{\mathbf{r}}}^{\pi}$ of the velocity of constituent π from its mass averaged velocity $\overline{\mathbf{v}}^{\pi}$ due to a change of density.

Note that in the sum on the right-hand side of [2.81] and [2.82] only the interactions exerted on the π phase from the α phases appear, while those from the π phase on the α phases are missing.

$$\mathbf{I}^{\pi} = \hat{\mathbf{t}}^{\pi} = \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi}^{k} \int_{da^{\pi\alpha}} \mathbf{t}_m \cdot \mathbf{n}^{\pi\alpha} da_m$$

[2. 83]

accounts for the exchange of momentum due to mechanical interaction with other phases. Again the sum on the right-hand side extends only to the interactions exerted from the α phase on the π phase.

The sum of [2.80] and [2.83]

$$\rho_{\pi} \mathbf{I}^{\pi} + \rho_{\pi} \mathbf{e}^{\pi}(\rho \, \dot{\mathbf{r}})$$

[2. 84]

represents a supply quantity based on the volume *dv*. This sum may be interpreted as volume density of a volume bounded local diffusive interaction *D*, between the π phase and the other constituents.

Finally

$$\overline{\mathbf{G}}^{\pi} = \mathbf{0}$$

[2. 85]

With the above definitions, the averaged linear momentum balance equation may be written as

$$\frac{\partial}{\partial t}\left(\rho_{\pi} \overline{\mathbf{v}}^{\pi}\right) + div \left(\rho_{\pi} \overline{\mathbf{v}}^{\pi} \otimes \overline{\mathbf{v}}^{\pi}\right) - div \, \mathbf{t}^{\pi} - \rho_{\pi}\left[\overline{\mathbf{g}}^{\pi} + \mathbf{e}^{\pi}(\rho \, \dot{\mathbf{r}}) + \hat{\mathbf{t}}^{\pi}\right] = 0$$

[2. 86]

Recalling that averaged quantities are constant in *dv*, we make use of the relationship

$$div\left(\rho_\pi \bar{\mathbf{v}}^\pi \otimes \bar{\mathbf{v}}^\pi\right) = \bar{\mathbf{v}}^\pi \otimes \bar{\mathbf{v}}^\pi\ grad\ \rho_\pi + \rho_\pi grad\ \bar{\mathbf{v}}^\pi \cdot \bar{\mathbf{v}}^\pi + \rho\, \bar{\mathbf{v}}^\pi div\ \bar{\mathbf{v}}^\pi \qquad [2.\ 87]$$

of the definition of π phase acceleration

$$\bar{\mathbf{a}}^\pi = \dot{\bar{\mathbf{v}}}^\pi = \frac{\partial \bar{\mathbf{v}}^\pi}{\partial t} + grad \bar{\mathbf{v}}^\pi \cdot \bar{\mathbf{v}}^\pi \qquad [2.\ 88]$$

as well as of the averaged macroscopic mass balance eq. [2.52].

It follows hence that

$$div\,\mathbf{t}^\pi + \rho_\pi\left(\bar{\mathbf{g}}^\pi - \bar{\mathbf{a}}^\pi\right) + \rho_\pi\left[\mathbf{e}^\pi(\rho\,\dot{\mathbf{r}}) + \hat{\mathbf{t}}^\pi\right] = \mathbf{0} \qquad [2.\ 89]$$

The quantity

$$\rho_\pi \bar{\mathbf{a}}^\pi \qquad [2.\ 90]$$

is the volume density of the inertia force, which is also a volume bounded quantity. The stress tensor $\mathbf{t}^\pi$, introduced in [2.78] needs some comments. W. O. Williams [Wi78] has argued that $\mathbf{t}^\pi$ in the form used above and in the traditional formulation of mixture theory should be the sum of the stress tensor in the π phase itself and of the cross stress tensors [Wi78],[No93] of the type $\frac{1}{2}\mathbf{t}^{\pi\alpha}$, which describe the forces exerted by the other constituents $\alpha \neq \pi$ on the π phase. If *da* is a surface element in the porous body then $\int_{da} \mathbf{t}^{\pi\alpha} \cdot \mathbf{n}\, da_m = \mathbf{F}^{\pi\alpha}(da) + \mathbf{F}^{\alpha\pi}(da)$, where $\mathbf{F}^{\pi\alpha}$ is the contact force exerted by the π phase on the α phase across *da* and $\mathbf{F}^{\alpha\pi}$ the force exerted by the α phase on the π phase across *da*. Note that only their sum is balanced by a stress tensor because the interaction between the π phase interior to a diaphragm with the α phase exterior to the same diaphragm is not the same as the interaction between the α phase interior to the diaphragm with the π phase exterior to the diaphragm [No93].Williams and Noll consider additional identities of the type

$$div\,\mathbf{t}^{\pi\alpha} - \mathbf{d}^{\alpha\pi} - \mathbf{d}^{\pi\alpha} = \mathbf{0} \qquad [2.\ 91]$$

where $\mathbf{d}^{\alpha\pi}$, $\mathbf{d}^{\pi\alpha}$ are the densities of the diffusive interactions *D*, i.e. of the volume distributed force exerted by the π phase on the α phase and vice versa. These identities come from the equations of balance of force and are regarded in [Wi78] as identities giving the constitutive descriptions of $\mathbf{d}^{\alpha\pi} + \mathbf{d}^{\pi\alpha}$. In accordance with the above definition [Wi78] of the tensor $\mathbf{t}^\pi$ the densities of the diffusive interaction *D* in [2.80] and [2.82] should be a combination of the type $\frac{1}{2}\left(\mathbf{d}^{\pi\alpha} - \mathbf{d}^{\alpha\pi}\right)$ for the π phase and each other constituent α. Neither the stress tensor defined through [2.78] nor the diffusive interaction forces appear to take into account all the interaction terms from the π phase on the α phases mentioned here. Therefore we must take $\mathbf{t}^{\pi\alpha} = \mathbf{0}$ as a constitutive assumption which means that the only contact forces applied to a portion of the π phase inside a diaphragm are those applied by the π phase external to the diaphragm [H79-1].

With the assumption that $\mathbf{t}^{\pi\alpha} = \mathbf{0}$, it follows that the interaction densities are equal and opposite, from the identities [2.91].

Hence $\frac{1}{2}\left(\mathbf{d}^{\pi\alpha} - \mathbf{d}^{\alpha\pi}\right) = \mathbf{d}^{\pi\alpha}$, i.e. the supply terms considered [2.81], [2.82] and [2.83], express for $\mathbf{t}^{\pi\alpha} = \mathbf{0}$ the totality of the interactions from the α phases on the π phase and from the π phase on the α phases. In [SW79] examples with $\mathbf{t}^{\pi\alpha} \neq \mathbf{0}$ can be found. The assumption $\mathbf{t}^{\pi\alpha} = \mathbf{0}$ is hence a limiting one.

In the following we make a further assumption that $\rho_\pi\, \mathbf{e}^\pi(\rho\,\dot{\mathbf{r}}) \neq 0$ only for the fluid phases. The linear momentum balance equation for the solid becomes hence

$$div\,\mathbf{t}^s + \rho_s\left(\bar{\mathbf{g}}^s - \bar{\mathbf{a}}^s\right) + \rho_s\,\hat{\mathbf{t}}^s = \mathbf{0} \qquad \text{[2. 92]}$$

and for the fluids it has the form of [2.89]. The average linear momentum balance equations are subject to the constraint [2.26]:

$$\sum\nolimits_\pi \rho^\pi\left[\mathbf{e}^\pi(\rho\,\dot{\mathbf{r}}) + \hat{\mathbf{t}}^\pi\right] = 0 \qquad \text{[2. 93]}$$

2.3.4 Angular momentum balance equation

As indicated in section 2.3, all phases of the semi-saturated porous medium are considered microscopically non-polar. The following microscopic variables are necessary for the balance equation [2.13] when angular momentum balance is considered

$$\begin{aligned} \boldsymbol{\psi} &= \mathbf{r}\times\dot{\mathbf{r}} \\ \mathbf{i} &= \mathbf{r}\times\mathbf{t}_m \\ \mathbf{b} &= \mathbf{r}\times\mathbf{g} \\ \mathbf{G} &= \mathbf{0} \end{aligned} \qquad \text{[2. 94]}$$

Hence we obtain the microscopic angular momentum balance equation in the form

$$\frac{\partial}{\partial t}\left[\rho(\mathbf{r}\times\dot{\mathbf{r}})\right] + div\left[\rho(\mathbf{r}\times\dot{\mathbf{r}})\otimes\dot{\mathbf{r}}\right] - div\left(\mathbf{r}\times\mathbf{t}_m\right) - \mathbf{r}\times\rho\,\mathbf{g} = 0 \qquad \text{[2. 95]}$$

Using [2.51] and [2.75], as well as taking into account that

$$\frac{\partial}{\partial t}\left[\rho(\mathbf{r}\times\dot{\mathbf{r}})\right] = \frac{\partial\rho}{\partial t}(\mathbf{r}\times\dot{\mathbf{r}}) + \rho\left(\frac{\partial\mathbf{r}}{\partial t}\times\dot{\mathbf{r}}\right) + \rho\left(\mathbf{r}\times\frac{\partial\dot{\mathbf{r}}}{\partial t}\right)$$

$$\begin{aligned} div\,[\rho(\mathbf{r}\times\dot{\mathbf{r}})\otimes\dot{\mathbf{r}}] &= (grad\;\;\rho\cdot\dot{\mathbf{r}})(\mathbf{r}\times\dot{\mathbf{r}}) + (\rho\;div\;\;\dot{\mathbf{r}})(\mathbf{r}\times\dot{\mathbf{r}}) \\ &\quad + \rho\;\dot{\mathbf{r}}\cdot grad\;\;\mathbf{r}\times\dot{\mathbf{r}} + \rho\mathbf{r}\times\dot{\mathbf{r}}\cdot grad\;\;\mathbf{r} \end{aligned} \qquad [2.\,96]$$

and

$$div(\mathbf{r}\times\mathbf{t}_m) = grad\,\mathbf{r}\times\mathbf{t}_m + \mathbf{r}\times\;div\,\mathbf{t}_m \qquad [2.\,97]$$

one obtains

$$\left[\frac{D\rho}{Dt} + \rho\,div\,\dot{\mathbf{r}}\right](\mathbf{r}\times\dot{\mathbf{r}}) - \mathbf{r}\times[div\,\mathbf{t}_m + \rho(\mathbf{b}-\ddot{\mathbf{r}})] - grad\,\mathbf{r}\times\mathbf{t}_m = 0 \qquad [2.\,98]$$

After application of the mass balance equation [2.51] and of the linear momentum balance equation [2.76], as well as of the relation

$$grad\,\mathbf{r} = \mathbf{I} \qquad [2.\,99]$$

where $\mathbf{I}$ is the identity tensor, equation [2.98] reduces to

$$\mathbf{I}\times\mathbf{t}_m = 0 \qquad [2.\,100]$$

which implies the symmetry of the stress tensor

$$\mathbf{t}_{\mathrm{m}} = (\mathbf{t}_{\mathrm{m}})^{\mathrm{T}} \qquad [2.\,101]$$

In a similar way, it can be shown, with an appropriate method chosen for the development of the average angular momentum equation [deB91], [H79-1], that for non-polar media, also at macroscopic level, the partial stress tensor is symmetric

$$\mathbf{t}^{\pi} = (\mathbf{t}^{\pi})^{T} \qquad [2.\,102]$$

and that the sum of the coupling vectors of angular momentum between the phases vanishes. For the rather lengthy development see [deB91] and [H79-1].

2.3.5 Balance of energy equation

For the energy balance, the following components must be taken into account in the generic microscopic balance equation [2.13]:

$$\begin{aligned} &\psi = E + \frac{1}{2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}} \\ &\mathbf{i} = \mathbf{t}_m\,\dot{\mathbf{r}} - \mathbf{q} \\ &b = \mathbf{g}\cdot\dot{\mathbf{r}} + h \\ &G = 0 \end{aligned} \qquad [2.\,103]$$

where $E(\mathbf{r},t)$ is the specific intrinsic energy, $\mathbf{q}(\mathbf{r},t)$ is the heat flux vector and $h(\mathbf{r},t)$ is the intrinsic heat source.

Hence, the microscopic energy balance equation has the form

$$\frac{\partial}{\partial t}\left(\rho E+\rho\frac{1}{2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}\right)+div\left[\rho\left(E+\frac{1}{2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}\right)\dot{\mathbf{r}}\right]-div(\mathbf{t}_m\dot{\mathbf{r}}-\mathbf{q})-\rho(\mathbf{g}\cdot\dot{\mathbf{r}}+h)=0 \tag{2. 104}$$

Taking into account symmetry of the stress tensor [2.101], $\mathbf{t}_\mathrm{m} = \mathbf{t}_\mathrm{m}^\mathrm{T}$, the definition of the velocity gradient tensor [2.45], $\mathbf{L} = grad\,\dot{\mathbf{r}}$, and relation [deB91]

$$\mathbf{t}_\mathrm{m}\mathbf{:W=0} \tag{2. 105}$$

we obtain

$$\frac{D}{Dt}(\rho E)+\rho E\,div\,\dot{\mathbf{r}}+\frac{D}{Dt}\left(\rho\frac{1}{2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}\right)+\frac{1}{2}\rho\,\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}\,div\,\dot{\mathbf{r}}$$
$$=\rho\,\ddot{\mathbf{r}}\cdot\dot{\mathbf{r}}+\mathbf{t}_m:\mathrm{D}-div\,\mathbf{q}+\rho\,h \tag{2. 106}$$

Taking into account the microscopic mass balance equation [2.51] and the microscopic linear momentum balance equation [2.76], the final form of the conservation law of energy is obtained as

$$\rho\frac{DE}{Dt}=\mathbf{t}_m:\mathbf{D}-div\,\mathbf{q}+\rho h \tag{2. 107}$$

The average quantities necessary for the macroscopic balance equation [2.23] are the following [deB91] and [H79-1]

$$\overline{\psi}^\pi=\overline{E}^\pi+\frac{1}{2}\overline{\mathbf{v}}^\pi\cdot\overline{\mathbf{v}}^\pi \tag{2. 108}$$

where $\overline{\mathrm{E}}^\pi$ accounts for the averaged specific energy of the volume element and for the averaged kinetic energy related to the deviation, $\tilde{\dot{\mathbf{r}}}^\pi$, from the mean velocity in *dv*.

The flux term is obtained after substitution of the generic quantities in [2.21] using [2.103] and [2.108]:

$$\tilde{i}^\pi=\frac{1}{da}\int_{da}\left[\mathbf{t}_m\dot{\mathbf{r}}-\mathbf{q}-\rho\left(E+\frac{1}{2}\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}-\overline{E}^\pi-\frac{1}{2}\overline{\mathbf{v}}^\pi\cdot\overline{\mathbf{v}}^\pi\right)\tilde{\dot{\mathrm{r}}}^\pi\right]\cdot\mathbf{n}\,\gamma^\pi da_m \tag{2. 109}$$

After further transformation by use of [2.77] and the deviation definition $\zeta^\pi(\mathbf{x},\xi,t)=\zeta^\pi(\mathbf{r},t)-\overline{\zeta}^\pi(\mathbf{x},t)$ applied for the π phase velocity

$$\tilde{\mathbf{v}}^\pi=\tilde{\dot{\mathbf{r}}}^\pi=\dot{\mathbf{r}}^\pi-\overline{\dot{\mathbf{r}}}^\pi=\dot{\mathbf{r}}^\pi-\overline{\mathbf{v}}^\pi \tag{2. 110}$$

the following form for $\tilde{i}^\pi$ is obtained

$$\tilde{i}^\pi=\tilde{\mathbf{t}}^\pi\cdot\overline{\mathbf{v}}^\pi+\frac{1}{da}\int_{da}\left[\mathbf{t}_m\tilde{\dot{\mathbf{r}}}-\mathbf{q}-\rho\left(E+\frac{1}{2}\tilde{\dot{\mathbf{r}}}^\pi\cdot\tilde{\dot{\mathbf{r}}}^\pi\right)\tilde{\dot{\mathbf{r}}}^\pi\right]\cdot\mathbf{n}\,\gamma^\pi da_m \tag{2. 111}$$

The integral expression represents the averaged internal heat flux, $\tilde{\mathbf{q}}^\pi$. Following [2.21], a macroscopic heat flux vector can be defined such that

$$\tilde{q}^{\pi} = \tilde{\mathbf{q}}^{\pi} \cdot \mathbf{n}$$

and eq. [2.111] can be written in simplified form

$$\tilde{i}^{\pi} = \tilde{\mathbf{t}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi} - \tilde{q}^{\pi}$$

where the negative sign takes into account the opposite direction of $\mathbf{q}^{\pi}$ and $\mathbf{n}$ [deB91]. The term for the external energy supply is

$$\overline{b}^{\pi} = h^{\pi} + \mathbf{g}^{\pi} \cdot \overline{\mathbf{v}}^{\pi} \tag{2. 112}$$

where h^{π} results from the sum of the averaged heat sources, h and the averaged work done by external volume forces due to the velocity difference $\tilde{\dot{\mathbf{r}}}^{\pi}$. The supply terms [2.19] and [2.20] are dealt with next.

$$e^{\pi}(\rho\psi) = e^{\pi}\left(\rho E + \frac{1}{2}\rho\,\dot{\mathbf{r}} \cdot \dot{\mathbf{r}}\right) = \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} \rho\left(E + \frac{1}{2}\dot{\mathbf{r}} \cdot \dot{\mathbf{r}}\right)(\mathbf{w} - \dot{\mathbf{r}}) \cdot \mathbf{n}^{\pi\alpha} da_{m} \tag{2. 113}$$

Upon use of the deviation term, [2.113] may be transformed as

$$e^{\pi}(\rho\psi) = \mathbf{e}^{\pi}\left(\rho\,\tilde{\dot{\mathbf{r}}}^{\pi}\right) \cdot \overline{\mathbf{v}}^{\pi} + \frac{1}{2} e^{\pi}(\rho)\,\overline{\mathbf{v}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi} + e^{\pi}\left(\rho\hat{E}\right) \tag{2. 114}$$

where

$$e^{\pi}\left(\rho\hat{E}\right) = e^{\pi} = \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} \rho\left(E + \frac{1}{2}\tilde{\dot{\mathbf{r}}} \cdot \tilde{\dot{\mathbf{r}}}\right)(\mathrm{w} - \dot{\mathbf{r}}) \cdot \mathbf{n}^{\pi\alpha} da_{m} \tag{2. 115}$$

is the exchange term of internal energy due to phase change and possible mass exchange. Further, according to [2.19], we have

$$I^{\pi} = \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} (\mathbf{t}_{m}\,\dot{\mathbf{r}} - \mathbf{q}) \cdot \mathbf{n}^{\pi\alpha} da_{m} \tag{2. 116}$$

Taking into account [2.83] and the deviation term, we may write [2.116] as

$$I^{\pi} = \hat{\mathbf{t}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi} + \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} \left(\mathbf{t}_{m}\,\tilde{\dot{\mathbf{r}}}^{\pi} - \mathbf{q}\right) \cdot \mathbf{n}^{\pi\alpha} da_{m} = \hat{\mathbf{t}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi} + Q^{\pi} \tag{2. 117}$$

The integral expression indicated as Q^{π} represents the exchange of energy due to mechanical interaction.

Finally

$$\overline{G}^{\pi} = 0 \tag{2. 118}$$

The macroscopic energy balance equation may now be written as

$$\frac{\partial}{\partial t}\left[\rho_{\pi}\left(\overline{E}^{\pi} + \frac{1}{2}\overline{\mathbf{v}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi}\right)\right] + div\left[\rho_{\pi}\left(\overline{E}^{\pi} + \frac{1}{2}\overline{\mathbf{v}}^{\pi} \cdot \overline{\mathbf{v}}^{\pi}\right)\overline{\mathbf{v}}^{\pi}\right]$$

$$-div\left(\mathrm{t}^{\pi}\overline{\mathbf{v}}^{\pi}-\tilde{\mathbf{q}}^{\pi}\right)-\rho_{\pi}\left(h^{\pi}+\mathbf{g}^{\pi}\cdot\overline{\mathbf{v}}^{\pi}\right)-\rho_{\pi}\mathbf{e}^{\pi}\left(\rho\,\tilde{\dot{\mathbf{r}}}^{\pi}\right)\cdot\overline{\mathbf{v}}^{\pi}$$

$$-\frac{1}{2}\rho_{\pi}\,e^{\pi}(\rho)\overline{\mathbf{v}}^{\pi}\cdot\overline{\mathbf{v}}^{\pi}-\rho_{\pi}\,e^{\pi}\left(\rho\hat{E}\right)-\rho_{\pi}\,\hat{\mathbf{t}}^{\pi}\cdot\overline{\mathbf{v}}^{\pi}-\rho_{\pi}Q^{\pi}=0\,. \qquad [2.\ 119]$$

Using the mass balance equation [2.52] for the generic π phase, the definition of material derivatives, the linear momentum balance equation [2.89] and [2.45], the energy balance equation may be written as follows

$$\rho_{\pi}\frac{D^{\pi}\overline{E}^{\pi}}{Dt}=\mathbf{t}^{\pi}:\mathbf{D}^{\pi}+\rho_{\pi}h^{\pi}-div\,\tilde{\mathbf{q}}^{\pi}+\rho_{\pi}R^{\pi} \qquad [2.\ 120]$$

where

$$\rho_{\pi}\,R^{\pi}=\rho_{\pi}\left[e^{\pi}\left(\rho\,\hat{E}\right)-e^{\pi}(\rho)\overline{E}^{\pi}+Q^{\pi}\right] \qquad [2.\ 121]$$

represents the exchange of energy between π phase and other phases of the medium due to phase change and mechanical interaction. Equation [2.120] coincides with the energy balance equation in the mixture theory as shown in [deB91].

For energy balance, [2.26] has the form:

$$\sum_{\pi}\rho_{\pi}\left[e^{\pi}\left(\rho\hat{E}\right)+\mathrm{e}^{\pi}\left(\rho\,\tilde{\dot{\mathrm{r}}}\right)\cdot\overline{\mathrm{v}}^{\pi}+\frac{1}{2}e^{\pi}(\rho)\overline{\mathrm{v}}^{\pi}\cdot\overline{\mathrm{v}}^{\pi}+\hat{\mathrm{t}}^{\pi}\cdot\overline{\mathrm{v}}^{\pi}+Q^{\pi}\right]=0 \qquad [2.\ 122]$$

and physically means that the total balance of energy exchange between all the phases is zero. Phase change and the corresponding supply terms will be considered in the following, only for the fluid phases.

2.3.6 Entropy inequality

Exploitation of entropy inequality is a tool for developing constitutive equations in a systematic manner, leading to a consistent thermodynamic description of the material behaviour at macroscale. The use of entropy inequality further assures that the second law of thermodynamics is not violated. The procedure was proposed by Coleman and W. Noll [CN63]. It is, for instance, exploited in [SW79], and recently by Gray and Hassanizzadeh [G91-2] for the development of constitutive equations for unsaturated flow in dry or partially saturated soil, including interfacial phenomena. Although we use, throughout this book, existing constitutive relations which are closer to current laboratory practice, we quote here the entropy inequalities from [deB91] both for the microscale and for the macroscale.

The variables in the microscopic balance equation [2.13] are now

$$\psi = \lambda \quad \mathbf{i} = \Phi, \quad \mathrm{b} = \mathrm{s}, \quad \mathrm{G} = \varphi \qquad [2.\ 123]$$

where λ is the specific entropy, Φ the entropy flux vector and s an intrinsic entropy source. The net production φ denotes an increase of entropy. The balance equation becomes then

$$\frac{\partial}{\partial t}(\rho\lambda) + div\,(\rho\lambda\,\dot{\mathrm{r}}) - div\,\mathbf{\Phi} - \rho\, s = \rho\varphi \qquad [2.\ 124]$$

This equation may be transformed in the usual manner, also making use of the mass balance equation to obtain

$$\rho\frac{D\lambda}{Dt} - \rho s - div\,\mathbf{\Phi} = \varphi \qquad [2.\ 125]$$

By identifying the entropy flux $\mathbf{\Phi}$ and the entropy source *s* respectively with the energy flux vector $\mathbf{q}$ and the energy source *h*, both divided by the absolute temperature θ [deB91], [2.125] may be written as

$$\rho\frac{D\lambda}{Dt} - \frac{1}{\theta}\rho\, h + div\frac{1}{\theta}\mathbf{q} = \rho\varphi \qquad [2.\ 126]$$

According to the second law of thermodynamics, the entropy production is zero for reversible processes, while for irreversible processes

$$\rho\varphi \geq 0 \qquad [2.\ 127]$$

Equations [2.126] and [2.127] yield the entropy inequality for single component media

$$\rho\frac{\mathrm{D}\lambda}{\mathrm{Dt}} - \frac{1}{\theta}\rho\,\mathrm{h} + \mathrm{div}\frac{1}{\theta}\,\mathbf{q} \geq 0 \qquad [2.\ 128]$$

The macroscopic variables are identified as follows

$$\overline{\psi}^{\pi} = \overline{\lambda}^{\pi} = \frac{1}{\rho_{\pi} dv}\int_{dv} \rho\lambda\,\gamma^{\pi} dv_m \qquad [2.\ 129]$$

is the averaged specific entropy of constituent π,

$$\tilde{i}^{\pi} = \tilde{\Phi}^{\pi} = \frac{1}{da}\int_{da}\left(\mathbf{\Phi} - \rho\,\tilde{\lambda}^{\pi}\,\tilde{\mathbf{r}}^{\pi}\right)\cdot\mathbf{n}\,\gamma^{\pi} da_m \qquad [2.\ 130]$$

is the averaged entropy supply density, for which an entropy supply vector can be defined, such that

$$\tilde{\Phi}^{\pi} = \mathbf{\Phi}^{\pi}\cdot\mathbf{n} \qquad [2.\ 131]$$

$$e^{\pi}(\rho\psi) = e^{\pi}(\rho\lambda) = \frac{1}{\rho_{\pi} dv}\sum_{\alpha\neq\pi}\int_{da^{\pi\alpha}} \rho\lambda\,(\mathbf{w} - \dot{\mathbf{r}})\cdot\mathbf{n}^{\pi\alpha} da_m \qquad [2.\ 132]$$

is the entropy supply due to mass exchange.

$$I^{\pi} = \frac{1}{\rho_{\pi} dv} \sum_{\alpha \neq \pi} \int_{da^{\pi\alpha}} \mathbf{\Phi} \cdot \mathbf{n}^{\pi\alpha} da_{m} \qquad [2.\ 133]$$

denotes the entropy supply due to mechanical interactions. Further

$$\bar{b}^{\pi} = \bar{s}^{\pi} \qquad [2.\ 134]$$

is the averaged entropy source and

$$\overline{G}^{\pi} = \overline{\varphi}^{\pi} \qquad [2.\ 135]$$

the averaged total entropy increase.

If the sum of both supply terms [2.132] and [2.133] is indicated as $\frac{1}{\rho_{\pi}} \hat{\lambda}^{\pi}$ and the usual transformation is applied, we obtain

$$\rho_{\pi} \frac{\overset{\pi}{D} \overline{\lambda}^{\pi}}{Dt} + \rho_{\pi}\, e^{\pi}(\rho) \overline{\lambda}^{\pi} - div\, \mathbf{\Phi}^{\pi} - \rho_{\pi}\, \bar{s}^{\pi} - \hat{\lambda}^{\pi} = \rho_{\pi} \overline{\varphi}^{\pi} \qquad [2.\ 136]$$

Equation [2.26] is simply

$$\sum_{\pi} \hat{\lambda}^{\pi} = 0 \qquad [2.\ 137]$$

We define now as for the microscopic situation

$$\sum_{\pi} \rho_{\pi} \overline{\varphi}^{\pi} \geq 0 \qquad [2.\ 138]$$

By assuming that the absolute temperature θ and the external acceleration g are microscopically constant, the entropy supply vector may be written as

$$\mathbf{\Phi}^{\pi} = \frac{1}{\theta^{\pi}} \mathbf{q}^{\pi} \qquad [2.\ 139]$$

and equation [2.134] as

$$\bar{s}^{\pi} = \frac{1}{\theta^{\pi}} h^{\pi} \qquad [2.\ 140]$$

The entropy inequality for the mixture, which is the quantity of interest here, taking into account [2.137] and [2.138], finally becomes

$$\sum_{\pi} \left[\rho_{\pi} \frac{\overset{\pi}{D} \overline{\lambda}^{\pi}}{Dt} + \rho_{\pi} e^{\pi}(\rho) \overline{\lambda}^{\pi} + div \left(\frac{1}{\theta^{\pi}} \mathbf{q}^{\pi} \right) - \frac{1}{\theta^{\pi}} \rho_{\pi}\, h^{\pi} \right] \geq 0 \qquad [2.\ 141]$$

Again, this corresponds to the form used in the mixture theory as shown in [deB91].

Before further transformations of the macroscopic balance equations are made, we introduce the constitutive equations for the constituents.

2.4 Constitutive equations

To complete the description of the mechanical behaviour, we now need to specify the constitutive equations. The balance equations developed in the previous sections allows for the introduction of quite elaborate constitutive theories, especially if the balance equations presented in the previous sections for the bulk material are extended to the interfaces, as done by Gray and Hassanizadeh in [G91-1] and [G91-2] for the aspects concerning multiphase flow. For the solid phase, second-grade material theories are also possible, where the gradients of relevant thermodynamic properties, such as densities, are considered as independent variables [Ehl89].

The constitutive models selected are based on quantities currently measurable in laboratory or field experiments and which have been extensively validated both with reference to known exact solutions and to experiments. Many of these constitutive models correspond to linearization of more complex arguments.

2.4.1 Stress tensor in the fluid phases

By applying entropy inequality for the bulk material [H80-3] [G91-1], it can been shown that the stress tensor in the fluid phases is

$$\mathbf{t}^{\pi} = -\eta^{\pi} p^{\pi} \mathbf{I} \qquad [2.\ 142]$$

where $\mathbf{I}$ is the identity tensor and p^{π} is the macroscopic pressure of the π phase.

The volume fraction η^{π} appears in equation [2.142] because $\mathbf{t}^{\pi}$ is the force exerted on the fluid phase per unit area of multiphase medium. It should be noted that the stress vector in the fluid phase does not have any dissipating part. The macroscopic effects of deviatoric stress components will be accounted for in linear momentum balance equations through momentum exchange terms.

2.4.2 Gaseous mixture of dry air and water vapour

The moist air in the pore system is usually assumed to be a perfect mixture of two ideal gases, i.e. dry air and water vapour. Hence the ideal gas law, relating the partial pressure $p_{g\pi}$ of species π, the mass concentration $\rho^{g\pi}$ of species π in the gas phase and the absolute temperature θ is used. The equations of state of a perfect gas, applied to dry air (*ga*), vapour (*gw*) and moist air (*g*) are

$$p^{ga} = \rho^{ga}\,\theta\,R/M_a$$
$$p^{gw} = \rho^{gw}\theta\,R/M_w \qquad [2.\ 143]$$

$$\rho^g = \rho^{ga} + \rho^{gw}$$
$$p^g = p^{ga} + p^{gw}$$
$$M_g = \left(\frac{\rho^{gw}}{\rho^g}\frac{1}{M_w} + \frac{\rho^{ga}}{\rho^g}\frac{1}{M_a}\right)^{-1} \qquad [2.\ 144]$$

where M_π is the molar mass of constituent π and R is the universal gas constant.

The second equations in [2.144] expresses Dalton's law [MS93]. For the averaging process it is reminded that dry air, vapour and moist air occupy the same volume fraction, nS_g.

2.4.3 Sorption equilibrium

If an oven-dry porous medium is exposed to moist air, the weight of such solid increases because the moisture is adsorbed on the inner surfaces of the pores starting with the finest ones. In the cases of interest here, the water is usually present as a condensed liquid that, because of the surface tension, is separated from its vapour by a concave meniscus (capillary water). There is then a relationship between the relative humidity, the water content (saturation) and the capillary pressure in the pores.

The capillary pressure is defined as the pressure difference between the gas phase and the liquid phase, by the capillary pressure equation

$$p^c = p^g - p^w \qquad [2.\ 145]$$

where p^w is the pressure of the liquid-phase (water). In [G91-2] it is shown that [2.145] is not just a definition, but a derived relationship between two independent quantities p^c and $p^g - p^w$, at equilibrium.

For the relationship between the relative humidity (RH) and the capillary pressure in the pores, Kelvin-Laplace law is assumed to be valid:

$$RH = \frac{p^{gw}}{p^{gws}} = \exp\left(\frac{p^c\,M_w}{\rho^w\,R\theta}\right) \qquad [2.\ 146]$$

The water vapour saturation pressure p^{gws}, which is a function of the temperature only, can be obtained from the Clausius-Clapeyron equation indicated below, or from empirical formulas such as the one proposed by in [AS93].

Assuming zero contact angle between the liquid phase and the solid phase, as is usually accepted for pore water, the capillary pressure can be obtained through the Laplace equation from the pore radius *r:*

$$p^c = \frac{2\sigma}{r} \qquad [2.\ 147]$$

where σ is the surface tension.

These considerations are applicable if the water is present in the pores, as a condensed liquid (capillary region). When, instead, the water is present as one or more molecular layers adsorbed on the surface of a solid because of the Van der Waals and/or other interactions, the capillary pressure no longer has an obvious meaning, even if it can be retained, referring to the broader concept of water potential or moisture stress. In such a case a direct relationship between the water content and the relative humidity is assumed to hold such as the BET equation [AS93].

2.4.4 Clausius-Clapeyron equation

As indicated above, this equation links the water vapour saturation pressure with temperature:

$$p^{gws}(\theta) = p^{gws0} \exp\left[-\frac{M_w \Delta H_{gw}}{R}\left(\frac{1}{\theta} - \frac{1}{\theta_0}\right)\right] \qquad [2.\ 148]$$

where θ_0 is a reference temperature, p^{gws} is the water vapour saturation pressure at θ, p^{gws0} is the water vapour saturation pressure at θ_0 and ΔH_{gw} is the specific enthalpy of evaporation. The equation is obtained from the second law of thermodynamics and is valid in the vicinity of θ_0. In the following, we denote *T* as the temperature difference above a reference value such that.

$$T = \theta\text{-}\theta_0 \qquad [2.\ 149]$$

2.4.5 Pore size distribution

As it turns out from equations [2.146] and [2.147], the problem is to know the pore size distribution of the considered porous medium, to relate the size of the largest pore filled (from which the capillary pressure depends) with the actual water content. This relationship is obtained through experimental tests, usually centrifuge tests, sorption isotherm measurements or mercury porosimetry.

The question is somewhat complex, because both the Laplace equation [2.147] and the Kelvin equation [2.146] are obtained from a force equilibrium, evaluated in a cylindrical capillary tube, and the porous medium is considered as a bundle of capillary tubes that do not intersect. The real porous media are more correctly represented as three-dimensional networks of sites (or bodies) interconnected by narrower bonds (or throats) and then intrusion, extrusion, adsorption and desorption are subjected to hysteresis. In this case, the actual value of capillary pressure can be only interpreted as a measurable quantity describing complex adsorbed water-solid matrix interaction. The determination of pore size distribution from sorption isotherms, results of centrifuge tests and mercury porosimetry should then be done following the percolation theory approach [BS78].

The Rayleigh distribution or the log-normal distributions are often a good estimation of the pore size and often such distribution can be bi-modal or multi-modal.

For soils, we need the Kelvin-Laplace equation [2.146], the Clausius-Clapeyron equation [2.148] and the capillary pressure relationship

$$S_\pi = S_\pi\left(p^c, T\right) \qquad [2.\ 150]$$

which is directly obtained in laboratory.

2.4.6 Equation of state for water

The equation of state for water has been given by Fernandez [Fer72] as

$$\rho^w = \rho^{w0} \exp\left[-\beta_w T + C_w\left(p^w - p^{w0}\right)\right] \qquad [2.\ 151]$$

where the superscript 0 indicates an initial steady state at standard conditions; β_w is the thermal expansion coefficient and C_w is the compressibility coefficient. By retaining the first-order terms of the series expansion of [2.151] we obtain

$$\rho^w = \rho^{w0}\left[1 - \beta_w T + C_w\left(p^w - p^{w0}\right)\right] \qquad [2.\ 152]$$

and

$$\frac{1}{\rho^{w0}} \frac{D^w \rho^w}{\mathrm{Dt}} = \frac{1}{K_w} \frac{D^w p^w}{\mathrm{D}t} - \beta_w \frac{D^w T}{\mathrm{D}t} \qquad [2.\ 153]$$

where $K_w = \frac{1}{C_w}$ is the bulk modulus of water and C_w is the compressibility coefficient.

Equation [2.153] can also be obtained from the mass conservation in differential form:

$$\frac{D^w\left(\rho^w V^w\right)}{Dt}=0 \qquad [2.\ 154]$$

In fact, by carrying out the differentiation of a product and keeping in mind that $\rho^w=\rho^w\left(p^w,T\right)$, we can write

$$\frac{1}{\rho^w}\frac{D^w\rho^w}{Dt}=-\frac{1}{V^w}\frac{D^wV^w}{Dt}=\frac{1}{\rho^w}\left(\frac{\partial\rho^w}{\partial p^w}\frac{D^w p^w}{Dt}+\frac{\partial\rho^w}{\partial T}\frac{D^wT}{Dt}\right) \qquad [2.\ 155]$$

Since

$$\frac{1}{\rho^{wo}}\frac{\partial\rho^w}{\partial p^w}=\frac{1}{K_w} \qquad [2.\ 156]$$

$$\frac{1}{\rho^{wo}}\frac{\partial\rho^w}{\partial T}=-\beta_w \qquad [2.\ 157]$$

it follows that

$$\frac{1}{\rho^{w0}}\frac{D^w\rho^w}{Dt}=\frac{1}{K_w}\frac{D^w p^w}{Dt}-\beta_w\frac{D^wT}{Dt} \qquad [2.\ 158]$$

2.4.7 Darcy's law

Darcy's law, generalized to allow for relative permeability,

$$\eta^\pi\bar{\mathbf{v}}^{\pi s}=\frac{k^{r\pi}\mathbf{k}}{\mu^\pi}\left(-grad\ p^\pi+\rho^\pi\,\mathbf{g}\right) \qquad [2.\ 159]$$

where $\mathbf{k}$ is the permeability of the medium, μ is the dynamic viscosity, $k^{r\pi}$ is the relative permeability, a dimensionless parameter varying from zero to one. It is assumed valid for the transport of both water and gas in slow phenomena.

For each particular porous medium, the relations $k^{r\pi}\left(S_w\right)$ are either predicted by models based on some more or less realistic capillary assumption or experimentally determined in laboratory as well as field conditions. For typical curves of relative permeability to water and air the reader is referred to Corey [Cor57].

The relative permeability goes to zero before the saturation reaches the value zero. The water saturation at which the relative permeability goes to zero is called the residual water saturation or the displacement residual water saturation.

Relationships used in the following are e.g. those by Brooks and Corey [BC66]:

$$k^{rw}=S_e^{\frac{(2+3\lambda)}{\lambda}} \qquad [2.\ 160]$$

$$k^{ra} = (1 - S_e)^2 \left(1 - S_e^{\frac{(2+\lambda)}{\lambda}} \right) \qquad [2.\ 161]$$

$$p^c = \frac{p^b}{S_e^{\frac{1}{\lambda}}} \qquad [2.\ 162]$$

where

$S_e = \dfrac{S_w - S_{wc}}{1 - S_{wc}}$ is the effective saturation, S_{wc} is the irreducible saturation, λ is the pore size distribution index and p^b is the bubbling pressure.

2.4.8 Fick's law

Diffusive-dispersive mass flux is governed by Fick's law

$$\mathrm{J}_\alpha^\pi = -\rho^\alpha \, \mathbf{D}_\alpha^\pi \, grad \left(\frac{\rho^\pi}{\rho^\alpha} \right) \qquad [2.\ 163]$$

where D_α^π is the effective dispersion tensor, π is diffusing phase, α is the phase in which diffusion takes place (α = *w*, *g*). D_α^π is a function of the tortuosity factor, which accounts for the tortuous nature of the pathway in soil; because of mechanical dispersion, D_α^π is also correlated with seepage velocity.

For dry air and water vapour (binary system) we have in particular, by the first of equations [2.144], that

$$\begin{aligned} \mathbf{J}_g^{ga} &= -\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g \, grad \left(\frac{p^{ga}}{p^g} \right) = \\ &= \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g \, grad \left(\frac{p^{gw}}{p^g} \right) = -\mathbf{J}_g^{gw} \end{aligned} \qquad [2.\ 164]$$

It is worthwhile to emphasise that gas diffusion can take place even in the absence of a gas pressure gradient, i.e. when its mass weighted velocity $\overline{\mathbf{v}}^g$ is zero.

2.4.9 Stress tensor in the solid phase and total stress

From the entropy inequality written in [G91-1] for unsaturated flow, including interfacial phenomena, it can be shown that the stress vector in the solid phase is

$$\mathbf{t}^s = (1 - n)(\mathbf{t}_e^s - \mathbf{I} p^s) \qquad [2.\ 165]$$

pressure in the solid phase is

$$p^s = p^w\, S_w + p^g\, S_g \tag{2. 166}$$

and

$$\boldsymbol{\sigma}' = (1-n)\,\mathbf{t}^s_e \tag{2. 167}$$

is the effective stress tensor.

Introduction of [2.166] into [2.165] yields

$$\mathbf{t}^s = (1-n)\left[\mathbf{t}^s_e - \mathbf{I}\left(S_w\, p^w + S_g\, p^g\right)\right] \tag{2. 168}$$

The volume fraction $(1-n)$ indicates that $\mathbf{t}^s$ is the stress exerted on the solid phase per unit area of a multiphase medium. The sum of [2.168] and of [2.142] written for gas and for water gives the total stress $\boldsymbol{\sigma}$ acting on a unit area of a multiphase medium:

$$\begin{aligned} \boldsymbol{\sigma} &= \mathbf{t}^s + \mathbf{t}^w + \mathbf{t}^g = \\ &= (1-n)\left[\mathbf{t}^s_e - \mathbf{I}\left(S_w p^w + S_g p^g\right)\right] - S_w n \mathbf{I} p^w - S_g n \mathbf{I} p^g = \\ &= (1-n)\mathbf{t}^s_e - \mathbf{I}\left(S_w p^w + S_g p^g\right) \end{aligned} \tag{2. 169}$$

This can be put in the usual soil mechanics form as

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - \mathbf{I}\left(S_w p^w + S_g p^g\right) \tag{2. 170}$$

or

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{I}\left(S_w p^w + S_g p^g\right) \tag{2. 171}$$

From this last equation, it follows that the relationship between effective stress and total stress, in partially saturated porous media, is no longer independent of the soil type because of the saturations, while in fully saturated soils, where $S_g = 0$ and $S_w = 1$, the effective stress principle [2.170] is unique for all soil types.

An expression of the effective stress principle was obtained by Bishop and Blight [BB63] using a phenomenological approach.

The effective stress is responsible for all major deformations in the skeleton and is linked to the strain rate tensor $\mathbf{D}^s$ by means of a constitutive relationship

$$\frac{D\boldsymbol{\sigma}'}{Dt} = \mathbf{D}_T\left[\left(\mathbf{D}^s - \mathbf{D}^s_0\right)\right] \tag{2. 172}$$

where

$$\mathbf{D}_T = \mathbf{D}_T\left(\mathbf{D}^s, \boldsymbol{\sigma}', p^c, T\right) \tag{2. 173}$$

is a fourth order tensor and $\mathbf{D}^s_0$ represents the increment of all other strains not directly associated with stress changes.

Assuming a small strain, we can say that

$$\mathbf{D}^s = \boldsymbol{\varepsilon} dt \qquad [2.\ 174]$$

where $\boldsymbol{\varepsilon}$ is the linear strain tensor.

2.4.10 Solid density

When considering the solid phase as compressible, a relationship for the material time derivative of the solid density can be obtained from the mass conservation equation in differential form

$$\frac{D^s(\rho^s V^s)}{Dt} = 0 \qquad [2.\ 175]$$

By assuming that the solid density is a function of p^s [2.166], temperature and the first invariant of the effective stress

$$\frac{1}{\rho^s}\frac{D^s\rho^s}{Dt} = -\frac{1}{V^s}\frac{D^s V^s}{Dt} = \frac{1}{K_s}\frac{D^s p^s}{Dt} - \beta_s\frac{D^s T}{Dt} - \frac{1}{3(n-1)K_s}\frac{D^s(tr\boldsymbol{\sigma}')}{Dt} \qquad [2.\ 176]$$

where we have kept in mind that

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial p^s} = \frac{1}{K_s} \qquad [2.\ 177]$$

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial T} = -\beta_s \qquad [2.\ 178]$$

$$\frac{1}{\rho^s}\frac{\partial\rho^s}{\partial \mathbf{I}_{1\sigma'}} = -\frac{1}{3(n-1)K_s} \qquad [2.\ 179]$$

where K_s is the bulk modulus of the grain material, β_s is the thermal expansion coefficient for the solid and $\mathbf{I}_{1\sigma'}$ is the first stress invariant.

We introduce now the constitutive relationship for the first stress invariant as

$$\frac{D^s\mathbf{I}_{1\sigma'}}{Dt} = 3K_T\left(div\overline{\mathbf{v}}^s + \frac{1}{K_s}\frac{D^s p^s}{Dt} - \beta_s\frac{D^s T}{Dt}\right)$$

where K_T is the bulk modulus of the skeleton, different from that of the grain material and $-\frac{1}{K_s}\frac{D^s p^s}{Dt}$ represents an overall volumetric strain rate caused by uniform compression of particles (as opposed to the skeleton) by the average pressure p^s. In the soils this volumetric strain is relatively insignificant and can be ignored, but it is important in rock mechanics and in concrete, where the compressibility of the solid phase is comparable to that of the skeleton.

Defining the Biot's constant [BW57] as

$$\alpha = 1 - \frac{K_T}{K_s} \qquad [2.\ 180]$$

we obtain

$$\frac{1}{\rho^s}\frac{D^s\rho^s}{Dt} = \frac{1}{1-n}\left[(\alpha - n)\frac{1}{K_s}\frac{D^s p^s}{Dt} - \beta_s(\alpha - n)\frac{D^s T}{Dt} - (1-\alpha) div\, \overline{\mathbf{v}}^s\right] \qquad [2.\ 181]$$

For incompressible grain material $\frac{1}{K_s} = 0$, $\alpha = 1$. This does not imply that the solid skeleton is rigid, because of rearrangements of the voids.

2.4.11 Fourier's Law

A constitutive assumption for the heat flux is the generalized Fourier's Law

$$\tilde{\mathbf{q}} = -\chi_{eff}\, grad\, T \qquad [2.\ 182]$$

where χ_{eff} is the effective thermal conductivity tensor and $\tilde{\mathbf{q}}$ is the heat flux of the multiphase medium, the sum of the partial heat fluxes $\tilde{\mathbf{q}}^\pi$.

For isotropic media the generalized Fourier's Law becomes the well known empirical Fourier's Law

$$q = -\chi_{eff}\ grad\, T \qquad [2.\ 183]$$

where χ_{eff} is the effective thermal conductivity. The effective thermal conductivity can be predicted theoretically as well as determined experimentally.

For porous building materials the following linear relationship may be used, which represents with sufficient accuracy the data by Bomberg and Shirtliffe [BS78]

$$\chi_{eff} = \chi_{dry}\left(1 + 4\frac{nS^{\mathrm{w}}\rho^w}{(1-n)\rho^s}\right) \qquad [2.\ 184]$$

2.5 General field equations

The macroscopic balance laws are now transformed, and the constitutive equations introduced, to obtain the general field equations, which will be used in the subsequent chapters. The averaging symbol, overbar, will be omitted, because all quantities belong to the macroscopic situations.

2.5.1 Mass balance equation

2.5.1.1 Solid phase

The macroscopic mass balance equation for the solid phase [2.56], divided by ρ^s is

$$\frac{1-n}{\rho^s}\frac{D^s\rho^s}{Dt}-\frac{D^s n}{Dt}+(1-n)div\ \mathbf{v}^s=0 \qquad [2.\ 185]$$

2.5.1.2 Liquid phase

Upon introduction of the relative velocity [2.41] and the material time derivative with respect to the moving solid [2.37], equation [2.58] for liquid water becomes

$$\frac{D^s\ \rho_w}{Dt}+\mathbf{v}^{ws}\cdot grad\ \rho_w+\rho_w\ div\left(\mathbf{v}^s+\mathbf{v}^{ws}\right)=-\dot{m} \qquad [2.\ 186]$$

Introduction of intrinsic phase averaged densities with the appropriate volume fractions, use of vector identity [2.55] written for water and division by $S_w\ \rho^w$ allows us to transform last equation into

$$\frac{D^s n}{Dt}+\frac{n}{\rho^w}\frac{D^s\rho^w}{Dt}+\frac{n}{S_w}\frac{D^s S_w}{Dt}+\frac{1}{S_w\ \rho^w}div\left(n\ S_w\ \rho^w\ \mathbf{v}^{ws}\right)+n\ div\ \mathbf{v}^s=-\frac{\dot{m}}{S_w\rho^w} \qquad [2.\ 187]$$

Summation with [2.185], to eliminate $\frac{D^s n}{Dt}$, gives

$$\begin{bmatrix}\frac{(1-n)}{\rho^s}\frac{D^s\rho^s}{Dt}+div\ \mathbf{v}^s+\frac{n}{\rho^w}\frac{D^s\ \rho^w}{Dt}+\\ +\frac{n}{S_w}\frac{D^s\ S_w}{Dt}+\frac{1}{S_w\rho^w}div\left(n\ S_w\ \rho^w\ \mathbf{v}^{ws}\right)\end{bmatrix}=-\frac{1}{S_w\rho^w}\dot{m} \qquad [2.\ 188]$$

Introduction of [2.158] and [2.181] for the material derivatives of the solid and water densities and of [2.166] gives

$$\begin{aligned}&\frac{\alpha-n}{K_s}\frac{D^s}{Dt}\left(S^w p^w+S^g\ p^g\right)-\beta_s(\alpha-n)\frac{D^s T}{Dt}+\alpha\ div\ \mathbf{v}^s\\ &+n\left(\frac{1}{K_w}\frac{D^s p^w}{Dt}-\beta_w\frac{D^s\ T}{Dt}\right)+\frac{n}{S_w}\frac{D^s S_w}{Dt}+\frac{1}{S_w\rho^w}div\left(n\ S_w\rho^w\mathbf{v}^{ws}\right)\\ &=-\frac{1}{S_w\rho^w}\dot{m}\end{aligned} \qquad [2.\ 189]$$

Because $\frac{D^s S_g}{Dt}=-\frac{D^s S_w}{Dt}$, carrying out derivatives of p^π

$$\begin{aligned}&\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\frac{D^s p^w}{Dt}+\frac{\alpha-n}{K_s}S_w S_g\frac{D^s p^g}{Dt}+\alpha\, S_w div\,\mathbf{v}^s+\\&-\beta_{sw}\frac{D^sT}{Dt}+\left(\frac{\alpha-n}{K_s}p^w S_w-\frac{\alpha-n}{K_s}p^g S_w+n\right)\frac{D^s S_w}{Dt}+\\&+\frac{1}{\rho^w}div\left(n\,S_w\rho^w\mathbf{v}^{ws}\right)=-\frac{\dot{m}}{\rho^w}\end{aligned}\tag*{[2. 190]}$$

where

$$\beta_{sw}=S_w\left[(\alpha-n)\beta_s+n\beta_w\right]\tag*{[2. 191]}$$

For incompressible grains ($\alpha=1$ and $\frac{1}{K_s}=0$) this equation may be simplified as follows

$$\frac{n\,S_w}{K_w}\frac{\overset{s}{D}\,p^w}{Dt}+S_w div\,\mathbf{v}^s-\beta_{sw}\frac{\overset{s}{D}\,T}{Dt}+n\frac{\overset{s}{D}\,S_w}{Dt}+\frac{1}{\rho^w}div\left(n\,S_w\rho^w\mathbf{v}^{ws}\right)=-\frac{\dot{m}}{\rho^w}\tag*{[2. 192]}$$

2.5.1.3 Gaseous phase

The mass balance equation for gas as a mixture of dry air and water vapour is dealt with next.

In the same way of the liquid phase, starting from [2.68] we obtain

$$\begin{aligned}&\frac{\alpha-n}{K_s}S_w S_g\frac{D^s p^w}{Dt}+\frac{\alpha-n}{K_s}S_g^2\frac{D^s p^g}{Dt}+\alpha S_g div\,\mathbf{v}^s+\\&+\frac{nS_g}{\rho^g}\frac{D^s\left[\frac{1}{\theta R}\left(p^{ga}M_a+p^{gw}M_w\right)\right]}{Dt}+\\&-\left(\frac{\alpha-n}{K_s}p^c S_g+n\right)\frac{D^s S_w}{Dt}+\frac{1}{\rho^g}div\left(nS_g\rho^g\mathbf{v}^{gs}\right)+\\&-\beta_s(\alpha-n)S_g\frac{D^sT}{Dt}=\frac{1}{\rho^g}\dot{m}\end{aligned}\tag*{[2. 193]}$$

For incompressible grains ($\alpha=1$ and $\frac{1}{K_s}=0$) this equation may be simplified as follows

$$\begin{aligned}&-n\frac{D^sS_w}{Dt}-\beta_s(1-n)S_g\frac{D^sT}{Dt}+S_g div\,\mathbf{v}^s\\&+\frac{nS_g}{\rho^g}\frac{D^s}{Dt}\left[\frac{1}{\theta R}\left(p^{ga}M_a+p^{gw}M_w\right)\right]\\&+\frac{1}{\rho^g}div\left(n\,S_g\,\rho^g\,\mathbf{v}^{gs}\right)=\frac{\dot{m}}{\rho^g}\end{aligned} \qquad [2.\ 194]$$

For heat transfer analysis, in partially saturated porous media, it is more convenient to consider the mass balance equation for dry air separately from that of vapour [Bag93] [Gaw95] and to sum the mass balance equations for both water species, liquid water and water vapour. In this way, the mass rate of water evaporation $\dot{m}$ disappears from the mass balance equations. But an evolution equation needed for $\dot{m}$ and this will be given by the energy balance equation. Note that, in this way, no constitutive model for the mass rate of water evaporation is needed.

2.5.1.4 Gaseous phase: dry air

The mass balance equation for dry air [2.60] is transformed in the following equation

$$\frac{D^s(nS_g\rho^{ga})}{Dt}+div\,\mathbf{J}_g^{ga}+nS_g\rho^{ga}div\,\mathbf{v}^g=0 \qquad [2.\ 195]$$

and then it is transformed as the mass balance equation for gas. The resulting equation is divided by $\rho^{ga}S_g$ and summed with [2.185] we obtained

$$\begin{aligned}&\frac{\alpha-n}{K_s}S_wS_g\frac{\overset{s}{D}p^w}{Dt}+\frac{\alpha-n}{K_s}S_g^2\frac{\overset{s}{D}p^{ga}}{Dt}+\alpha S_g div\mathbf{v}^s+\frac{nS_g}{\rho^{ga}}\frac{\overset{s}{D}\rho^{ga}}{Dt}+\frac{1}{\rho^{ga}}div\mathbf{J}_g^{ga}+\\&-\left(\frac{\alpha-n}{K_s}p^cS_g+n\right)\frac{\overset{s}{D}S_w}{Dt}+\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right)-\beta_s(\alpha-n)S_g\frac{\overset{s}{D}T}{Dt}=0\end{aligned} \qquad [2.\ 196]$$

For incompressible grains ($\alpha=1$ and $\frac{1}{K_s}=0$) this equation may be simplified as follows

$$\begin{aligned}&S_g div\mathbf{v}^s+\frac{nS_g}{\rho^{ga}}\frac{D^s\rho^{ga}}{Dt}+\frac{1}{\rho^{ga}}div\mathbf{J}_g^{ga}+\\&-n\frac{D^sS_w}{Dt}+\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right)-\beta_s(1-n)S_g\frac{D^sT}{Dt}=0\end{aligned} \qquad [2.\ 197]$$

Introducing now the constitutive equations for ρ^{ga} and for $\mathbf{J}_g^{ga}$ to obtain

$$\begin{aligned}&-n\frac{D^sS_w}{Dt}-\beta_s(1-n)S_g\frac{D^sT}{Dt}+S_g div\,\mathbf{v}^s+\frac{S_g n}{\rho^{ga}}\frac{D^s}{Dt}\left(\frac{M_a}{\theta R}p^{ga}\right)\\&-\frac{1}{\rho^{ga}}div\left[\rho^g\frac{M_aM_w}{M_g^2}\mathrm{D}_g\,grad\left(\frac{p^{ga}}{p^g}\right)\right]+\frac{1}{\rho^{ga}}div\left(n\,S_g\rho^{ga}\mathbf{v}^{gs}\right)=0\end{aligned}\qquad [2.\ 198]$$

2.5.1.5 Gaseous phase: vapour

The way to derive the mass balance equation for vapour is identical to that of dry air and results, for the case of incompressible solid grains, in

$$\begin{aligned}&-n\frac{D^SS_w}{Dt}-\beta_s(1-n)S_g\frac{D^ST}{Dt}+S_g div\,\mathbf{v}^s+\frac{S_g n}{\rho^{gw}}\frac{D^S}{Dt}\left(\frac{M_w}{\theta R}p^{gw}\right)\\&-\frac{1}{\rho^{gw}}div\left[\rho^g\frac{M_aM_w}{M_g^2}\mathbf{D}_g\,grad\left(\frac{p^{gw}}{p^g}\right)\right]+\frac{1}{\rho^{gw}}div\left(n\,S_g\rho^{gw}\mathbf{v}^{gs}\right)=\frac{\dot{m}}{\rho^{gw}}\end{aligned}\qquad [2.\ 199]$$

This equation is now multiplied by ρ^{gw} and added to the mass balance equation of liquid water, in turn multiplied by ρ^w. This sum gives the mass balance equation for the water species, liquid and vapour, without mass rate of water evaporation as

$$\begin{aligned}&n\left(\rho^w-\rho^{gw}\right)\frac{D^sS_w}{Dt}-\beta_{swg}\frac{D^sT}{Dt}+\left(\rho^{gw}S_g+\rho^wS_w\right)div\,\mathbf{v}^s\\&+\frac{n\,\rho^wS_w}{K_w}\frac{D^sp^w}{Dt}+S_g\,n\frac{D^s}{Dt}\left(\frac{M_w}{\theta R}p^{gw}\right)-div\left[\rho^g\frac{M_aM_w}{M_g^2}\mathbf{D}_g\,grad\left(\frac{p^{gw}}{p^g}\right)\right]\\&+div\left(n\,S_g\rho^{gw}\mathbf{v}^{gs}\right)+div\left(n\,S_w\rho^w\mathbf{v}^{ws}\right)=0\end{aligned}\qquad [2.\ 200]$$

where

$$\beta_{swg}=\beta_s(1-n)\left(S_g\rho^{gw}+\rho^wS_w\right)+n\,\beta_w\rho^wS_w\qquad [2.\ 201]$$

In these equations Darcy's law for the fluid velocities relative to the solid has still to be introduced. This law was introduced in section 2.4.7 and will be derived again in its generalized form in the next section from the linear momentum balance equations.

2.5.2 Linear momentum balance equation

2.5.2.1 Fluids

A more suitable form for the linear momentum balance equation for the fluid-phases [2.89] is now obtained by introducing kinematic equations and constitutive relationships. Equations [2.43] and [2.44] allow us to write

$$\mathbf{a}^{\pi} = \mathbf{a}^{s} + \mathbf{a}^{\pi s} + \mathbf{v}^{\pi s} \cdot grad\ \mathbf{v}^{\pi} \qquad [2.\ 202]$$

where $\mathbf{a}^{\pi s}$ is the relative acceleration.

Introduction in [2.89] of [2. 202], [2.142] and the momentum exchange term

$$\rho_{\pi}\hat{\mathbf{t}}^{\pi} = -\mathbf{R}^{\pi}\eta^{\pi}\mathbf{v}^{\pi\alpha} + p^{\pi}grad\eta^{\pi} \qquad [2.\ 203]$$

along with the intrinsic phase averaged density yields

$$\begin{aligned} &-\eta^{\pi}\rho^{\pi}\left(\mathbf{a}^{s} + \mathbf{a}^{\pi s} + \mathbf{v}^{\pi s} \cdot grad\,\mathbf{v}^{\pi}\right) - div\left(\eta^{\pi}p^{\pi}\mathbf{I}\right) + \\ &+\eta^{\pi}p^{\pi}e^{\pi}\left(\rho\dot{\mathbf{r}}\right) + \eta^{\pi}p^{\pi}\mathbf{g} - \mathbf{R}^{\pi}\eta^{\pi}\mathbf{v}^{\pi s} = \mathbf{0} \end{aligned} \qquad [2.\ 204]$$

By neglecting the term dependent on the gradient of the fluid velocity, the effects of phase change and by applying a vector identity, for the divergence of the stress tensor in the fluid-phase, we obtain the relative velocity of the fluid as

$$\eta^{\pi}\mathbf{v}^{\pi s} = \left(\mathbf{R}^{\pi}\right)^{-1}\eta^{\pi}\left[-grad\,p^{\pi} + \rho^{\pi}\left(\mathbf{g} - \mathbf{a}^{s} - \mathbf{a}^{\pi s}\right)\right] \qquad [2.\ 205]$$

By introducing the following

$$\eta^{\pi}\left(\mathbf{R}^{\pi}\right)^{-1} = \frac{\mathbf{k}}{\mu^{\pi}}\left(\rho^{\pi}, \eta^{\pi}, T\right) \qquad [2.\ 206]$$

at a macroscopic level we assume the resulting permeability as a product of the intrinsic permeability times the relative permeability $k^{r\pi}$,

$$\mathbf{k}^{\pi} = k^{r\pi}\mathbf{k} \qquad [2.\ 207]$$

so the linear momentum balance for fluids becomes

$$\eta^{\pi}\mathbf{v}^{\pi s} = \frac{\mathbf{k}\,k^{r\pi}}{\mu}\left[-grad\ p^{\pi} + \rho^{\pi}(\,\mathbf{g} - \mathbf{a}^{s} - \mathbf{a}^{\pi s})\right] \qquad [2.\ 208]$$

Finally, neglecting the soil acceleration and the relative acceleration terms, it yields Darcy's law in the form [2.159]

$$\eta^{\pi}\overline{\mathbf{v}}^{\pi s} = \frac{\mathbf{k}k^{r\pi}}{\mu^{\pi}}\left(-grad\ p^{\pi} + \rho^{\pi}\ \mathbf{g}\right) \qquad [2.\ 209]$$

Due to the simplifications introduced, this law is valid as a first approximation for slow flow of a macroscopically inviscid fluid through a porous medium with incompressible grains.

2.5.2.2 Solid-phase

Taking into account equations [2. 165], [2.166], [2.167], the linear momentum balance equation for the solid-phase [2.92] becomes

$$\begin{aligned} &div\left[\boldsymbol{\sigma}'-\mathbf{I}\,(1-n)\left(S_w p^w + S_g p^g\right)\right]+ \\ &+(1-n)\rho^s\,\mathbf{g}-(1-n)\rho^s\,\mathbf{a}^s+\mathbf{R}^w\eta^w\mathbf{v}^{ws}+\mathbf{R}^g\,\eta^g\mathbf{v}^{wg}=0 \end{aligned} \qquad [2.\ 210]$$

2.5.2.3 Multiphase medium

By summing the momentum balance equations [2.210], written for water and gas phase respectively, with that of the solid phase [2.210], by taking into account the definition of total stress [2.169], assuming continuity of stress at the fluid-solid interfaces and by introducing the averaged density of the multiphase medium

$$\rho=(1-n)\rho^s+n\,S_w\,\rho^w+n\,S_g\,\rho^g \qquad [2.\ 211]$$

we obtain the linear momentum balance equation for the whole multiphase medium

$$\begin{aligned} &-\rho\,\mathbf{a}^s-n\,S_w\,\rho^w\left[\mathbf{a}^{ws}+\mathbf{v}^{ws}\cdot grad\ \mathbf{v}^w\right]+ \\ &-n\,S_g\,\rho^g\left[\mathbf{a}^{gs}+\mathbf{v}^{gs}\cdot grad\ \mathbf{v}^g\right]+ \\ &+div\,\boldsymbol{\sigma}+\rho\,\mathbf{g}=0 \end{aligned} \qquad [2.\ 212]$$

2.5.3 Energy balance equation

The energy balance equation for the single phase is

$$\rho_\pi C_p^\pi \frac{\overset{\pi}{D}\theta^\pi}{Dt}=\rho_\pi h^\pi-div\tilde{\mathbf{q}}^\pi+\rho_\pi R^\pi-\rho_\pi e^\pi(\rho)H^\pi \qquad [2.\ 213]$$

where $H^\pi=H^\pi\left(\overline{p}^\pi,\theta^\pi\right)$ is the specific enthalpy of the phase π and $C_p^\pi=\left(\frac{\partial H^\pi}{\partial\theta^\pi}\right)_{\overline{p}}$ is the specific heat at constant pressure.

We assume that the phases of a partially saturated porous medium are locally in a state of thermodynamic equilibrium. This means that the averaged temperatures of all phases are assumed equal at each point in the multiphase system:

$$\theta^s=\theta^w=\theta^g=0 \qquad [2.\ 214]$$

Because of $T=\theta-\theta_0$ with θ_0 a fixed reference value, all derivatives of θ can be substituted with those of T.

For the continuum multiphase, with the impose of thermodynamic equilibrium, the energy balance equation is

$$\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t}+\left(\rho_w C_p^w \mathbf{v}^w+\rho_g C_p^g \mathbf{v}^g\right)\cdot gradT-div\left(\chi_{eff}\, gradT\right)=-\dot{m}\Delta H_{vap} \qquad [2.\ 215]$$

where

$$\left(\rho C_p\right)_{eff}=\rho_s C_p^s+\rho_w C_p^w+\rho_g C_p^g$$

$$\chi_{eff}=\chi^s+\chi^w+\chi^g$$

$$\Delta H_{vap}=H^{gw}-H^w$$

2.6 Physical approach: extended Biot's theory

The governing equations, using Biot's theory [B41-1] [B41-2] [B55] [B56-1] [B56-2] [B63], are again derived but extended to the case of non-isothermal two-phase flow in deforming porous media. This extension was made in [Sch95] [SZ93] for the case of slow phenomena. Also, inertia forces are taken into account, as was done in [Zie90] for the isothermal case with the air phase at atmospheric pressure.

The physical approach works directly with macroscopic variables. However, the distinction between a macroscopic and microscopic domain is not so clear as in the previous sections, because macroscopic variables are sometimes directly used in the microscopic domain.

For the sake of simplicity, small displacements are assumed for the solid phase. The governing equations in the form needed for finite strain analysis are those of the previous section. For all queries regarding the assumed hypotheses the interested reader is referred to the first part of this chapter.

2.6.1 The physical model

The voids of the skeleton are filled partly with water and partly with moist air (mixture of dry air and water vapour), which is referred to as gas. The degree of water saturation S_w is given as the ratio between the pore space occupied by the water and the total pore volume in a representative elementary volume element (REV), Figure 2.1. We have

$$S_w=\frac{dv^w}{dv^w+dv^g} \qquad [2.\ 216]$$

In the following equations the super or subscript π refers to the generic phase, π = *s* to the solid phase, π = *w* to water and π = *g* to gas. The volume of the REV is *dv*, while the partial volumes are dv^s, dv^w and dv^g. Their sum is dv while the sum of the respective fluid volumes is $dv^f=dv^w+dv^g$. The definition of the degree of gas saturation S_g is

$$S_g = \frac{dv^g}{dv^w + dv^g} \tag{2. 217}$$

and both degrees of saturation sum to one, i.e.

$$S_w + S_g = 1 \tag{2. 218}$$

The porosity n is defined as the ratio between the volume of voids and the total volume of the REV,

$$n = \frac{dv^w + dv^g}{dv} \tag{2. 219}$$

As in the first part of this chapter, the stress is defined as tension positive for the solid phase, while pore pressure is defined as compressive positive for fluids. The water pressure p^w and the gas pressure p^g are related through the capillary pressure p^c

$$p^c = p^g - p^w \tag{2. 220}$$

The capillary pressure is a function of the water saturation and temperature:

$$p^c = p^c(S_w, T) \tag{2. 221}$$

The relation [2.221] is determined experimentally and usually shows hysteresis characteristics, which are ignored in this case. It can be numerically inverted to obtain

$$S_\pi = S_\pi(p^c, T) \tag{2. 222}$$

The constitutive law of the solid phase is introduced through the concept of effective stress:

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{I}\, p^s \tag{2. 223}$$

which stipulates that the main characteristics of the solid phase constitutive relation can be written in terms of $\boldsymbol{\sigma}'$ where $\boldsymbol{\sigma}$ is the total stress tensor, $\mathbf{I}$ the second order unit tensor and p^s is the average pressure of both the water and air surrounding the grains. In the case of immiscible two-phase flow, we need a simple averaging technique for the calculation of p^s as described in section 2.2. Thus the modified effective stress principle may be obtained as stated previously. The effective stress resulting from equation [2.223] is also referred to as Bishop's stress.

$$\overline{\boldsymbol{\sigma}} = \frac{1}{dv}\int_{dv} \boldsymbol{\sigma}\, dv_m = \frac{1}{dv}\left[\int_{dv^s} \boldsymbol{\sigma}\, dv_m + \int_{dv^f} \boldsymbol{\sigma}\, dv_m\right] \qquad [2.\ 224]$$

where $\overline{\boldsymbol{\sigma}}$ is the macroscopic total stress tensor.

For the fluid phases, the stress tensor is given by

$$\boldsymbol{\sigma}^\pi = \tau^\pi - \mathbf{I}\, p^\pi \qquad [2.\ 225]$$

where $\boldsymbol{\sigma}^\pi$ is the intrinsic phase averaged stress tensor in the π phase and τ^π is the shear stress. Under the assumption that the shear stress τ^π is negligible in fluids, we obtain

$$\overline{\boldsymbol{\sigma}} = (1-n)\boldsymbol{\sigma}^s - n\,\mathbf{I}\left[S_g p^g + S_w p^w\right] \qquad [2.\ 226]$$

The term in square brackets represents the intrinsically averaged (or mean) pressure p^s of the fluid phases, i.e.

$$p^s = \left(S_g\ p^g + S_w\ p^w\right) \qquad [2.\ 227]$$

This weighted pore pressure produces a stress state in the grains, but for the moment, we assume the grains will not undergo any deformation due to this stress, i.e. we introduce the hypothesis of incompressible grains. The deformation of the solid skeleton, which depends on the effective stress, will be a function of the grain rearrangement only.

Equation [2.226] can be modified to

$$\begin{aligned} \boldsymbol{\sigma} &= (1-n)\boldsymbol{\sigma}^s - n\,\mathbf{I}\, p^s \\ &= (1-n)\left(\boldsymbol{\sigma}^s + \mathbf{I}\, p^s\right) - (1-n)\mathbf{I}\, p^s - n\,\mathbf{I}\, p^s \\ &= \boldsymbol{\sigma}' - \mathbf{I}\, p^s \end{aligned} \qquad [2.\ 228]$$

where the overbar for the total stress has been omitted.

The stress tensor is split into two components: the pore pressure effect and the part which deforms the solid skeleton, i.e. the effective stress. This effective stress is given by

$$\boldsymbol{\sigma}' = (1-n)\left(\boldsymbol{\sigma}^s + \mathbf{I}\, p^s\right) \qquad [2.\ 229]$$

Equation [2.228] results in a splitting of the stress tensor similar to that of Terzaghi's principle and in presence of several fluid phases, the splitting is

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{I}\left(S_w\ p^w + S_g\ p^g\right) \qquad [2.\ 230]$$

For greater generality, a corrective term known as Biot's constant has to be introduced to account for the deformability of the grains [BW57]. Therefore a more general expression of the effective stress is assumed as follows

$$\boldsymbol{\sigma}'' = \boldsymbol{\sigma} + \mathbf{I}\,\alpha\left(S_w p^w + S_g p^g\right) \qquad [2.\,231]$$

where the corrective coefficient α will be determined in section 2.6.2. Note that this equation differs substantially from the previous one, for the determination of α we need the constitutive equations of the solid phase. This effective stress is indicated by $\boldsymbol{\sigma}''$ as in [Zie90].

Another, more intuitive way of deriving equation [2.229] follows Bishop [B59] and Skempton [Ske61]. Here the microscopic and macroscopic aspects are somewhat mixed. We consider for this purpose the mean stresses, i.e.

$$\hat{\sigma} = tr\,\frac{\boldsymbol{\sigma}}{3} \qquad [2.\,232]$$

and

$$\hat{\sigma}' = tr\,\frac{\boldsymbol{\sigma}'}{3} \qquad [2.\,233]$$

If the pores (Figure 2. 4) are filled with water and air, then due to the surface tension effect we have

$$p^w < p^g \qquad [2.\,234]$$

If the degree of saturation is relatively low, the water is present as menisci and the corresponding pressure acts over an area χ per unit gross area, [AD56].

Consequently, the equivalent pore pressure is given by

$$\chi\, p^w + (1-\chi)\, p^g \qquad [2.\,235]$$

and the equivalent pore pressure may be written as

$$p^g - \chi\left(p^g - p^w\right) \qquad [2.\,236]$$

or

$$p^w + (1-\chi)\left(p^g - p^w\right) \qquad [2.\,237]$$

For the fully saturated case, Bishop suggested the following expression for the mean effective stress $\hat{\sigma}'$

$$\hat{\sigma}' = \hat{\sigma} + \left[p^g - \chi\left(p^g - p^w\right)\right] \qquad [2.\,238]$$

For the full stress tensor, this equation assumes the form

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{I}\left[p^g - \chi\left(p^g - p^w\right)\right] \qquad [2.\,239]$$

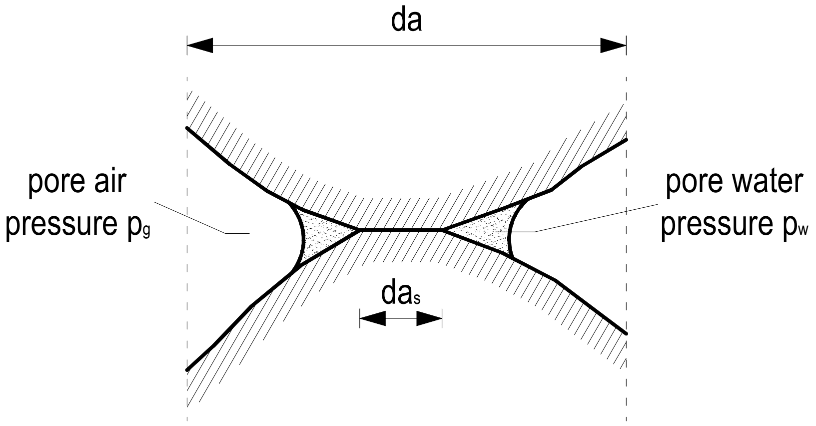

Figure 2. 4: *Contact area between two grains in the partially saturated case*

The coefficient χ is not the same as for problems involving shear strength and consolidation [Ske61]. For a given degree of saturation the coefficient χ must be determined experimentally for both types of problems.

In general the pressure is implied as being an absolute value, but in many soil mechanics problems relative pressures are used and p^g is often assumed to be equal to the atmospheric pressure. If this is the case and the atmospheric pressure is assumed as the reference pressure then the effective stress principle becomes

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathbf{I}\,\chi\, p^w \qquad [2.\,240]$$

The comparison between [2.230] and [2.239] is noteworthy. [2.230] may be written as a function of the degree of saturation S_w

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - \mathbf{I}\left[p^g - S_w\left(p^g - p^w\right)\right] \qquad [2.\,241]$$

and coincides with equation [2.239] if $\chi = S_w$.

The coefficient χ is related to the area of contact between solid and fluids, whereas the degrees of saturation S_π depend on the volume occupied by the π phase. We define the volume fraction as

$$\eta^\pi = \frac{dv^\pi}{dv} \qquad [2.\,242]$$

and cross sectional area fraction as

$$\alpha^{\pi} = \frac{da^{\pi}}{da} \qquad [2.\ 243]$$

For the case of microstructurally isotropic constituents, such that α^{π} is independent of the orientation of the surface, and assuming that

$$\alpha^{\pi} = \alpha^{\pi}\left(\eta^{\pi}\right) \qquad [2.\ 244]$$

it can be shown that [Mor72]

$$\alpha^{\pi} = \eta^{\pi} \qquad [2.\ 245]$$

This conclusion coincides with the basic supposition of Delesse's law. If this assumption regarding the area and volume fraction is valid, then little difference exists between the definition of Bishop's coefficient χ and the degree of water saturation S_{π}. Bishop's equation [2.238] has been experimentally validated by means of a triaxial tests carried out on soil samples [Ske61].

The assumption

$$\chi = S_w \qquad [2.\ 246]$$

is acceptable for many materials as shown experimentally in [BB63].

However, other expressions may also be used, e.g. by Gudehus for clay [Gud95]

$$\chi = S(2 - S) \qquad [2.\ 247]$$

If the solid phase is completely surrounded by a single wetting fluid phase, which is the only one in direct contact with the porous medium, then Li and Zienkiewicz [LZ92] use equation [2.240] with $\chi = 1$, as in the case of a fully saturated porous medium. This assumption is widely used when the two fluids are water and bitumen: only water is in contact with the solid grains.

A new expression for the effective stress principle in fully saturated conditions only, involving four parameters, has been proposed by Lade and de Boer [LB96] and experimentally tested. This formulation, based on principles of mechanics is valid for all types of materials. A distinction is made between the compressibilities of the grain particles and the skeleton due to total stresses and pore pressures.

Two distinct expressions are then obtained for effective stresses in granular material and in solid rock with interconnected pores respectively. For various special conditions these expressions become similar to the expressions found in the literature, in particular to the expression used here with Biot's constant α. Lade and de Boer [LB96] conclude that Terzaghi's proposed effective stress principle works well for stress magnitudes encountered in most geotechnical applications, but significant deviations occur at very high stresses.

2.6.2 Constitutive equations

Only a few equations, needed for the remaining part of this section, are recalled. In particular an expression for Biot's constant α is derived.

The averaged pore pressure p^s of the fluids occupying the void space induces a hydrostatic stress distribution in the solid phase. The ensuing deformation is a purely volumetric strain

$$\varepsilon_v^s = -\frac{p^s}{K_s} \qquad [2.\ 248]$$

where K_s is the averaged bulk modulus of the solid grains.

As stated previously, the effective stress causes all relevant deformation of the solid skeleton. The constitutive relationship may be written as

$$d\,\boldsymbol{\sigma}' = \mathbf{D}_{\mathrm{T}}\left[\left(d\,\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^c - d\boldsymbol{\varepsilon}_v^s - d\boldsymbol{\varepsilon}^\circ\right)\right] \qquad [2.\ 249]$$

where $d\boldsymbol{\sigma}'$ is the stress responsible for all deformations, except for the grain compressibility, $d\boldsymbol{\varepsilon}$ represents the total strain of the solid, $\mathbf{D}_T$ is the tangent constitutive tensor

$$\mathbf{D}_T = \mathbf{D}_T\left(\boldsymbol{\sigma}', \boldsymbol{\varepsilon}, \dot{\boldsymbol{\varepsilon}}\right) \qquad [2.\ 250]$$

$d\boldsymbol{\varepsilon}^c = g\left(\boldsymbol{\sigma}'\right)dt$ accounts for the creep strain, $d\boldsymbol{\varepsilon}^o$ represents all other strains in the solid skeleton not directly dependent on effective stress.

A modified effective stress $\boldsymbol{\sigma}''$ will now be introduced which will also account for grain compression. This allows the use of Biot's constant α. Omitting for brevity $d\boldsymbol{\varepsilon}^c$ and $d\varepsilon^o$ we obtain

$$d\boldsymbol{\sigma}' = \mathbf{D}_T\left[\left(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_v^s\right)\right] = \mathbf{D}_T\left[d\boldsymbol{\varepsilon}\right] + \mathbf{D}_T\left[\,\mathbf{I}\,\right]\frac{dp^s}{3K_s} \qquad [2.\ 251]$$

Consequently, the effective stress equation written in incremental form becomes

$$d\boldsymbol{\sigma} = d\boldsymbol{\sigma}' - \mathbf{I}\,dp^s = d\boldsymbol{\sigma}'' + \mathbf{D}_T\left[\,\mathbf{I}\,\right]\frac{dp^s}{3K_s} - \mathbf{I}\,dp^s \qquad [2.\ 252]$$

where $\boldsymbol{\sigma}''$ represents the stress responsible for all deformation of the solid.

For the following developments we use indicial notation and the Kronecker symbol δ instead of the unit tensor $\mathbf{I}$.

It can be immediately verified that equation [2.252] can be written as given by Zienkiewicz and Shiomi [ZS85]

$$d\,\sigma_{ij} = d\,\sigma''_{ij} - \frac{1}{3}\left(\delta_{mn}\delta_{nm} - \delta_{mn}D_{mnkl}\delta_{kl}\,\frac{1}{3K_s}\right)\delta_{ij}\,dp^s \qquad [2.\ 253]$$

For an isotropic, elastic material

$$\delta_{mn}D_{mnkl}\delta_{kl} = \frac{3E}{1-2\upsilon} = 9K_T \qquad [2.\ 254]$$

where E is the Young's modulus, υ is the Poisson's ratio and K_T is the bulk modulus of the overall skeleton.

Hence equation [2.253] can be written as

$$d\,\sigma_{ij} = d\,\sigma''_{ij} - \left(1 - \frac{K_T}{K_s}\right)\delta_{ij}\,d\,p^s = d\,\sigma''_{ij} - \alpha\,\delta_{ij}\,dp^s \qquad [2.\ 255]$$

where α is Biot's constant.

The resultant expression of the constitutive relationship is therefore

$$d\boldsymbol{\sigma}'' = \mathbf{D}_T\,[d\boldsymbol{\varepsilon}] \qquad [2.\ 256]$$

The intrinsic pore pressure p^π of the π fluid phase causes a purely volumetric strain of that phase, which is represented by

$$\boldsymbol{\varepsilon}_v^\pi = -\frac{p^\pi}{K_\pi} \qquad [2.\ 257]$$

2.6.3 Governing equations

In the following a material coordinate system is employed for the solid phase and a spatial coordinate system for the fluid phases; convective terms, unless specified otherwise, are neglected. Because of this choice of reference systems, the fluid velocities are conveniently referred to the solid phase by means of the relative velocities for water and gas respectively

$$\mathbf{v}^{ws} = \mathbf{v}^w - \mathbf{v}^s \qquad [2.\ 258]$$

$$\mathbf{v}^{gs} = \mathbf{v}^g - \mathbf{v}^s \qquad [2.\ 259]$$

and the accelerations, without convective terms, are

$$\mathbf{a}^w = \mathbf{a}^s + \mathbf{a}^{ws} \qquad [2.260]$$

$$\mathbf{a}^g = \mathbf{a}^s + \mathbf{a}^{gs} \qquad [2.261]$$

where $\mathbf{a}^{ws}$ is the acceleration of water relative to the solid phase and $\mathbf{a}^{gs}$ the relative acceleration of gas.

2.6.3.1 Linear momentum balance equation of the multiphase medium

The linear momentum balance equation for the multiphase system is the sum of the dynamics equations for the individual constituents, but relative to the solid phase via equations [2.260] and [2.261]

$$-\rho\, \mathbf{a}^s - n\, S_w \rho^w \mathbf{a}^{ws} - n\, S_g \rho^g \mathbf{a}^{gs} + div\, \boldsymbol{\sigma} + \rho\, \mathbf{g} = 0 \qquad [2.262]$$

where

$$\rho = (1-n)\rho^s + n\, S_w \rho^w + n\, S_g \rho^g \qquad [2.263]$$

is the averaged density of the multiphase systems, ρ^s is the intrinsic density of the solid phase, i.e. the density referred to the volume occupied by the solid phase only, as opposed to the volume occupied by the multiphase system, ρ^w is the intrinsic density of water, ρ^g the intrinsic density of gas and $\mathbf{g}$ an acceleration usually related to gravitational effects.

The linear momentum balance equation for each fluid phase yields the generalized form of Darcy's law, where the dissipative terms arising in a multiphase flow system at the interfaces are taken into account through the relative permeabilities

$$nS_w \mathbf{v}^{ws} = \frac{\mathbf{k}k^{rw}}{\mu_w}\left[-grad\ p^w + \rho^w\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{ws}\right)\right] \qquad [2.264]$$

$$nS_g\ \mathbf{v}^{gs} = \frac{\mathbf{k}k^{rg}}{\mu_g}\left[-grad\ p^g + \rho^g\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{gs}\right)\right] \qquad [2.265]$$

where $\mathbf{k}$ is the intrinsic permeability, k^{rw} and k^{rg} are the relative permeabilities of water and gas, μ_w and μ_g are the dynamic viscosities. The relative permeabilities vary between 0 and 1 and are a function of the degree of saturation; the dynamic viscosities are temperature dependent. In the generalized form of Darcy's law for the gas phase the body forces are usually neglected. The left end side of equations [2.264] and [2.265] are multiplied by the volume fractions nS_π because Darcy's law is expressed in terms of volume averaged relative velocities. These are the velocities measured from experimental work.

2.6.3.2 Mass balance equations

The summation of mass balance equations for the solid and fluid phases, with opportune arrangements, eliminates the time derivative of the porosity and yields the so-called continuity equation of the fluid phase i.e.

$$\begin{aligned}&\frac{(1-n)}{\rho^s}\frac{\partial\rho^s}{\partial t}+div\ \mathbf{v}^s+\frac{n}{\rho^\pi}\frac{\partial\rho^\pi}{\partial t}+\\&+\frac{n}{S_\pi}\frac{\partial S_\pi}{\partial t}+\frac{1}{S_\pi\rho^\pi}\left(nS_\pi\rho^\pi\mathbf{v}^{\pi s}\right)=\pm\frac{\dot{m}}{\rho^\pi S_\pi}\end{aligned} \qquad [2.\ 266]$$

We consider first the continuity equation for water. Introduction of the constitutive relationships for the time derivatives of water density [2.158] and solid density [2.181], along with the pressure in the solid phase [2.227], multiplication by S_w and then with the introduction of Darcy's law [2.264] and of the definition of capillary pressure [2.220] yields

$$\begin{aligned}&\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\frac{\partial p^w}{\partial t}+\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^g}{\partial t}+\alpha S_w div\ \mathbf{v}^s\\&-\beta_{sw}\frac{\partial T}{\partial t}+\left(\frac{n-\alpha}{K_s}S_wp^c+n\right)\frac{\partial S_w}{\partial t}\\&+\frac{1}{\rho^w}div\left\{\rho^w\frac{\mathbf{k}k^{rw}}{\mu_w}\left[-grad\ p^w+\rho^w\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{ws}\right)\right]\right\}=-\frac{\dot{m}}{\rho^w}\end{aligned} \qquad [2.\ 267]$$

In the same way the continuity equation for gas is obtained

$$\begin{aligned}&\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^w}{\partial t}+\frac{\alpha-n}{K_s}S_g{}^2\frac{\partial p^g}{\partial t}-\left(n+\frac{\alpha-n}{K_s}p^cS_g\right)\frac{\partial S_w}{\partial t}^s\\&-\beta_s(\alpha-n)S_g\frac{\partial T}{\partial t}+\alpha\,S_g div\ \mathbf{v}^s+\frac{nS_g}{\rho^g}\frac{\partial}{\partial t}\left(\frac{p^gM_g}{\theta R}\right)\\&+\frac{1}{\rho^g}div\left\{\rho^g\frac{\mathbf{k}k^{rg}}{\mu_g}\left[-grad\ p^g+\rho^g\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{gs}\right)\right]\right\}=-\frac{\dot{m}}{\rho^g}\end{aligned} \qquad [2.\ 268]$$

where M_g is the molar mass of gas.

2.6.3.3 Energy balance equation

By subtracting the kinetic energy from a global energy balance, the balance equation of thermal energy may be written for constituent π as [Bir60]

$$\frac{\partial}{\partial t}\left(\rho^{\pi} E^{\pi}\right) = -div\left(\rho^{\pi} E^{\pi} \mathbf{v}^{\pi}\right) - div\,\tilde{\mathbf{q}}^{\pi} - \bar{p}^{\pi} div\,\mathbf{v}^{\pi} + \boldsymbol{\tau}^{\pi} : grad\,\mathbf{v}^{\pi} + \rho^{\pi} R^{\pi} \qquad [2.\ 269]$$

where E^{π} is the specific internal energy, $\boldsymbol{\tau}$ is the deviatoric part of the stress tensor and $\bar{p}^{\pi}$ the hydrostatic part of the stress tensor.

The left-hand side represents the rate of accumulation of internal energy in a control volume. The right-hand terms express respectively the rate of internal energy change due to convection and to conduction, the reversible rate of internal energy increase due to pressure, the irreversible rate of internal energy increase by viscous dissipation and the contribution of heat sources.

In small strain the energy balance equation becomes

$$\rho^{\pi} \frac{\partial E^{\pi}}{\partial t} + \rho^{\pi} \mathbf{v}^{\pi} \cdot grad\,E^{\pi} = -div\,\tilde{\mathbf{q}}^{\pi} - \bar{p}^{\pi} div\,\mathbf{v}^{\pi} + \tau^{\pi} \cdot grad\,\mathbf{v}^{\pi} + \rho^{\pi} R^{\pi} \qquad [2.\ 270]$$

The irreversible part of the internal energy increase by viscous dissipation is neglected in what follows. It is convenient to express this equation in terms of temperature and heat capacity instead of internal energy [Bir60]. This is done through the concept of enthalpy. Hence with sufficient accuracy for geomechanical applications the energy balance equation can be rewritten as

$$\rho^{\pi} C_p^{\pi} \left(\frac{\partial T^{\pi}}{\partial t} + \mathbf{v}^{\pi} \cdot grad\,T^{\pi} \right) = -div\,\tilde{\mathbf{q}}^{\pi} + \rho^{\pi} R^{\pi} \qquad [2.\ 271]$$

for $\pi = s, w$, which for the purpose of the energy balance only may be considered as incompressible, and

$$\rho^{\pi} C_p^{g} \left(\frac{\partial T^{g}}{\partial t} + \mathbf{v}^{g} \cdot grad\,T^{g} \right) = -div\,\tilde{\mathbf{q}}^{g} + \frac{\partial p^{g}}{\partial t} + \mathbf{v}^{g} \cdot grad\,p^{g} + \rho^{g} R^{g} \qquad [2.\ 272]$$

where C_p^g is the specific heat at constant pressure.

Some insignificant terms which are related to the mechanical work induced by density variations due to temperature changes of the water and solid phases have been neglected.

Gas pressure changes are usually very slow and their gradients small in geomaterials, hence the time derivatives of gas pressure, as well as the convective terms, are negligible with respect to other terms in equation [2.272]. Also, because gas pressure changes are usually small when compared to atmospheric pressure, the specific heat at constant pressure may be utilised instead of specific heat at constant volume.

A local equilibrium state is assumed to hold, i.e.

$$T^s = T^w = T^g = T \qquad [2.\ 273]$$

We also introduce the constitutive equation for heat fluxes [2.182], and add together equations [2.271] and [2.272], and introduce the appropriate heat sources to obtain the following form of the energy balance equation

$$(\rho C_p)_{eff} \frac{\partial T}{\partial t} + \left(\rho^w C_p^w \mathbf{v}^w + \rho^g C_p^g \mathbf{v}^g\right) \cdot grad\, T - div\left(\chi_{eff}\, grad\, T\right) = -\dot{m}\Delta H_{vap} \qquad [2.\ 274]$$

where ΔH_{vap} is the latent heat of evaporation and the convective heat flux in the solid phase has been neglected.

2.7 Quasi static case

The relationship shown in 2.6.3 are now presented for quasi static loading conditions, which is the starting point of this work. The quasi static model is implemented in the finite element code Comes-Geo [GS96], [LS98], [SPS6].

The equations are hence rewritten in the quasi static case by neglecting the terms dependent on the accelerations $\mathbf{a}^w, \mathbf{a}^s, \mathbf{a}^{ws}, \mathbf{a}^g, \mathbf{a}^{gs}$.

This model developed by considering the air dissolved in liquid water can be found in Gawin and Sanavia [G10-1] and [G10-2].

2.7.1 Governing equations

2.7.1.1 Linear momentum balance equation of the multiphase medium

The equation [2.262] becomes

$$div\, \boldsymbol{\sigma} + \rho\, \mathbf{g} = 0 \qquad [2.\ 275]$$

where

$$\rho = (1-n)\rho^s + n\, S_w \rho^w + n\, S_g \rho^g \qquad [2.\ 276]$$

is the averaged density of the multiphase systems

ρ^s is the intrinsic density of the solid phase

ρ^w is the intrinsic density of water

ρ^g the intrinsic density of gas

$\mathbf{g}$ is the gravity acceleration

2.7.1.2 Mass balance equations

The equations [2.267] and [2.268] becomes

$$\begin{aligned}&\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\frac{\partial p^w}{\partial t}+\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^g}{\partial t}+\alpha S_w div\,\mathbf{v}^s\\&-\beta_{sw}\frac{\partial T}{\partial t}+\left(\frac{n-\alpha}{K_s}S_wp^c+n\right)\frac{\partial S_w}{\partial t}\\&+\frac{1}{\rho^w}div\left\{\rho^w\frac{\mathbf{k}k^{rw}}{\mu_w}\left[-grad\ p^w+\rho^w\mathbf{g}\right]\right\}=0\end{aligned}\qquad [2.\ 277]$$

In the same way the continuity equation for gas is obtained

$$\begin{aligned}&\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^w}{\partial t}+\frac{\alpha-n}{K_s}S_g{}^2\frac{\partial p^g}{\partial t}-\left(n+\frac{\alpha-n}{K_s}p^cS_g\right)\frac{\partial S_w}{\partial t}^{s}\\&-\beta_s(\alpha-n)S_g\frac{\partial T}{\partial t}+\alpha\,S_g div\,\mathbf{v}^s+\frac{nS_g}{\rho^g}\frac{\partial}{\partial t}\left(\frac{p^gM_g}{\theta R}\right)\\&+\frac{1}{\rho^g}div\left\{\rho^g\frac{\mathbf{k}k^{rg}}{\mu_g}\left[-grad\ p^g+\rho^g\mathbf{g}\right]\right\}=0\end{aligned}\qquad [2.\ 278]$$

2.7.1.3 Energy balance equation

The equation [2.274] not change for the quasi static case but, using Darcy' law, it can be rewritten in a complete mode as follow

$$\begin{aligned}&(\rho C_p)_{eff}\frac{\partial T}{\partial t}+\rho^wC_p^w\left[\frac{\mathbf{k}\,\mathrm{k}^{\mathrm{rw}}}{\mu^{\mathrm{w}}}\left[-grad(p^g)+grad(p^c)+\rho^w\mathbf{g}\right]\right]\cdot grad\,T\\&\rho^gC_p^g\left[\frac{\mathbf{k}\,\mathrm{k}^{\mathrm{r}g}}{\mu^g}\left[-grad(p^g)+\rho^g\mathbf{g}\right]\right]\cdot grad\,T-div(\chi_{eff}\ grad\,T)=-\dot{m}\Delta H_{vap}\end{aligned}\qquad [2.\ 279]$$

2.7.1.4 Boundary and initial conditions

For the quasi static model closure the initial and boundary conditions are needed.

The initial conditions specify the full fields of primary state variables at time $t=t_0$, in the whole analysed domain Ω and on its boundary Γ and the boundary conditions can be either imposed value on Γ_π or fluxes on Γ_π^q where

$$\Gamma = \Gamma_\pi \cup \Gamma_\pi^q \quad \pi = g,c,T,\mathbf{u} \qquad [2.\ 280]$$

The initial conditions values for gas pressure, water pressure, temperature and displacements are:

$$\begin{aligned} p^g &= p_0^g && \text{on} \quad \Omega_g \cup \Gamma_g \\ p^c &= p_0^c && \text{on} \quad \Omega_c \cup \Gamma_c \\ T &= T_0 && \text{on} \quad \Omega_T \cup \Gamma_T \\ \mathbf{u} &= \mathbf{u}_0 && \text{on} \quad \Omega_u \cup \Gamma_u \end{aligned} \qquad [2.\ 281]$$

The boundary conditions can be of Dirichlet's type on ∂B_π for $t \geq t_0$:

$$\begin{aligned} p^g &= \hat{p}^g && \text{on } \Gamma_g \\ p^c &= \hat{p}^c && \text{on } \Gamma_c \\ T &= \hat{T} && \text{on } \Gamma_T \\ \mathbf{u} &= \hat{\mathbf{u}} && \text{on } \Gamma_u \end{aligned} \qquad [2.\ 282]$$

or of Cauchy's type on ∂B_π^q for $t \geq t_0$:

$$\left(nS_g \rho^{ga} v^{gs} + \mathbf{J}_d^{ga}\right) \cdot \mathbf{n} = q^{ga} \quad \text{on } \Gamma_g^q \qquad [2.\ 283]$$

$$\left(nS_w \rho^w v^{ws} + nS_g \rho^{gw} v^{gs} + \mathbf{J}_d^{gw}\right) \cdot \mathbf{n} = q^{gw} + q^w + \beta_c\left(\rho^{gw} - \rho_\infty^{gw}\right) \quad \text{on } \Gamma_c^q \qquad [2.\ 284]$$

$$\left(nS_w \rho^w \mathbf{v}^{ws} \Delta H_{vap} - \chi_{eff}\, gradT\right) \cdot \mathbf{n} = q^T + q^w + \alpha_c\left(T - T_\infty\right) + e\sigma_0\left(T^4 - T_\infty^4\right) \quad \text{on } \Gamma_T^q \qquad [2.\ 285]$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_u^q \qquad [2.\ 286]$$

where

$\mathbf{n}(\mathbf{x},t)$ is the unit normal vector

$q^{ga}(\mathbf{x},t)$ is the imposed fluxes of dry air

$q^{gw}(\mathbf{x},t)$ is the imposed fluxes of vapour

$q^{w}(\mathbf{x},t)$ is the imposed fluxes of liquid water

$q^{T}(\mathbf{x},t)$ is the imposed heat flux

$\bar{\mathbf{t}}(\mathbf{x},t)$ is the imposed traction vector related to the total Cauchy stress tensor

$\rho_\infty^{gw}(\mathbf{x},t)$ is the mass concentration of water vapour

$T_\infty(\mathbf{x},t)$ is the temperature in the far field of undisturbed gas phase

$e(\mathbf{x},t)$ is the emissivity of the interface

$\sigma_0(\mathbf{x},t)$ is the Stefan-Boltzmann constant

$b_c(\mathbf{x},t)$ is the convective heat exchange coefficients

$a_c(\mathbf{x},t)$ is the convective mass exchange coefficients

The boundary conditions with only imposed fluxes are called Neumann boundary conditions. The purely convective boundary conditions for heat and moisture exchange are also called Robin boundary conditions.

2.8 Dynamic case

In this work the dynamic formulation of the field governing equations is needed. From the general formulation the final system of equations is obtained by several simplifications.

2.8.1 Governing equations

2.8.1.1 Linear momentum balance equation of the multiphase medium

According with Lewis and Schrefler [LS98] the linear momentum balance equation for the whole multiphase medium has the following generalised form:

$$\begin{aligned} & div\boldsymbol{\sigma} + \rho\left(\mathbf{b} - \mathbf{a}^s\right) - nS_w\rho^w\left(\mathbf{a}^{ws} + \mathbf{v}^{ws} \cdot grad\mathbf{v}^w\right) + \\ & - nS_g\rho^g\left(\mathbf{a}^{gs} + \mathbf{v}^{gs} \cdot grad\mathbf{v}^g\right) = 0 \end{aligned} \qquad [2.\ 287]$$

where $\boldsymbol{\sigma}$ is the total stress, $\mathbf{b}$ is the body force and ρ is the averaged density of the multiphase medium written as

$$\rho = (1-n)\rho^s + nS_w\rho^w + nS_g\rho^g \qquad [2.\ 288]$$

in which ρ^s is the density of the solid grain, ρ^w is the density of water and ρ^g is the density of gas.

2.8.1.2 Water species mass balance equation

There are several components that contribute to the water species mass balance equation:

1. Vapour advective flux

$$div\left(nS_g\rho^{gw}\mathbf{v}^{gws}\right) \qquad [2.\ 289]$$

2. Water advective flux

$$div\left(nS_w\rho^w\mathbf{v}^{ws}\right) \qquad [2.\ 290]$$

3. Vapour diffusional flux

$$div\mathbf{J}_g^{gw} \qquad [2.\ 291]$$

6. Term linked to water vapour density changes

$$nS_g\frac{\partial \rho^{gw}}{\partial t} \qquad [2.\ 292]$$

5. Term linked to the saturation changes

$$\left[\rho^w\left(\frac{\alpha-n}{K_s}p^w S_w-\frac{\alpha-n}{K_s}p^g S_w+n\right)-\rho^{gw}\left(\frac{\alpha-n}{K_s}p^c S_g+n\right)\right]\frac{\partial S_w}{\partial t} \qquad [2.\ 293]$$

7. Term linked to the temperature changes

$$-\beta_{swg}\frac{\partial T}{\partial t} \qquad [2.\ 294]$$

where

$$\beta_{swg}=n\beta_w\rho^w S_w+\beta_s(\alpha-n)\left(S_g\rho^{gw}+\rho^w S_w\right) \qquad [2.\ 295]$$

8. Volumetric strain of solid skeleton

$$\left[\rho^w S_w+\rho^{gw}S_g\right]\alpha div\mathbf{v}^s \qquad [2.\ 296]$$

9. Term linked to the vapour pressure changes

$$\left[\rho^w\frac{\alpha-n}{K_s}S_w S_g+\rho^{gw}\frac{\alpha-n}{K_s}S_g^2\right]\frac{\partial p^{gw}}{\partial t} \qquad [2.\ 297]$$

10. Term linked to the water pressure changes

$$\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)+\rho^{gw}\frac{\alpha-n}{K_s}S_w S_g\right]\frac{\partial p^w}{\partial t} \qquad [2.\ 298]$$

The sum of point 1,3 and 4 is the mass balance equation of vapour:

$$nS_g\frac{\partial \rho^{gw}}{\partial t}+div\,\mathbf{J}_g^{gw}+div\left(nS_g\rho^{gw}\mathbf{v}^{gws}\right)=\dot{m} \qquad [2.\ 299]$$

The final mass balance equation of water species becomes:

$$\begin{aligned}
&\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)+\rho^{gw}\frac{\alpha-n}{K_s}S_w S_g\right]\frac{\partial p^w}{\partial t}\\
&+\left(\rho^w\frac{\alpha-n}{K_s}S_w S_g+\rho^{gw}\frac{\alpha-n}{K_s}S_g^2\right)\frac{\partial p^{gw}}{\partial t}+\left[\rho^w S_w+\rho^{gw}S_g\right]\alpha div\mathbf{v}^s-\beta_{swg}\frac{\partial T}{\partial t}\\
&+\left[\rho^w\left(\frac{\alpha-n}{K_s}p^w S_w-\frac{\alpha-n}{K_s}p^g S_w+n\right)-\rho^{gw}\left(\frac{\alpha-n}{K_s}p^c S_g+n\right)\right]\frac{\partial S_w}{\partial t}\\
&+nS_g\frac{\partial \rho^{gw}}{\partial t}+div\mathbf{J}_g^{gw}+div\left(nS_w\rho^w\mathbf{v}^{ws}\right)+div\left(nS_g\rho^{gw}\mathbf{v}^{gws}\right)=0
\end{aligned} \qquad [2.\ 300]$$

2.8.1.3 Dry air mass balance equation

There are several components that contribute to the dry air mass balance equation:

1. Term linked to the saturation changes

$$-\beta_s(\alpha-n)S_g\frac{\partial T}{\partial t} \tag{2. 301}$$

2. Dry air advective flux

$$\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right) \tag{2. 302}$$

3. Term linked to saturation changes

$$-\left(\frac{\alpha-n}{K_s}p^cS_g+n\right)\frac{\partial S_w}{\partial t} \tag{2. 303}$$

4. Dry air diffusional flux

$$\frac{1}{\rho^{ga}}div\mathbf{J}_g^{ga} \tag{2. 304}$$

5. Term linked to the water vapour density changes

$$\frac{nS_g}{\rho^{ga}}\frac{\partial\rho^{ga}}{\partial t} \tag{2. 305}$$

6. Volumetric strain of solid skeleton

$$\alpha S_g\,div\;\mathbf{v}^s \tag{2. 306}$$

7. Term linked to the dry air pressure changes

$$\frac{\alpha-n}{K_s}S_g^2\frac{\partial p^{ga}}{\partial t} \tag{2. 307}$$

8. Term linked to the water pressure changes

$$\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^w}{\partial t} \tag{2. 308}$$

The final mass balance equation of dty air becomes:

$$\begin{aligned}&\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^w}{\partial t}+\frac{\alpha-n}{K_s}S_g^2\frac{\partial p^{ga}}{\partial t}+\alpha S_g div\,\mathbf{v}^s\\&+\frac{nS_g}{\rho^{ga}}\frac{\partial\rho^{ga}}{\partial t}+\frac{1}{\rho^{ga}}div\,\mathbf{J}_g^{ga}-\beta_s(\alpha-n)S_g\frac{\partial T}{\partial t}\\&-\left(\frac{\alpha-n}{K_s}p^cS_g+n\right)\frac{\partial S_w}{\partial t}+\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right)=0\end{aligned} \tag{2. 309}$$

2.8.1.4 Enthalpy balance equation

There are several components that contribute to the enthalpy balance equation of the multiphase medium:

1. Heat for temperature changes

$$\left(\rho C_p\right)_{eff} \frac{\partial T}{\partial t} \qquad [2.\ 310]$$

where $\left(\rho C_p\right)_{eff}$ is the specific heat of the mixture at constant pressure written as the sum of the specific heat at constant pressure of the single phases

$$\left(\rho C_p\right)_{eff} = \rho^s C_p^s + \rho^w C_p^w + \rho^g C_p^g \qquad [2.\ 311]$$

2. Convective heat flux in the fluids

$$\left(\rho_w C_p^w \mathbf{v}^{ws} + \rho_g C_p^g \mathbf{v}^{gs}\right) \cdot gradT \qquad [2.\ 312]$$

and the convective heat flux in the solid phase is neglected.

3. Fourier's Law for the heat flux

$$-div\left(\chi_{eff}\, gradT\right) \qquad [2.\ 313]$$

where χ_{eff} is the effective thermal conductivity of the mixture written as

$$\chi_{eff} = \chi^s + \chi^w + \chi^g$$

4. Source terms relate to phase change of water

$$-\dot{m}\Delta H_{vap} \qquad [2.\ 314]$$

where $\dot{m}$ is the mass exchange term between the two phases from the water mass conservation equation

$$\begin{aligned}\dot{m} = & -\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2 + \frac{nS_w}{K_w}\right)\right]\frac{\partial p^w}{\partial t} - \rho^w\frac{\alpha-n}{K_s}S_w S_g\frac{\partial p^g}{\partial t} \\ & -\rho^w S_w \alpha div\mathbf{v}^s + \beta_{sw}\frac{\partial T}{\partial t} - div\left(\rho^w n S_w \mathbf{v}^{ws}\right) \\ & -\begin{bmatrix}\rho^w\left(\frac{\alpha-n}{K_s}p^w S_w - \frac{\alpha-n}{K_s}p^g S_w + n\right) \\ -\rho^{gw}\left(\frac{\alpha-n}{K_s}p^c S_g + n\right)\end{bmatrix}\frac{\partial S_w}{\partial t}\end{aligned} \qquad [2.\ 315]$$

with $\beta_{sw} = S_w\left[(\alpha-n)\beta_s + n\beta_w\right]$ and ΔH_{vap} is the latent heat of evaporation.

The final enthalpy balance equation is:

$$
\begin{aligned}
&(\rho C_p)_{eff} \frac{\partial T}{\partial t} + \left(\rho_w C_p^w \mathbf{v}^{ws} + \rho_g C_p^g \mathbf{v}^{gs}\right) \cdot grad\ T \\
&- div\left(\chi_{eff}\ grad\ T\right) = -\dot{m}\Delta H_{vap}
\end{aligned}
\qquad [2.\ 316]
$$

introducing the source term, [2.316] becomes:

$$
\begin{aligned}
&(\rho C_p)_{eff} \frac{\partial T}{\partial t} + \left(\rho_w C_p^w \mathbf{v}^{ws} + \rho_g C_p^g \mathbf{v}^{gs}\right) \cdot gradT + \\
&- div\left(\chi_{eff}\, gradT\right) - \Delta H_{vap}\left[\rho^w\left(\frac{\alpha - n}{K_s} S_w^2 + \frac{nS_w}{K_w}\right)\right]\frac{\partial p^w}{\partial t} + \\
&- div\left(\rho^w n S_w \mathbf{v}^{ws}\right)\Delta H_{vap} + \\
&- \Delta H_{vap}\rho^w \frac{\alpha - n}{K_s} S_w S_g \frac{\partial p^g}{\partial t} - \Delta H_{vap}\rho^w S_w \alpha\, div\, \mathbf{v}^s + \Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t} + \\
&- \Delta H_{vap}\begin{bmatrix} \rho^w\left(\dfrac{\alpha - n}{K_s} p^w S_w - \dfrac{\alpha - n}{K_s} p^g S_w + n\right) + \\ - \rho^{gw}\left(\dfrac{\alpha - n}{K_s} p^c S_g + n\right) \end{bmatrix}\frac{\partial S_w}{\partial t} = 0
\end{aligned}
\qquad [2.\ 317]
$$

2.8.1.5 Summary of governing equations

Linear momentum balance equation of the mixture

$$
\begin{aligned}
&- \rho \mathbf{a}^s - nS_w \rho^w \left(\mathbf{a}^{ws} + \mathbf{v}^{ws} \cdot grad\ \mathbf{v}^w\right) + \\
&- nS_g \rho^g \left(\mathbf{a}^{gs} + \mathbf{v}^{gs} \cdot grad\ \mathbf{v}^g\right) + div\, \boldsymbol{\sigma} + \rho \mathbf{g} = \mathbf{0}
\end{aligned}
\qquad [2.\ 318]
$$

Water species (liquid and vapour) mass balance equation

With compressible solid grains:

$$
\begin{aligned}
&\left[\rho^w\left(\frac{\alpha - n}{K_s} S_w^2 + \frac{nS_w}{K_w}\right) + \rho^{gw}\frac{\alpha - n}{K_s} S_w S_g\right]\frac{\partial p^w}{\partial t} + \\
&+ \left(\rho^w \frac{\alpha - n}{K_s} S_w S_g + \rho^{gw}\frac{\alpha - n}{K_s} S_g^2\right)\frac{\partial p^{gw}}{\partial t} + \\
&+ \left[\rho^w S_w + \rho^{gw} S_g\right]\alpha\, div\, \mathbf{v}^s - \beta_{swg}\frac{\partial T}{\partial t} + \\
&+ \left[\rho^w\left(\frac{\alpha - n}{K_s} p^w S_w - \frac{\alpha - n}{K_s} p^g S_w + n\right) - \rho^{gw}\left(\frac{\alpha - n}{K_s} p^c S_g + n\right)\right]\frac{\partial S_w}{\partial t} + \\
&+ nS_g \frac{\partial \rho^{gw}}{\partial t} + div\, \mathbf{J}_g^{gw} + div\left(nS_w \rho^w \mathbf{v}^{ws}\right) + div\left(nS_g \rho^{gw} \mathbf{v}^{gws}\right) = 0
\end{aligned}
\qquad [2.\ 319]
$$

With incompressible solid grains $\alpha = 1, \dfrac{1}{K_s} = 0$:

$$\begin{aligned}&\rho^{w}\frac{nS_{w}}{K_{w}}\frac{\partial p^{w}}{\partial t}+\left[\rho^{w}S_{w}+\rho^{gw}S_{g}\right]\alpha\, div\,\mathbf{v}^{s}-\beta_{swg}\frac{\partial T}{\partial t}+n\left(\rho^{w}-\rho^{gw}\right)\frac{\partial S_{w}}{\partial t}+\\&+nS_{g}\frac{\partial\rho^{gw}}{\partial t}+div\,\mathbf{J}_{g}^{gw}+div\left(nS_{w}\rho^{w}\mathbf{v}^{ws}\right)+div\left(nS_{g}\rho^{gw}\mathbf{v}^{gws}\right)=0\end{aligned}\tag*{[2. 320]}$$

Dry air mass balance equation

With compressible solid grains:

$$\begin{aligned}&\frac{\alpha-n}{K_{s}}S_{w}S_{g}\frac{\partial p^{w}}{\partial t}+\frac{\alpha-n}{K_{s}}S_{g}^{2}\frac{\partial p^{ga}}{\partial t}+\alpha S_{g}\,div\,\mathbf{v}^{s}+\frac{nS_{g}}{\rho^{ga}}\frac{\partial\rho^{ga}}{\partial t}+\\&+\frac{1}{\rho^{ga}}div\,\mathbf{J}_{g}^{ga}-\left(\frac{\alpha-n}{K_{s}}p^{c}S_{g}+n\right)\frac{\partial S_{w}}{\partial t}+\\&+\frac{1}{\rho^{ga}}div\left(nS_{g}\rho^{ga}\mathbf{v}^{gs}\right)-\beta_{s}\left(\alpha-n\right)S_{g}\frac{\partial T}{\partial t}=0\end{aligned}\tag*{[2. 321]}$$

With incompressible solid grains $\alpha=1,\frac{1}{K_{s}}=0$:

$$\begin{aligned}&S_{g}\,div\,\mathbf{v}^{s}+\frac{nS_{g}}{\rho^{ga}}\frac{\partial\rho^{ga}}{\partial t}+\frac{1}{\rho^{ga}}div\,\mathbf{J}_{g}^{ga}-n\frac{\partial S_{w}}{\partial t}+\\&+\frac{1}{\rho^{ga}}div\left(nS_{g}\rho^{ga}\mathbf{v}^{gs}\right)+n\beta_{s}S_{g}\frac{\partial T}{\partial t}=0\end{aligned}\tag*{[2. 322]}$$

Enthalpy balance equation of the mixture

With compressible solid grains:

$$\begin{aligned}&\left(\rho C_{p}\right)_{eff}\frac{\partial T}{\partial t}+\left(\rho_{w}C_{p}^{w}\mathbf{v}^{ws}+\rho_{g}C_{p}^{g}\mathbf{v}^{gs}\right)\cdot grad\,T+\\&-div\left(\chi_{eff}\,grad\,T\right)-\Delta H_{vap}\left[\rho^{w}\left(\frac{\alpha-n}{K_{s}}S_{w}^{2}+\frac{nS_{w}}{K_{w}}\right)\right]\frac{\partial p^{w}}{\partial t}+\\&-\Delta H_{vap}\rho^{w}\frac{\alpha-n}{K_{s}}S_{w}S_{g}\frac{\partial p^{g}}{\partial t}-\Delta H_{vap}\rho^{w}S_{w}\alpha\, div\,\mathbf{v}^{s}+\\&-\Delta H_{vap}\left[\begin{array}{l}\rho^{w}\left(\dfrac{\alpha-n}{K_{s}}p^{w}S_{w}-\dfrac{\alpha-n}{K_{s}}p^{g}S_{w}+n\right)+\\-\rho^{gw}\left(\dfrac{\alpha-n}{K_{s}}p^{c}S_{g}+n\right)\end{array}\right]\frac{\partial S_{w}}{\partial t}+\\&-div\left(\rho^{w}nS_{w}v^{ws}\right)\Delta H_{vap}+\Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t}=0\end{aligned}\tag*{[2. 323]}$$

With incompressible solid grains $\alpha=1,\frac{1}{K_{s}}=0$:

$$
\begin{aligned}
&(\rho C_p)_{eff}\frac{\partial T}{\partial t}+\left(\rho_w C_p^w \mathbf{v}^{ws}+\rho_g C_p^g \mathbf{v}^{gs}\right)\cdot gradT+\\
&-div\left(\chi_{eff}\, gradT\right)-\Delta H_{vap}\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t}+\\
&-\Delta H_{vap}\rho^w S_w \alpha\, div\,\mathbf{v}^s+\Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t}+\\
&-\Delta H_{vap} n\left(\rho^w-\rho^{gw}\right)\frac{\partial S_w}{\partial t}-div\left(\rho^w n S_w v^{ws}\right)\Delta H_{vap}=0
\end{aligned}
\qquad [2.\ 324]
$$

The above system of equations for the analysis of T-H-M behaviour of a porous media in dynamics can be solved with appropriate boundary and initial conditions, see section 3.2.2.

2.8.1.6 Various simplifying approximations

We assumed different approximations for the general field equations:

1) Incompressible grain at the microscopic level $\left(\alpha=1, \frac{1}{K_s}=0\right)$

Linear momentum balance equation of the mixture (no difference)

$$
\begin{aligned}
&-\rho\mathbf{a}^s-nS_w\rho^w\left(\mathbf{a}^{ws}+\mathbf{v}^{ws}\cdot grad\,\mathbf{v}^w\right)\\
&-nS_g\rho^g\left(\mathbf{a}^{gs}+\mathbf{v}^{gs}\cdot grad\,\mathbf{v}^g\right)+div\boldsymbol{\sigma}+\rho\mathbf{g}=0
\end{aligned}
\qquad [2.\ 325]
$$

Water species (liquid and vapour) mass balance equation

$$
\begin{aligned}
&\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t}+\left[\rho^w S_w+\rho^{gw}S_g\right]\alpha\, div\,\mathbf{v}^s-\beta_{swg}\frac{\partial T}{\partial t}\\
&+n\left(\rho^w-\rho^{gw}\right)\frac{\partial S_w}{\partial t}+nS_g\frac{\partial \rho^{gw}}{\partial t}+div\,\mathbf{J}_g^{gw}\\
&+div\left(nS_w\rho^w\mathbf{v}^{ws}\right)+div\left(nS_g\rho^{gw}\mathbf{v}^{gws}\right)=0
\end{aligned}
\qquad [2.\ 326]
$$

Dry air mass balance equation

$$
\begin{aligned}
&S_g\, div\,\mathbf{v}^s+\frac{nS_g}{\rho^{ga}}\frac{\partial \rho^{ga}}{\partial t}+\frac{1}{\rho^{ga}}div\,\mathbf{J}_g^{ga}\\
&-n\frac{\partial S_w}{\partial t}+\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right)+n\beta_s S_g\frac{\partial T}{\partial t}=0
\end{aligned}
\qquad [2.\ 327]
$$

Enthalpy balance equation for the multiphase medium

$$\begin{aligned}
&(\rho C_p)_{eff}\frac{\partial T}{\partial t}+\left(\rho_w C_p^w \mathbf{v}^{ws}+\rho_g C_p^g \mathbf{v}^{gs}\right)\cdot gradT \\
&-div\left(\chi_{eff}\, gradT\right)-\Delta H_{vap}\rho^w \frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} \\
&-\Delta H_{vap}\,\rho^w S_w \alpha\, div\, \mathbf{v}^s+\Delta H_{vap}\,\beta_{sw}\frac{\partial T}{\partial t} \\
&-\Delta H_{vap}\, n\left(\rho^w-\rho^{gw}\right)\frac{\partial S_w}{\partial t}-div\left(\rho^w nS_w \mathbf{v}^{ws}\right)\Delta H_{vap}=0
\end{aligned}$$

[2. 328]

If the generalized Darcy's Law [2.264] and [2.265] valid for the transport of both water and gas in slow phenomena is considered:

$$\begin{aligned}
nS_w \mathbf{v}^{ws}&=\frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w+\rho^w\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{ws}\right)\right] \\
nS_g \mathbf{v}^{gs}&=\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^g+\rho^g\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{gs}\right)\right]
\end{aligned}$$

[2. 329]

where

$k^{r\pi}$ is the relative permeability, a dimensionless parameter varying from 1 to 0

$\mathbf{k}$ is the permeability tensor of the medium

μ^π is the dynamic viscosity

With the introduction of the Darcy's Law the final system becomes:

Linear momentum balance equation of the mixture (no difference)

$$\begin{aligned}
&-\rho\mathbf{a}^s-nS_w\rho^w\left(\mathbf{a}^{ws}+\mathbf{v}^{ws}\cdot grad\,\mathbf{v}^w\right) \\
&-nS_g\rho^g\left(\mathbf{a}^{gs}+\mathbf{v}^{gs}\cdot grad\,\mathbf{v}^g\right)+div\boldsymbol{\sigma}+\rho\mathbf{g}=0
\end{aligned}$$

[2. 330]

Water species (liquid and vapour) mass balance equation

$$\begin{aligned}
&\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t}+\left[\rho^w S_w+\rho^{gw}S_g\right]\alpha div\mathbf{v}^s-\beta_{swg}\frac{\partial T}{\partial t} \\
&+n\left(\rho^w-\rho^{gw}\right)\frac{\partial S_w}{\partial t}+nS_g\frac{\partial \rho^{gw}}{\partial t}+div\mathbf{J}_g^{gw} \\
&+div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w+\rho^w\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{ws}\right)\right]\right] \\
&+div\left[\rho^{gw}\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^{gw}+\rho^{gw}\left(\mathbf{g}-\mathbf{a}^s-\mathbf{a}^{gws}\right)\right]\right]=0
\end{aligned}$$

[2. 331]

Dry air mass balance equation

$$\begin{aligned}
&S_g div\mathbf{v}^s + \frac{nS_g}{\rho^{ga}}\frac{\partial \rho^{ga}}{\partial t} + \frac{1}{\rho^{ga}} div\mathbf{J}_g^{ga} - n\frac{\partial S_w}{\partial t} \\
&+ \frac{1}{\rho^{ga}} div\left[\rho^{ga}\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^g + \rho^g\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{gs}\right)\right]\right] + n\beta_s S_g\frac{\partial T}{\partial t} = 0
\end{aligned} \qquad [2.\ 332]$$

Enthalpy balance equation for the multiphase medium

$$\begin{aligned}
&\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t} - div\left(\chi_{eff}\, gradT\right) \\
&+\left\{\begin{array}{l}\rho_w C_p^w nS_w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{ws}\right)\right] + \\ +\rho_g C_p^g nS_g\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^g + \rho^g\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{gs}\right)\right]\end{array}\right\}\cdot gradT \\
&-\Delta H_{vap}\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} - \Delta H_{vap}\rho^w S_w \alpha div\mathbf{v}^s \\
&+\Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t} - \Delta H_{vap} n\left(\rho^w - \rho^{gw}\right)\frac{\partial S_w}{\partial t} \\
&- div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\left(\mathbf{g} - \mathbf{a}^s - \mathbf{a}^{ws}\right)\right]\right]\Delta H_{vap} = 0
\end{aligned} \qquad [2.\ 333]$$

2) Apparently small terms related to relative acceleration of the fluids and their convective terms are neglected to reduce the number of variables [Z99, page 21]. This is an approximation for dynamics of lower frequencies. Some loss of accuracy will be evident for problems in which high-frequency oscillations are important, these are of little importance for earthquake analyses [Z99, pages 25-31], [LS98].

Linear momentum balance equation of the mixture

$$-\rho\mathbf{a}^s + div\boldsymbol{\sigma} + \rho\mathbf{g} = 0 \qquad [2.\ 334]$$

Water species (liquid and vapour) mass balance equation

$$\begin{aligned}
&\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} + \left[\rho^w S_w + \rho^{gw} S_g\right]\alpha div\,\mathbf{v}^s - \beta_{swg}\frac{\partial T}{\partial t} + n\left(\rho^w - \rho^{gw}\right)\frac{\partial S_w}{\partial t} \\
&+ nS_g\frac{\partial \rho^{gw}}{\partial t} + div\,\mathbf{J}_g^{gw} + div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\left(\mathbf{g} - \mathbf{a}^s\right)\right]\right] + \\
&+ div\left[\rho^{gw}\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^{gw} + \rho^{gw}\left(\mathbf{g} - \mathbf{a}^s\right)\right]\right] = 0
\end{aligned} \qquad [2.\ 335]$$

Dry air mass balance equation

$$
\begin{aligned}
& S_g div \mathbf{v}^s + \frac{nS_g}{\rho^{ga}} \frac{\partial \rho^{ga}}{\partial t} + \frac{1}{\rho^{ga}} div \mathbf{J}_g^{ga} - n \frac{\partial S_w}{\partial t} \\
& + \frac{1}{\rho^{ga}} div \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left[- gradp^g + \rho^g \left(\mathbf{g} - \mathbf{a}^s \right) \right] \right] + n\beta_s S_g \frac{\partial T}{\partial t} = 0
\end{aligned}
\qquad [2.\ 336]
$$

Enthalpy balance equation for the multiphase medium

$$
\begin{aligned}
& \left(\rho C_p \right)_{eff} \frac{\partial T}{\partial t} - div \left(\chi_{eff}\ grad\ T \right) - \Delta H_{vap}\, \rho^w S_w \alpha\, div\ \mathbf{v}^s \\
& + \left\{ \begin{aligned} & \rho_w C_p^w n S_w \left[- gradp^w + \rho^w \left(\mathbf{g} - \mathbf{a}^s \right) \right] + \\ & + \rho_g C_p^g n S_g \frac{k^{rg}\mathbf{k}}{\mu^g} \left[- gradp^g + \rho^g \left(\mathbf{g} - \mathbf{a}^s \right) \right] \end{aligned} \right\} \cdot grad\ T \\
& - \Delta H_{vap}\, \rho^w \frac{nS_w}{K_w} \frac{\partial p^w}{\partial t} + \Delta H_{vap}\, \beta_{sw} \frac{\partial T}{\partial t} - \Delta H_{vap}\, n \left(\rho^w - \rho^{gw} \right) \frac{\partial S_w}{\partial t} \\
& - div \left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left[- gradp^w + \rho^w \left(\mathbf{g} - \mathbf{a}^s \right) \right] \right] \Delta H_{vap} = 0
\end{aligned}
\qquad [2.\ 337]
$$

3) Dynamic seepage forcing terms connected with the solid acceleration are neglected in the mass and enthalpy balance equations because their contribution to the equation is very small compared with other terms [LS98], [Z99]. The effect of dynamic seepage can be of importance in the high frequency range where the **u**-p formulation is no longer valid [Z99].

Linear momentum balance equation of the mixture (no difference)

$$
-\rho \mathbf{a}^s + div \boldsymbol{\sigma} + \rho \mathbf{g} = 0 \qquad [2.\ 338]
$$

Water species (liquid and vapour) mass balance equation

$$
\begin{aligned}
& \rho^w \frac{nS_w}{K_w} \frac{\partial p^w}{\partial t} + \left[\rho^w S_w + \rho^{gw} S_g \right] \alpha\, div\ \mathbf{v}^s - \beta_{swg} \frac{\partial T}{\partial t} \\
& + n \left(\rho^w - \rho^{gw} \right) \frac{\partial S_w}{\partial t} + nS_g \frac{\partial \rho^{gw}}{\partial t} + div\ \mathbf{J}_g^{gw} \\
& + div \left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(- gradp^w + \rho^w \mathbf{g} \right) \right] \\
& + div \left[\rho^{gw} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(- gradp^{gw} + \rho^{gw} \mathbf{g} \right) \right] = 0
\end{aligned}
\qquad [2.\ 339]
$$

Dry air mass balance equation (no difference)

$$S_g div\,\mathbf{v}^s + \frac{nS_g}{\rho^{ga}}\frac{\partial \rho^{ga}}{\partial t} + \frac{1}{\rho^{ga}} div\,\mathbf{J}_g^{ga} - n\frac{\partial S_w}{\partial t}$$
$$+ \frac{1}{\rho^{ga}} div\left[\rho^{ga}\frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g + \rho^g\mathbf{g}\right)\right] \qquad [2.\,340]$$
$$+ n\beta_s S_g\frac{\partial T}{\partial t} = 0$$

Enthalpy balance equation for the multiphase medium

$$\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t} - div\left(\chi_{eff}\,grad\,T\right) - \Delta H_{vap}\rho^w S_w \alpha\, div\,\mathbf{v}^s$$
$$+ \begin{bmatrix} \rho_w C_p^w n S_w \frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right) + \\ + \rho_g C_p^g n S_g \frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g + \rho^g\mathbf{g}\right) \end{bmatrix} \cdot grad\,T$$
$$- \Delta H_{vap}\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} + \Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t} \qquad [2.\,341]$$
$$- \Delta H_{vap} n\left(\rho^w - \rho^{gw}\right)\frac{\partial S_w}{\partial t}$$
$$- div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right)\right]\Delta H_{vap} = 0$$

With the assumptions described we obtain the **u**-p^c-p^g(-T) formulation of the generalised field equations system.

2.8.1.7 Limits of validity of the u-p(-T) approximation

It is important to know the degree of approximation of the model just derived.

As described in [Z99, pages 27-31], in Figure 2. **5** are shown zones of sufficient accuracy for various approximations:

B = Biot Theory,

Z = **u**-p approximation theory,

C = Consolidation theory.

where:

$$\pi_1 = \frac{\kappa\rho V_c^2}{\omega L^2}\ and\ \pi_2 = \frac{\omega^2 L^2}{V_c^2}, K = \frac{\hat{\kappa}}{\rho g}$$

$\hat{\kappa}$ is the kinematic permeability,

$$V_c^2 = \frac{\dfrac{(D+k_f)}{n}}{\rho}$$

$D = \dfrac{E(1-\nu)}{(1+\nu)(1-2\nu)}$ is called the one-dimensional constrained modulus

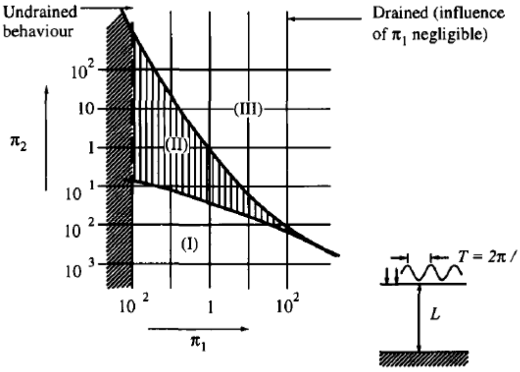

Figure 2. 5: *Zones of sufficient accuracy for various approximations.*

In Zone I: B = Z = C, slow phenomena (the acceleration of the fluid $\ddot{\mathbf{w}}$ and the acceleration of solid skeleton $\ddot{\mathbf{u}}$ can be neglected).

In Zone II: B = Z $\neq$ C, moderate speed ($\ddot{\mathbf{w}}$ can be neglected).

In Zone III, B $\neq$ Z $\neq$ C, fast phenomena ($\ddot{\mathbf{w}}$ cannot be neglected only full Biot equation valid).

We can, with reasonable confidence:

(i) assume fully undrained behaviour when π_1 = 97k' < 10^{-2} or the permeability k' < 10^{-4} m/s. (This is a very low value inapplicable for most materials used in dam construction).

(ii) We can assume **u**-p approximation as being valid when k' < 10^{-3} m/s to reproduce the complete frequency range. However, when k' < 10^{-1} m/s periods of less then 0.5 s are still well modelled.

The **u**-p formulation is particularly useful to implement the developed dynamics formulation starting from the quasi-static one (Comes-Geo),[GS96], [LS98], [SPS6] just introducing terms depending from the same independent variables.

2.8.1.8 Final system of equations to be implemented

With the following simplification:

1) Incompressible grain at the microscopic level $\left(\alpha = 1, \frac{1}{K_s} = 0\right)$

2) Small terms related to relative acceleration of the fluids and their convective terms are neglected [Z99, page 25], [LS98].

3) Dynamic seepage forcing terms connected with the solid acceleration are neglected in the mass and enthalpy balance equations [LS98], [Z99].

the final set of equation is:

Linear momentum balance equation of the mixture

$$-\rho \mathbf{a}^s + div\boldsymbol{\sigma} + \rho\mathbf{g} = 0 \qquad [2.\ 342]$$

Water species (liquid and vapour) mass balance equation

$$\begin{aligned}&\rho^w \frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} + \left[\rho^w S_w + \rho^{gw} S_g\right]\alpha div\mathbf{v}^s - \beta_{swg}\frac{\partial T}{\partial t} + n\left(\rho^w - \rho^{gw}\right)\frac{\partial S_w}{\partial t}\\ &+ nS_g\frac{\partial \rho^{gw}}{\partial t} + div\mathbf{J}_g^{gw} + div\left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right)\right]\\ &+ div\left[\rho^{gw}\frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^{gw} + \rho^{gw}\mathbf{g}\right)\right] = 0\end{aligned} \qquad [2.\ 343]$$

Dry air mass balance equation

$$\begin{aligned}&S_g div\,\mathbf{v}^s + \frac{nS_g}{\rho^{ga}}\frac{\partial \rho^{ga}}{\partial t} + \frac{1}{\rho^{ga}}div\mathbf{J}_g^{ga} - n\frac{\partial S_w}{\partial t} +\\ &+ \frac{1}{\rho^{ga}}div\left[\rho^{ga}\frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g + \rho^g\mathbf{g}\right)\right] + n\beta_s S_g\frac{\partial T}{\partial t} = 0\end{aligned} \qquad [2.\ 344]$$

Enthalpy balance equation for the multiphase medium

$$\begin{aligned}&\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t} - div\left(\chi_{eff}\,grad\,T\right) - \Delta H_{vap}\rho^w S_w \alpha div\,\mathbf{v}^s\\ &- \Delta H_{vap}\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} + \Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t}\\ &+ \begin{bmatrix}\rho_w C_p^w nS_w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right) +\\ + \rho_g C_p^g nS_g\frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g + \rho^g\mathbf{g}\right)\end{bmatrix}\cdot grad\,T\\ &- \Delta H_{vap} n\left(\rho^w - \rho^{gw}\right)\frac{\partial S_w}{\partial t} - div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right)\right]\Delta H_{vap} = 0\end{aligned} \qquad [2.\ 345]$$

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DISCRETIZATION OF GOVERNING EQUATIONS AND SOLUTION PROCEDURES

3.1 Introduction

In Chapter 2 the governing equations for the analysis of T-H-M behaviour of porous media in dynamics have been presented. The final system of equations, see section 2.8.1.8, is composed of:

- *Linear momentum balance equation of the mixture*
- *Water species (liquid and vapour) mass balance equativo*
- *Dry air mass balance equation*
- *Enthalpy balance equation for the multiphase medium*

and the independent variables chosen are:

- **u** displacement of the solid skeleton
- p^c *capillary pressure*
- p^g *gas pressure*
- *T temperature*

It is a non linear, coupled system of differential equations of first and second order, extremely difficult to solve by analytical methods.

In this chapter, numerical solution procedures are introduced for fluid-solid non isothermal interaction, in small-strain situations. The finite element method is used for the discretization in space and a generalized Newmark scheme is used for time discretization [ZT00].

3.2 Finite element spatial discretization

3.2.1 Weighted Residual Method

A boundary value problem of the type stated in the previous chapter can be represented as

$$\mathbf{A}(\mathbf{u}) = \mathbf{C}(\mathbf{u}) + \mathbf{p} = \mathbf{0} \qquad \text{on } \Omega \qquad [3.\ 1]$$

and

$$\mathbf{B}(\mathbf{u}) = \mathbf{D}(\mathbf{u}) + \mathbf{q} = \mathbf{0} \qquad \text{on } \Gamma \qquad [3.\ 2]$$

where $\mathbf{C}$ and $\mathbf{D}$ are differential operators and $\mathbf{p}$ and $\mathbf{q}$ are known functions, defined on the domain Ω and on the boundary Γ, independent of $\mathbf{u}$ which is the exact solution of the boundary value problems.

For most problems the exact solution can be very difficult or even impossible to obtain. Sometimes some form of approximation is needed, obtained here by finite element method. For instance one can construct an approximation

$$\bar{\mathbf{u}} = \sum_{i}^{r} \mathbf{N}_i \mathbf{a}_i = \mathbf{N}\mathbf{a} \approx \mathbf{u} \qquad [3.\ 3]$$

In which $\mathbf{N}_i$ are trial or shape functions in terms of the independent variables and $\mathbf{a}_i$ are the parameters which can be identified with the values of the unknown at defined points (nodes) in the domain.

If the approximation [3.3] is substituted into the [3.1] and [3.2] the equations are usually not satisfied and the residuals are

$$\mathbf{R}_\Omega = \mathbf{A}(\bar{\mathbf{u}}) = \mathbf{C}(\bar{\mathbf{u}}) + \mathbf{p} \qquad \text{on } \Omega \qquad [3.\ 4]$$

and

$$\mathbf{R}_\Gamma = \mathbf{B}(\bar{\mathbf{u}}) = \mathbf{D}(\bar{\mathbf{u}}) + \mathbf{q} \qquad \text{on } \Gamma \qquad [3.\ 5]$$

Those can be made zero with a numerical solution, in some weighted sense, by writing

$$\int_\Omega \mathbf{W}^T \mathbf{R}_\Omega d\Omega + \int_\Gamma \overline{\mathbf{W}}^T \mathbf{R}_\Gamma d\Gamma = 0 \qquad [3.\ 6]$$

or

$$\int_\Omega \mathbf{W}^T [\mathbf{C}(\bar{\mathbf{u}}) + \mathbf{p}] d\Omega + \int_\Gamma \overline{\mathbf{W}}^T [\mathbf{D}(\bar{\mathbf{u}}) + \mathbf{q}] d\Gamma = 0 \qquad [3.\ 7]$$

where the weighting functions $\mathbf{W}$ and $\overline{\mathbf{W}}$ can be chosen independently.

The Weighted Residual Method [ZT00] is applied in the following to the dynamic $\mathbf{u}$-p^c-p^g(-T) formulation of the generalised field equations for porous media summarized in section 2.8.1.7.

3.2.2 Initial and boundary conditions

There are various possible sets of primary variables to solve the problem described, in this work are chosen:

p^g *gas pressure* to describe the gas flow

p^c *capillary pressure* to describe the water species flow

T *temperature* for the heat flow equation

u *displacement vector* for mechanical behaviour

The initial and boundary conditions have to take into account any phase change which may take place.

The initial conditions describe the full field of variables at time zero in the domain **Ω** and the boundary Γ, and for the dynamic formulation we have to initialize also the velocity $\mathbf{V}$ of the solid skeleton:

$$\begin{aligned} &p^g = p_0^g \\ &p^w = p_0^w \\ &T = T_0 \\ &\mathbf{u} = \mathbf{u}_0 \\ &\mathbf{V} = \mathbf{V}_0 \end{aligned} \qquad [3.\ 8]$$

The Dirichlet boundary conditions are:

$$\begin{aligned} &p^g = \overline{p}^g && \text{on} \quad \Gamma_g \\ &p^w = \overline{p}^w && \text{on} \quad \Gamma_w \\ &T = \overline{T} && \text{on} \quad \Gamma_T \\ &\mathbf{u} = \overline{\mathbf{u}} && \text{on} \quad \Gamma_u \end{aligned} \qquad [3.\ 9]$$

The Neumann boundary conditions are:

$$div\, \boldsymbol{\sigma} - \mathbf{t} = \mathbf{0} \qquad \text{on } \Gamma_u^q \qquad [3.\ 10]$$

The fluxes of each phase may be required.

For water flux on on Γ_w^q:

$$\begin{bmatrix} \rho^w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-\,grad p^w + \rho^w \mathbf{g}\right)^T \\ +\,\rho^{gw} \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\,grad p^g + \rho^g \mathbf{g}\right)^T \\ -\,\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\dfrac{p^{gw}}{p^g}\right) \end{bmatrix} \cdot \mathbf{n} == q^w + q^{gw} + \beta_c\left(\rho^{gw} - \rho^{gw}{}_{\infty}\right) \qquad [3.\ 11]$$

For gas flux on Γ_g^q:

$$\begin{bmatrix} \rho^{ga} \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\,gradp^{\,g} + \rho^g \mathbf{g}\right)^T \\ -\,\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\dfrac{p^{gw}}{p^g}\right) \end{bmatrix} \cdot \mathbf{n} = q^{ga} \qquad [3.\ 12]$$

For heat flux on Γ_g^q:

$$\begin{bmatrix} \rho^{ga} \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\,gradp^{\,g} + \rho^g \mathbf{g}\right)^T \\ -\,\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\dfrac{p^{gw}}{p^g}\right) \end{bmatrix} \cdot \mathbf{n} = q^{ga} \qquad [3.\ 13]$$

where q^w, q^{gw}, q^{ga} , q^T are the imposed mass flux of water, vapour, dry air and heat, β_c is the convective mass transfer coefficient, $\rho^{gw}{}_\infty$ is the partial density of vapour in the surrounding air at a great distance from the interface, α_c is the convective heat transfer coefficient and T_∞ is the temperature in the far field of the undisturbed gas phase [LS98: pages 345-346, 357].

3.2.3 Linear momentum balance equation of the multiphase medium

Starting from the equilibrium equation [2.342]

$$\mathbf{L}^T\boldsymbol{\sigma} + \rho\mathbf{g} - \rho\ddot{\mathbf{u}} = \mathbf{0} \qquad \text{on } \Omega \qquad [3.\ 14]$$

where the differential operator $\mathbf{L}$ is defined as

$$\mathbf{L} = \begin{bmatrix} \dfrac{\partial}{\partial x} & 0 & 0 \\ 0 & \dfrac{\partial}{\partial y} & 0 \\ 0 & 0 & \dfrac{\partial}{\partial z} \\ \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial x} & 0 \\ 0 & \dfrac{\partial}{\partial z} & \dfrac{\partial}{\partial y} \\ \dfrac{\partial}{\partial z} & 0 & \dfrac{\partial}{\partial x} \end{bmatrix} \qquad [3.\ 15]$$

the stress tensor is written in vector form as

$$\boldsymbol{\sigma} = \left\{\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{yz}, \tau_{zx}\right\}^T \qquad [3.\ 16]$$

and

$$\rho = nS_w\rho_w + n(1-S_w)\rho_g + (1-n)\rho_s \quad [3.\ 17]$$

is the density of the total composite

The boundary condition are equation [3.9] and [3.10]

$$\begin{aligned} &\mathbf{l}^T\boldsymbol{\sigma} - \mathbf{t} = \mathbf{0} && \text{on } \Gamma_u^q \\ &\mathbf{u} = \overline{\mathbf{u}} && \text{on } \Gamma_u \end{aligned} \quad [3.\ 18]$$

where

$$\mathbf{l} = \begin{bmatrix} n_x & 0 & 0 \\ 0 & n_y & 0 \\ 0 & 0 & n_z \\ n_y & n_x & 0 \\ 0 & n_z & n_y \\ n_z & 0 & n_x \end{bmatrix}$$

Applying the integral equation [3.7] to the equilibrium equation and the boundary condition we have:

$$\begin{aligned} &\int_\Omega \mathbf{W}_u{}^T \mathbf{L}\boldsymbol{\sigma} d\Omega \\ &+ \int_\Omega \mathbf{W}_u{}^T (\rho\mathbf{g} - \rho\ddot{\mathbf{u}}) d\Omega \\ &+ \int_\Gamma \overline{\mathbf{W}}_u{}^T (\mathbf{l}\boldsymbol{\sigma} - \mathbf{t}) d\Gamma = \mathbf{0} \end{aligned} \quad [3.\ 19]$$

It is assume that the boundary condition on Γ_u is satisfied by the choice of the approximation of $\mathbf{u}$ and that the weighting functions are:

$$\begin{aligned} &\mathbf{W}_u = -\overline{\mathbf{W}}_u && \text{on } \Gamma_u^q \\ &\mathbf{W}_u = \mathbf{0} && \text{on } \Gamma_u \end{aligned} \quad [3.\ 20]$$

Using Green's Theorem [ZT00], the first term of the [3.19] can be replaced by the following

$$\int_\Omega \mathbf{W}_u{}^T \mathbf{L}\,\boldsymbol{\sigma}\, d\Omega = -\int_\Omega (\mathbf{L}\mathbf{W}_u)^T \boldsymbol{\sigma}\, d\Omega + \oint_\Gamma \mathbf{W}_u{}^T \mathbf{l}\boldsymbol{\sigma}\, d\Gamma \quad [3.\ 21]$$

So the equation [3.19] becomes:

$$\begin{aligned} &\int_\Omega (\mathbf{L}\mathbf{W}_u)^T \boldsymbol{\sigma} d\Omega + \int_\Omega \mathbf{W}_u{}^T \rho\ddot{\mathbf{u}} d\Omega \\ &- \int_\Omega \mathbf{W}_u{}^T \rho\mathbf{g} d\Omega - \int_\Gamma \overline{\mathbf{W}}_u{}^T \mathbf{t} d\Gamma = \mathbf{0} \end{aligned} \quad [3.\ 22]$$

Now the domain Ω is divided into subdomains and the primary variables are expressed by their nodal values and the shape functions:

$$\begin{aligned}
\mathbf{u}^e &= \mathbf{N}_u^e \overline{\mathbf{u}}^e = \sum_{i=1}^{m} \mathbf{N}_{ui}^e \overline{\mathbf{u}}_i^{\,e} \\
p^{g^e} &= \mathbf{N}_g^e \overline{\mathbf{p}}^{\mathbf{g}^e} = \sum_{j=1}^{n} N_{g\,j}^e \overline{p}_j^{g^e} \\
p^{c^e} &= \mathbf{N}_c^e \overline{\mathbf{p}}^{\mathbf{c}^e} = \sum_{l=1}^{p} N_{c\,l}^e \overline{p}_l^{c^e} \\
T^e &= \mathbf{N}_T^e \overline{\mathbf{T}}^e = \sum_{k=1}^{q} N_{Tk}^e \overline{T}_k^{\,e}
\end{aligned} \qquad [3.\ 23]$$

where *e* denotes the number of elements, *i, j, l, k* denote the nodes of the element and *m, n ,p, q* denote the number of nodes per element for the shape functions.

So

$$\overline{\mathbf{u}}_i^{\,e} = \left[u_{ix}, u_{iy}, u_{iz}\right]^T \qquad [3.\ 24]$$

is the displacement at node i

$$\overline{\mathbf{u}}^e = \left[\overline{\mathbf{u}}_1^{e^T} \ldots\ldots\ldots \overline{\mathbf{u}}_m^{e^T}\right] \qquad [3.\ 25]$$

is the nodal displacement vector

$$\mathbf{N}_u^e = \left[N_{u1}^e \mathbf{I}_3 \ldots\ldots\ldots N_{um}^e \mathbf{I}_3\right] \qquad [3.\ 26]$$

is the shape function for the displacement and $\mathbf{I}_3$ is a 3x3 identity matrix.

We can say the same for the other variables.

The sum of all elements can be represented in terms of global shape functions as

$$\begin{aligned}
\mathbf{u} &= \mathbf{N}_u \overline{\mathbf{u}} \\
p^g &= \mathbf{N}_g \overline{\mathbf{p}}^g \\
p^c &= \mathbf{N}_c \overline{\mathbf{p}}^c \\
T &= \mathbf{N}_T \overline{\mathbf{T}}
\end{aligned} \qquad [3.\ 27]$$

The shape functions for the displacement and for the other variables can be different, it is usually necessary to use higher order of interpolation for displacement then the other when there are incompressible or nearly incompressible undrained problems [ZQ86].

The standard Bubnov-Galerkin procedure [ZT00] is applied replacing the weighting functions by the corresponding shape functions.

$$\begin{aligned}
\mathbf{W_g} &= \mathbf{N_g} \\
\mathbf{W_w} &= \mathbf{N_w} \\
\mathbf{W_T} &= \mathbf{N_T} \\
\mathbf{W_u} &= \mathbf{N_u}
\end{aligned} \qquad [3.\ 28]$$

Substituting the [3.27] and [3.28] in the [3.22] we arrive at:

$$\begin{aligned}&\int_{\Omega}(\mathbf{LN}_u)^T\boldsymbol{\sigma}d\Omega+\int_{\Omega}\mathbf{N}_u{}^T\rho\mathbf{N}_u\ddot{\mathbf{u}}d\Omega\\&-\int_{\Omega}\mathbf{N}_u{}^T\rho\mathbf{g}d\Omega-\int_{\Gamma}\mathbf{N}_u{}^T\mathbf{t}d\Gamma=\mathbf{0}\end{aligned}\qquad [3.\ 29]$$

Now we introduce in [3.29] the effective stress [2.170] in the following form

$$\boldsymbol{\sigma}=\boldsymbol{\sigma}'-\mathbf{m}\alpha\left(S_w p^w+S_g p^g\right)\qquad [3.\ 30]$$

where the vector $\mathbf{m}$ has the form $\mathbf{m}^T=[1,1,1,0,0,0]$

$$\begin{aligned}&\int_{\Omega}(\mathbf{LN}_u)^T\boldsymbol{\sigma}''d\Omega+\int_{\Omega}\mathbf{N}_u{}^T\rho\mathbf{N}_u\ddot{\mathbf{u}}d\Omega\\&-\int_{\Omega}(\mathbf{LN}_u)^T\mathbf{m}\,\alpha\left[S_w\left(\mathbf{N}_g\overline{\mathbf{p}}^g-\mathbf{N}_c\overline{\mathbf{p}}^c\right)+S_g\mathbf{N}_g\overline{\mathbf{p}}^g\right]d\Omega\\&-\int_{\Omega}\mathbf{N}_u{}^T\rho\mathbf{g}d\Omega-\int_{\Gamma}\mathbf{N}_u{}^T\mathbf{t}d\Gamma=\mathbf{0}\end{aligned}\qquad [3.\ 31]$$

As regards the first term of the [3.31], for <u>the isotropic elastic case</u> the constitutive relationship can be written as:

$$\begin{aligned}\boldsymbol{\sigma}'&=\mathbf{D}_e\boldsymbol{\varepsilon}=\mathbf{D}_e(\boldsymbol{\varepsilon}_m+\boldsymbol{\varepsilon}_T)\\&=\mathbf{D}_e(\mathbf{Lu}_m+\boldsymbol{\varepsilon}_T)\\&=\mathbf{D}_e\left[\mathbf{LN}_u\overline{\mathbf{u}}-\mathbf{m}\frac{\beta_s}{3}\left(\mathbf{N}_t\overline{\mathbf{T}}-T_0\right)\right]\end{aligned}\qquad [3.\ 32]$$

where $\mathbf{D}_e$ is the constitutive tensor, $\mathbf{Lu}_m$ is the mechanical strain, $\boldsymbol{\varepsilon}_T$ is the thermal strain.

With

$$\mathbf{LN}_u=\mathbf{B}\qquad [3.\ 33]$$

[3.32] becomes:

$$\boldsymbol{\sigma}'=\mathbf{D}_e\mathbf{B}\overline{\mathbf{u}}-\mathbf{D}_e\left[\mathbf{m}\frac{\beta_s}{3}\left(\mathbf{N}_t\overline{\mathbf{T}}-T_0\right)\right]\qquad [3.\ 34]$$

So the first term of the [3.31] can be rewrite as:

$$\int_{\Omega}(\mathbf{LN}_u)^T\boldsymbol{\sigma}'d\Omega=\int_{\Omega}\left(\mathbf{B}^T\mathbf{D}_e\mathbf{B}\overline{\mathbf{u}}\right)d\Omega-\int_{\Omega}\mathbf{B}^T\mathbf{D}_e\left[\mathbf{m}\frac{\beta_s}{3}\left(\mathbf{N}_t\overline{\mathbf{T}}-T_0\right)\right]d\Omega\qquad [3.\ 35]$$

defining

$$\mathbf{K}_e=\int_{\Omega}\left(\mathbf{B}^T\mathbf{D}_e\mathbf{B}\right)d\Omega$$

the Linear Elastic Stiffness matrix, [3.35] becomes:

$$\int_{\Omega}(\mathbf{LN}_u)^T\boldsymbol{\sigma}'d\Omega=\mathbf{K}_e\overline{\mathbf{u}}-\int_{\Omega}\mathbf{B}^T\mathbf{D}_e\left[\mathbf{m}\frac{\beta_s}{3}\left(\mathbf{N}_t\overline{\mathbf{T}}-T_0\right)\right]d\Omega\qquad [3.\ 36]$$

For solid phase with non linear behavior only Tangential Stiffness Matrix $\mathbf{K}_T$ can be defined. So if

$$P(\overline{\mathbf{u}}) = \int_{\Omega} B^T \boldsymbol{\sigma}' d\Omega \tag{3. 37}$$

represents the internal force, K_T can be defined as

$$\begin{aligned} \mathbf{K}_T &= \int_{\Omega} \mathbf{B}^T \mathbf{D} \mathbf{B} d\Omega = \frac{\partial \mathbf{P}(\overline{\mathbf{u}})}{\partial \overline{\mathbf{u}}} \\ \frac{\partial \mathbf{P}(\overline{\mathbf{u}})}{\partial t} &= \frac{\partial \mathbf{P}(\overline{\mathbf{u}})}{\partial \overline{\mathbf{u}}} \frac{\partial \overline{\mathbf{u}}}{\partial t} = \mathbf{K}_T \frac{\partial \overline{\mathbf{u}}}{\partial t} \end{aligned} \tag{3. 38}$$

We can highlight the independent variables in [3.23]:

$$\begin{aligned} &\int_{\Omega} (\mathbf{L}\mathbf{N}_u)^T \boldsymbol{\sigma}' d\Omega \\ &- \int_{\Omega} (\mathbf{L}\mathbf{N}_u)^T \mathbf{m} \alpha \mathbf{N}_g \overline{\mathbf{p}}^g d\Omega \\ &+ \int_{\Omega} (\mathbf{L}\mathbf{N}_u)^T \mathbf{m} \alpha \mathbf{N}_c S_w \overline{\mathbf{p}}^c d\Omega \\ &+ \int_{\Omega} \mathbf{N}_u{}^T \rho \mathbf{N}_u \ddot{\overline{\mathbf{u}}} d\Omega \\ &- \int_{\Omega} \mathbf{N}_u{}^T \rho \mathbf{g} d\Omega - \int_{\Gamma} \mathbf{N}_u{}^T \mathbf{t} d\Gamma = \mathbf{0} \end{aligned} \tag{3. 39}$$

and [3.39] is rewritten as:

$$\int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma}' d\Omega - \mathbf{Q}\overline{\mathbf{p}}^g + \mathbf{R}\overline{\mathbf{p}}^c + \mathbf{M}\ddot{\overline{\mathbf{u}}} = \mathbf{f}_u \tag{3. 40}$$

where

$\mathbf{B} = \mathbf{L}\mathbf{N}_u$ is the strain operator

$\mathbf{Q} = \int_{\Omega} (\mathbf{L}\mathbf{N}_u)^T \mathbf{m} \alpha \mathbf{N}_g d\Omega$ is the first coupling matrix

$\mathbf{R} = \int_{\Omega} (\mathbf{L}\mathbf{N}_u)^T \mathbf{m} \alpha \mathbf{N}_c S_w d\Omega$ is the second coupling matrix

$\mathbf{M} = \int_{\Omega} \mathbf{N}_u{}^T \rho \mathbf{N}_u d\Omega$ is the mass matrix

$\mathbf{f}_u = \int_{\Omega} \mathbf{N}_u{}^T \rho \mathbf{g} d\Omega + \int_{\Gamma} \mathbf{N}_u{}^T \mathbf{t} d\Gamma$ is the right - hand term

So has been carried out the discretization in space of the momentum equilibrium equation and has been obtained an ordinary differential equation in time. We will operate in the same way for the other three balance equations.

3.2.4 Water species mass balance equation

Starting from the general [2.300] equation and using Fick's Law [2.164]

$$\mathbf{J}_g^{gw} = -\rho^g \frac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\frac{p^{gw}}{p^g}\right) \tag{3. 41}$$

we obtain

$$\begin{aligned}
& div\left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w + \rho^w\mathbf{g}\right)\right] \\
& + div\left[\rho^{gw} \frac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g + \rho^g\mathbf{g}\right)\right] \\
& + \left(\rho^w S_w + \rho^{gw} S_g\right)\alpha \mathbf{m}^T \mathbf{L}\frac{\partial \mathbf{u}}{\partial t} \\
& - \beta_{swg}\frac{\partial T}{\partial t} + \begin{bmatrix} \rho^w\left(\frac{\alpha - n}{K_s} p^w S_w - \frac{\alpha - n}{K_s} p^c S_w + n\right) + \\ - \rho^{gw}\left(\frac{\alpha - n}{K_s} p^c S_g + n\right) \end{bmatrix}\frac{\partial S_w}{\partial t} \\
& + nS_g\frac{\partial \rho^{gw}}{\partial t} + \left[\rho^w\left(\frac{\alpha - n}{K_s} S_w^2 + \frac{nS_w}{K_w}\right) + \rho^{gw}\frac{\alpha - n}{K_s} S_w S_g\right]\frac{\partial p^w}{\partial t} \\
& + \frac{\alpha - n}{K_s}\left(\rho^w S_w S_g + \rho^{gw} S_g^2\right)\frac{\partial p^g}{\partial t} \\
& - div\left[\rho^g \frac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\frac{p^{gw}}{p^g}\right)\right] = 0
\end{aligned} \tag{3. 42}$$

The boundary conditions for water species mass balance equation are imposed value and fluxes:

$$p^c = \overline{p}^c \qquad \text{on } \Gamma_w \tag{3. 43}$$

$$\begin{bmatrix} \frac{k^{rw}\mathbf{k}}{\mu^w}\left(-\rho^w gradp^w + {\rho^w}^2\mathbf{g}\right)^T \\ + \frac{k^{rg}\mathbf{k}}{\mu^g}\left(-\rho^{gw} gradp^{gw} + \rho^g\rho^{gw}\mathbf{g}\right)^T \\ - \left[\rho^g \frac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\, grad\left(\frac{p^{gw}}{p^g}\right)\right] \end{bmatrix} \cdot \mathbf{n} = \qquad \text{on } \Gamma_w^q$$
$$= q^w + q^{gw} + \beta_c\left(\rho^{gw} - {\rho^{gw}}_\infty\right) \tag{3. 44}$$

Applying the integral equation [3.7] to [3.42] and the boundary conditions [3.43], [3.44], we have:

$$
\begin{aligned}
&\int_\Omega \mathbf{W}_w{}^T \left\{ \begin{array}{l} div\left[\rho^w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]+ \\ +div\left[\rho^{gw}\ \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g+\rho^g\mathbf{g}\right)\right]+ \\ -div\left[\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga} grad\left(\dfrac{p^{gw}}{p^g}\right)\right] \end{array} \right\} d\Omega \\
&+\int_\Omega \mathbf{W}_w{}^T\left(\rho^w S_w+\rho^{gw}S_g\right)\alpha\mathbf{m}^T\mathbf{L}\frac{\partial \mathbf{u}}{\partial t}d\Omega \\
&+\int_\Omega \mathbf{W}_w{}^T nS_g\frac{\partial \rho^{gw}}{\partial t}d\Omega-\int_\Omega \mathbf{W}_w{}^T\beta_{swg}\frac{\partial T}{\partial t}d\Omega \\
&+\int_\Omega \mathbf{W}_w{}^T\left[\rho^w\left(\frac{\alpha-n}{K_s}p^wS_w-\frac{\alpha-n}{K_s}p^cS_w+n\right)-\rho^{gw}\left(\frac{\alpha-n}{K_s}p^cS_g+n\right)\right]\frac{\partial S_w}{\partial t}d\Omega \\
&+\int_\Omega \mathbf{W}_w{}^T\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)+\rho^{gw}\frac{\alpha-n}{K_s}S_wS_g\right]\frac{\partial p^w}{\partial t}d\Omega \\
&+\int_\Omega \mathbf{W}_w{}^T\frac{\alpha-n}{K_s}\left(\rho^wS_wS_g+\rho^{gw}S_g^2\right)\frac{\partial p^g}{\partial t}d\Omega \\
&+\int_\Gamma \overline{\mathbf{W}}_w{}^T\left\{ \begin{array}{l} \left[\begin{array}{l} \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-\rho^w gradp^w+\rho^{w^2}\mathbf{g}\right)^T+\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\rho^{gw}gradp^{gw}+\rho^g\rho^{gw}\mathbf{g}\right)^T \\ -\rho^g\dfrac{M_aM_w}{M_g^2}\mathbf{D}_g^{ga}\nabla\left(\dfrac{p^{gw}}{p^g}\right) \end{array}\right]\cdot\mathbf{n} \\ -q^w-q^{gw}-\beta_c\left(\rho^{gw}-\rho^{gw}{}_\infty\right) \end{array}\right\}d\Gamma=0
\end{aligned}
\qquad [3.\ 45]
$$

It is assume that the weighting functions are:

$$
\begin{array}{ll} \mathbf{W}_w=-\overline{\mathbf{W}}_w & \text{on } \Gamma_w^q \\ \mathbf{W}_w=0 & \text{on } \Gamma_w \end{array} \qquad [3.\ 46]
$$

Using Green’s Theorem [ZT00] in the first term of the [3.45], it can be replaced by the following equation:

$$
\int_\Omega \mathbf{W}_w{}^T\left\{ \begin{array}{l} div\left[\rho^w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]+div\left[\rho^{gw}\ \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g+\rho^g\mathbf{g}\right)\right] \\ -div\left[\rho^g\dfrac{M_aM_w}{M_g^2}\mathbf{D}_g^{ga}grad\left(\dfrac{p^{gw}}{p^g}\right)\right] \end{array}\right\}d\Omega=
$$

$$
\begin{aligned}
&= -\int_{\Omega} (\nabla \mathbf{W}_w)^T \left\{ \begin{array}{l} \left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(-gradp^w + \rho^w \mathbf{g} \right) \right] + \left[\rho^{gw} \quad \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right) \right] \\ - \left[\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \left(\frac{p^{gw}}{p^g} \right) \right] \end{array} \right\} d\Omega \\
&+ \oint_{\Gamma} \mathbf{W}_w{}^T \left\{ \begin{array}{l} \left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(-gradp^w + \rho^w \mathbf{g} \right) \right] + \left[\rho^{gw} \quad \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right) \right] \\ - \left[\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \left(\frac{p^{gw}}{p^g} \right) \right] \end{array} \right\} \mathbf{n} d\Gamma
\end{aligned}
\qquad [3.\ 47]
$$

So the equation [3.45] becomes:

$$
\begin{aligned}
&-\int_{\Omega} (\nabla \mathbf{W}_w)^T \left[\begin{array}{l} \rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(-gradp^w + \rho^w \mathbf{g} \right) \\ + \rho^{gw} \quad \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right) \\ - \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \left(\frac{p^{gw}}{p^g} \right) \end{array} \right] d\Omega \\
&+ \int_{\Omega} \mathbf{W}_w{}^T \left(\rho^w S_w + \rho^{gw} S_g \right) \alpha \mathbf{m}^T \mathbf{L} \frac{\partial \mathbf{u}}{\partial t} d\Omega \\
&+ \int_{\Omega} \mathbf{W}_w{}^T n S_g \frac{\partial \rho^{gw}}{\partial t} d\Omega - \int_{\Omega} \mathbf{W}_w{}^T \beta_{swg} \frac{\partial T}{\partial t} d\Omega \\
&+ \int_{\Omega} \mathbf{W}_w{}^T \left[\rho^w \left(\frac{\alpha - n}{K_s} p^w S_w - \frac{\alpha - n}{K_s} p^c S_w + n \right) - \rho^{gw} \left(\frac{\alpha - n}{K_s} p^c S_g + n \right) \right] \frac{\partial S_w}{\partial t} d\Omega \\
&+ \int_{\Omega} \mathbf{W}_w{}^T \left[\rho^w \left(\frac{\alpha - n}{K_s} S_w^2 + \frac{n S_w}{K_w} \right) + \rho^{gw} \frac{\alpha - n}{K_s} S_w S_g \right] \frac{\partial p^w}{\partial t} d\Omega \\
&+ \int_{\Omega} \mathbf{W}_w{}^T \frac{\alpha - n}{K_s} \left(\rho^w S_w S_g + \rho^{gw} S_g^2 \right) \frac{\partial p^g}{\partial t} d\Omega \\
&+ \int_{\Gamma} \mathbf{W}_w{}^T \left[q^w + q^{gw} + \beta_{\mathrm{c}} \left(\rho^{gw} - \rho^{gw}{}_{\infty} \right) \right] d\Gamma = 0
\end{aligned}
\qquad [3.\ 48]
$$

Now the primary variables are expressed by their nodal values and the shape functions:

$$
\begin{aligned}
&\mathbf{u} = \mathbf{N}_u \bar{\mathbf{u}} \\
&p^g = \mathbf{N}_g \bar{\mathbf{p}}^g \\
&p^c = \mathbf{N}_c \bar{\mathbf{p}}^c \\
&T = \mathbf{N}_T \bar{\mathbf{T}}
\end{aligned}
\qquad [3.\ 49]
$$

The standard Bubnov-Galerkin procedure [ZT00] is applied replacing the weighting functions by the corresponding shape functions.

$$
\begin{aligned}
&\mathbf{W_g} = \mathbf{N_g} \\
&\mathbf{W_w} = \mathbf{N_w} \\
&\mathbf{W_T} = \mathbf{N_T} \\
&\mathbf{W_u} = \mathbf{N_u}
\end{aligned}
\qquad [3.\ 50]
$$

The diffusive term is now transformed using Kelvin's equation [2.146]

$$p^{gw} = p^{gws}(T)e^{\left(\frac{p^c M_w}{\rho^w RT}\right)}$$

So $grad\,\frac{p^{gw}}{p^g}$ becomes:

$$\begin{aligned}
grad\,\frac{p^{gw}}{p^g} &= grad\,\frac{p^{gw}\left(p^c,T\right)}{p^g}\\
&= \frac{1}{p^g}\,gradp^{gw} + p^{gw}gradp^{g^{-1}}\\
&= \frac{1}{p^g}\,gradp^{gw} - \frac{p^{gw}}{{p^g}^2}\,gradp^g =\\
&= \frac{1}{p^g}\left(\frac{\partial p^{gw}}{\partial p^c}\,gradp^c + \frac{\partial p^{gw}}{\partial T}\,gradT\right) - \frac{p^{gw}}{{p^g}^2}\,gradp^g
\end{aligned} \qquad [3.\ 51]$$

Substituting the [3. 49], [3.50] and [3.49] in the [3.51] we arrive at:

$$\begin{aligned}
&\int_\Omega (\mathbf{LN}_w)^T \left\{\begin{array}{l}
-\left[\rho^w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-\mathbf{L}\left(\mathbf{N}_g\overline{\mathbf{p}}^g - \mathbf{N}_c\overline{\mathbf{p}}^c\right) + \rho^w\mathbf{g}\right)\right]\\
-\left[\rho^{gw}\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\mathbf{LN}_g\overline{\mathbf{p}}^g + \rho^g\mathbf{g}\right)\right]\\
+\left[\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\,\dfrac{1}{p^g}\dfrac{\partial p^{gw}}{\partial p^c}\mathbf{LN}_c\overline{\mathbf{p}}^c\right]\\
+\left[\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\left(\dfrac{1}{p^g}\dfrac{\partial p^{gw}}{\partial T}\mathbf{LN}_T\overline{\mathbf{T}}\right)\right]\\
-\left[\rho^g \dfrac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}\left(\dfrac{p^{gw}}{{p^g}^2}\mathbf{LN}_g\overline{\mathbf{p}}^g\right)\right]
\end{array}\right\} d\Omega\\
&+\int_\Omega \mathbf{N}_w{}^T\left(\rho^w S_w + \rho^{gw}S_g\right)\alpha\,\mathbf{m}^T\mathbf{L}\,\mathbf{N}_u\dot{\overline{\mathbf{u}}}\,d\Omega\\
&+\int_\Omega \mathbf{N}_w{}^T nS_g\,\dot{\rho}^{gw}\,d\Omega - \int_\Omega \mathbf{N}_w{}^T\beta_{swg}\,\mathbf{N}_T\dot{\overline{T}}\,d\Omega\\
&+\int_\Omega \mathbf{N}_w{}^T\left[\begin{array}{l}
\rho^w\left(\begin{array}{l}\dfrac{\alpha-n}{K_s}\left(\mathbf{N}_g\overline{\mathbf{p}}^g - \mathbf{N}_c\overline{\mathbf{p}}^c\right)S_w\\
-\dfrac{\alpha-n}{K_s}\mathbf{N}_c\overline{\mathbf{p}}^c S_w + n\end{array}\right)\\
-\rho^{gw}\left(\dfrac{\alpha-n}{K_s}\mathbf{N}_c\overline{\mathbf{p}}^c S_g + n\right)
\end{array}\right]\left(\frac{\partial S_w}{\partial T}\mathbf{N}_T\dot{\overline{\mathbf{T}}} + \frac{\partial S_w}{\partial p^c}\mathbf{N}_c\dot{\overline{\mathbf{p}}}^c\right)d\Omega\\
&+\int_\Omega \mathbf{N}_w{}^T\left[\begin{array}{l}
\rho^w\left(\dfrac{\alpha-n}{K_s}S_w^2 + \dfrac{nS_w}{K_w}\right)\\
+\rho^{gw}\,\dfrac{\alpha-n}{K_s}S_w S_g
\end{array}\right]\left(\mathbf{N}_g\dot{\overline{\mathbf{p}}}^g - \mathbf{N}_c\dot{\overline{\mathbf{p}}}^c\right)d\Omega\\
&+\int_\Omega \mathbf{N}_w{}^T\,\frac{\alpha-n}{K_s}\left(\rho^w S_w S_g + \rho^{gw}S_g^2\right)\mathbf{N}_g\dot{\overline{\mathbf{p}}}^g\,d\Omega\\
&+\int_\Gamma \mathbf{N}_w{}^T\left[q^w + q^{gw} + \beta_{\mathrm{c}}\left(\rho^{gw} - \rho^{gw}{}_\infty\right)\right]d\Gamma = 0
\end{aligned} \qquad [3.\ 52]$$

With the assumption of incompressible grain at microscopic level $\left(\alpha=1, \frac{1}{K_s}=0\right)$ and by neglecting the variation of the vapour density, the equation [3.52] becomes:

$$
\begin{aligned}
&\int_\Omega (\mathbf{LN}_w)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial p^c} - \rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \mathbf{LN}_c \overline{\mathbf{p}}^c \right) \mathbf{LN}_c \overline{\mathbf{p}}^c d\Omega \\
&- \int_\Omega (\mathbf{LN}_w)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{p^{gw}}{{p^g}^2} - \rho^{gw} \frac{k^{rg}\mathbf{k}}{\mu^g} - \rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \right) \mathbf{LN}_g \overline{\mathbf{p}}^g d\Omega \\
&+ \int_\Omega (\mathbf{LN}_w)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial T} \mathbf{LN}_T \overline{\mathbf{T}} d\Omega \\
&+ \int_\Omega \mathbf{N}_w{}^T \left(\rho^w S_w + \rho^{gw} S_g\right) \alpha \mathbf{m}^T \mathbf{LN}_u \dot{\overline{\mathbf{u}}} d\Omega \\
&+ \int_\Omega \mathbf{N}_w{}^T \left[n\left(\rho^w - \rho^{gw}\right) \frac{\partial S_w}{\partial T} - \beta_{swg} \right] \mathbf{N}_T \dot{\overline{\mathbf{T}}} d\Omega \\
&+ \int_\Omega \mathbf{N}_w{}^T \left[n\left(\rho^w - \rho^{gw}\right) \frac{\partial S_w}{\partial p^c} - \rho^w \frac{n S_w}{K_w} \right] \mathbf{N}_c \dot{\overline{\mathbf{p}}}^c d\Omega \\
&+ \int_\Omega N_w{}^T \rho^w \frac{n S_w}{K_w} \mathbf{N}_g \dot{\overline{\mathbf{p}}}^g d\Omega + \\
&+ \int_\Omega (\mathbf{LN}_w)^T \mathbf{g} \left(\rho^{w2} \frac{k^{rw}\mathbf{k}}{\mu^w} - \rho^{gw} \rho^g \frac{k^{rg}\mathbf{k}}{\mu^g} \right) d\Omega \\
&+ \int_\Gamma \mathbf{N}_w{}^T \left[q^w + q^{gw} + \beta_{\mathrm{c}} \left(\rho^{gw} - \rho^{gw}{}_\infty \right) \right] d\Gamma = 0
\end{aligned}
\qquad [3.\ 53]
$$

We can rewrite the equation [3.53] in such a way:

$$
\mathbf{U}\,\dot{\overline{\mathbf{p}}}^g + \mathbf{S}\,\dot{\overline{\mathbf{p}}}^c + \mathbf{T}\,\dot{\overline{\mathbf{T}}} + \mathbf{Q}'\,\dot{\overline{\mathbf{u}}} - \mathbf{I}\,\overline{\mathbf{p}}^g + \mathbf{H}\,\overline{\mathbf{p}}^c + \mathbf{E}\,\overline{\mathbf{T}} + \mathbf{f}_w = 0 \qquad [3.\ 54]
$$

where

$$
\begin{aligned}
\mathbf{I} &= \int_\Omega (\mathbf{LN}_w)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{p^{gw}}{{p^g}^2} - \rho^{gw} \frac{k^{rg}\mathbf{k}}{\mu^g} - \rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \right) \mathbf{LN}_g d\Omega \\
\mathbf{H} &= \int_\Omega (\mathbf{LN}_w)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial p^c} - \rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \mathbf{LN}_c \overline{p}^c \right) \mathbf{LN}_c d\Omega \\
\mathbf{E} &= \int_\Omega (\mathbf{LN}_w)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial T} \mathbf{LN}_T T d\Omega \\
\mathbf{U} &= \int_\Omega \mathbf{N}_w{}^T \rho^w \frac{n S_w}{K_w} \mathbf{N}_g d\Omega \\
\mathbf{S} &= \int_\Omega \mathbf{N}_w{}^T \left[n\left(\rho^w - \rho^{gw}\right) \frac{\partial S_w}{\partial p^c} - \rho^w \frac{n S_w}{K_w} \right] \mathbf{N}_c d\Omega \\
\mathbf{T} &= \int_\Omega \mathbf{N}_w{}^T \left[n\left(\rho^w - \rho^{gw}\right) \frac{\partial S_w}{\partial T} - \beta_{swg} \right] \mathbf{N}_T d\Omega \\
\mathbf{Q}' &= \int_\Omega \mathbf{N}_w{}^T \left(\rho^w S_w + \rho^{gw} S_g\right) \alpha m^T L\mathbf{N}_u d\Omega \\
\mathbf{f}_w &= \int_\Omega (\mathbf{LN}_w)^T \mathbf{g} \left(\rho^{w2} \frac{k^{rw}\mathbf{k}}{\mu^w} - \rho^{gw} \rho^g \frac{k^{rg}\mathbf{k}}{\mu^g} \right) d\Omega + \int_\Gamma \mathbf{N}_w{}^T \left[q^w + q^{gw} + \beta_{\mathrm{c}} \left(\rho^{gw} - \rho^{gw}_\infty \right) \right] d\Gamma
\end{aligned}
\qquad [3.\ 55]
$$

3.2.5 Dry air mass balance equation

Starting from the general equation [2.321] and using Fick's Law [2.164]

$$\begin{aligned}&\mathbf{J}_g^{ga} = -\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \frac{p^{ga}}{p^g} = \\ &= \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \frac{p^{gw}}{p^g} = -\mathbf{J}_g^{gw}\end{aligned} \qquad [3.\ 56]$$

we obtain

$$\begin{aligned}&\rho^{ga} \frac{\alpha - n}{K_s} S_w S_g \frac{\partial p^w}{\partial t} + \rho^{ga} \frac{\alpha - n}{K_s} S_g^2 \frac{\partial p^{ga}}{\partial t} \\ &+ \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L} \dot{\overline{\mathbf{u}}} + n S_g \frac{\partial \rho^{ga}}{\partial t} \\ &+ div\left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \frac{p^{gw}}{p^g} \right) \\ &- \rho^{ga} \left(\frac{\alpha - n}{K_s} p^c S_g + n \right) \frac{\partial S_w}{\partial t} \\ &+ div\left(\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right) \right) \\ &- \beta_s \rho^{ga} (\alpha - n) S_g \frac{\partial T}{\partial t} = 0\end{aligned} \qquad [3.\ 57]$$

The boundary conditions for dry air mass balance equation are imposed value and fluxes:

$$p^g = \overline{p}^g \qquad \text{on } \Gamma_g \qquad [3.\ 58]$$

$$\begin{bmatrix} \rho^{ga} \dfrac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right)^T \\ -\rho^g \dfrac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \left(\dfrac{p^{gw}}{p^g} \right) \end{bmatrix} \cdot \mathbf{n} = q^{ga} \qquad \text{on } \Gamma_g^q \qquad [3.\ 59]$$

Applying the integral equation [3.7] to the [3.57] and the above boundary conditions we have:

$$\begin{aligned}&\int_\Omega \mathbf{W}_g{}^T div\left(\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right) \right) d\Omega \\ &+ \int_\Omega \mathbf{W}_g{}^T div\left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \frac{p^{gw}}{p^g} \right) d\Omega\end{aligned}$$

$$
\begin{aligned}
&+\int_\Omega \mathbf{W}_g^{\;T} \frac{\alpha-n}{K_s} \rho^{ga} S_w S_g \frac{\partial p^w}{\partial t} d\Omega \\
&+\int_\Omega \mathbf{W}_g^{\;T} \frac{\alpha-n}{K_s} \rho^{ga} S_g^2 \frac{\partial p^{ga}}{\partial t} d\Omega \\
&+\int_\Omega \mathbf{W}_g^{\;T} \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L} \dot{\mathbf{u}} d\Omega \\
&+\int_\Omega \mathbf{W}_g^{\;T} n S_g \frac{\partial \rho^{ga}}{\partial t} d\Omega \\
&-\int_\Omega \mathbf{W}_g^{\;T} \rho^{ga} \left(\frac{\alpha-n}{K_s} p^c S_g + n \right) \frac{\partial S_w}{\partial t} d\Omega \\
&-\int_\Omega \mathbf{W}_g^{\;T} \rho^{ga} \beta_s (\alpha-n) S_g \frac{\partial T}{\partial t} d\Omega \\
&+\int_\Gamma \overline{\mathbf{W}}_g^{\;T} \left\{ \begin{bmatrix} \rho^{ga} \dfrac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^g + \rho^g \mathbf{g} \right)^T \\ -\rho^g \dfrac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad \dfrac{p^{gw}}{p^g} \end{bmatrix} \cdot \mathbf{n} - q^{ga} \right\} d\Gamma = 0
\end{aligned}
\tag*{[3. 60]}
$$

It is assume that the weighting functions are:

$$
\begin{aligned}
&\mathbf{W}_g = -\overline{\mathbf{W}}_g && \text{on } \Gamma_g^q \\
&\mathbf{W}_g = 0 && \text{on } \Gamma_g
\end{aligned}
\tag*{[3. 61]}
$$

Using Green's Theorem [ZT00], the first term of [3.60] can be replaced by the following equality:

$$
\begin{aligned}
&\int_\Omega \mathbf{W}_g^{\;T} div \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^{\,g} + \rho^g \mathbf{g} \right) \right] d\Omega + \\
&+\int_\Omega \mathbf{W}_g^{\;T} div \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad\, \frac{p^{gw}}{p^g} \right) d\Omega \\
&= -\int_\Omega \left(\mathbf{L}\mathbf{W}_g \right)^T \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^{\,g} + \rho^g \mathbf{g} \right) \right] d\Omega + \\
&-\int_\Omega \left(\mathbf{L}\mathbf{W}_g \right)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad\, \frac{p^{gw}}{p^g} \right) d\Omega + \\
&+\int_\Gamma \mathbf{W}_g^{\;T} \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \left(-gradp^{\,g} + \rho^g \mathbf{g} \right) \right] \cdot \mathbf{n} d\Gamma + \\
&+\int_\Gamma \mathbf{W}_g^{\;T} \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} grad\, \frac{p^{gw}}{p^g} \right) \cdot \mathbf{n} d\Gamma
\end{aligned}
\tag*{[3. 62]}
$$

So the equation [3.60] becomes:

$$\begin{aligned}
&-\int_\Omega (\mathbf{LW}_g)^T \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g}\left(-grad p^g + \rho^g \mathbf{g}\right)\right] d\Omega + \\
&-\int_\Omega (\mathbf{LW}_g)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga}\, grad \frac{p^{gw}}{p^g} \right) d\Omega + \\
&+\int_\Omega \mathbf{W}_g{}^T \frac{\alpha - n}{K_s} \rho^{ga} S_w S_g \frac{\partial p^w}{\partial t} d\Omega + \\
&+\int_\Omega \mathbf{W}_g{}^T \frac{\alpha - n}{K_s} \rho^{ga} S_g^2 \frac{\partial p^{ga}}{\partial t} d\Omega + \\
&+\int_\Omega \mathbf{W}_g{}^T \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L}\dot{\bar{\mathbf{u}}} d\Omega + \int_\Omega \mathbf{W}_g{}^T n S_g \frac{\partial \rho^{ga}}{\partial t} d\Omega \\
&\int_\Omega \mathbf{W}_g{}^T \rho^{ga} \left(\frac{\alpha - n}{K_s} p^c S_g + n \right) \frac{\partial S_w}{\partial t} d\Omega + \\
&-\int_\Omega \mathbf{W}_g{}^T \rho^{ga} \beta_s (\alpha - n) S_g \frac{\partial T}{\partial t} d\Omega + \int_\Gamma \mathbf{W}_g{}^T q^{ga} d\Gamma = 0
\end{aligned} \qquad [3.63]$$

Now the primary variables are expressed by their nodal values and the shape functions

$$\begin{aligned}
&\mathbf{u} = \mathbf{N}_u \bar{\mathbf{u}} \\
&p^g = \mathbf{N}_g \bar{\mathbf{p}}^g \\
&p^c = \mathbf{N}_c \bar{\mathbf{p}}^c \\
&T = \mathbf{N}_T \bar{\mathbf{T}}
\end{aligned} \qquad [3.64]$$

The standard Bubnov-Galerkin procedure [ZT00] is applied replacing the weighting functions by the corresponding shape functions.

$$\begin{aligned}
&\mathbf{W_g} = \mathbf{N_g} \\
&\mathbf{W_w} = \mathbf{N_w} \\
&\mathbf{W_T} = \mathbf{N_T} \\
&\mathbf{W_u} = \mathbf{N_u}
\end{aligned} \qquad [3.65]$$

The diffusive term is now transformed using Kelvin's equation [2.146]

$$p^{gw} = p^{gws}(T) e^{\left(\frac{p^c M_w}{\rho^w RT}\right)}$$

So the $grad \frac{p^{gw}}{p^g}$ becomes:

$$\begin{aligned}
&grad \frac{p^{gw}}{p^g} = grad \frac{p^{gw}(p^c, T)}{p^g} = \frac{1}{p^g} grad p^{gw} + p^{gw} grad p^{g^{-1}} = \\
&= \frac{1}{p^g} grad p^{gw} - \frac{p^{gw}}{p^{g^2}} grad p^g =
\end{aligned}$$

$$= \frac{1}{p^g}\left(\frac{\partial p^{gw}}{\partial p^c} gradp^c + \frac{\partial p^{gw}}{\partial T} gradT\right) - \frac{p^{gw}}{{p^g}^2} gradp^g \qquad [3.\ 66]$$

Substituting the [3. 64], [3.65] and [3.66] in the [3.63], we arrives at:

$$\begin{aligned}
&-\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \left[\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g}\left(-\mathbf{L}\mathbf{N}_g \bar{\mathbf{p}}^g + \rho^g \mathbf{g}\right)\right] d\Omega \\
&-\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g}\frac{\partial p^{gw}}{\partial p^c} \mathbf{L}\mathbf{N}_c \bar{\mathbf{p}}^c\right) d\Omega \\
&-\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g}\frac{\partial p^{gw}}{\partial T} \mathbf{L}\mathbf{N}_T \bar{\mathbf{T}}\right) d\Omega \\
&+\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \left(\rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{p^{gw}}{{p^g}^2} \mathbf{L}\mathbf{N}_g \bar{\mathbf{p}}^g\right) d\Omega \\
&+\int_\Omega \mathbf{N}_g{}^T \frac{\alpha - n}{K_s} \rho^{ga} S_w S_g \left(\mathbf{N}_g \dot{\bar{\mathbf{p}}}^g - \mathbf{N}_c \dot{\bar{\mathbf{p}}}^c\right) d\Omega \\
&+\int_\Omega \mathbf{N}_g{}^T \frac{\alpha - n}{K_s} \rho^{ga} S_g^2 \dot{p}^{ga} d\Omega \\
&+\int_\Omega \mathbf{N}_g{}^T \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L}\mathbf{N}_u \dot{\bar{\mathbf{u}}} d\Omega \\
&+\int_\Omega \mathbf{N}_g{}^T n S_g \dot{\rho}^{ga} d\Omega \\
&-\int_\Omega \mathbf{N}_g{}^T \rho^{ga} \left(\frac{\alpha - n}{K_s} \mathbf{N}_c \dot{\bar{\mathbf{p}}}^c S_g + n\right)\left(\frac{\partial S_w}{\partial T} \mathbf{N}_T \dot{\bar{\mathbf{T}}} + \frac{\partial S_w}{\partial p^c} \mathbf{N}_c \dot{\bar{\mathbf{p}}}^c\right) d\Omega \\
&-\int_\Omega \mathbf{N}_g{}^T \rho^{ga} \beta_s (\alpha - n) S_g \mathbf{N}_T \dot{\bar{\mathbf{T}}} d\Omega \qquad [3.\ 67] \\
&+\int_\Gamma \mathbf{N}_g{}^T q^{ga} d\Gamma = 0
\end{aligned}$$

With the assumption of incompressible grain at microscopic level $\left(\alpha = 1, \frac{1}{K_s} = 0\right)$ and by neglecting the variation of the dry air density, the equation [3.67] becomes:

$$\begin{aligned}
&\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \left(\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} + \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{p^{gw}}{{p^g}^2}\right) (\mathbf{L}\mathbf{N}_g) \bar{\mathbf{p}}^g d\Omega \\
&-\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g}\frac{\partial p^{gw}}{\partial p^c} (\mathbf{L}\mathbf{N}_c) \bar{\mathbf{p}}^c d\Omega \\
&-\int_\Omega (\mathbf{L}\mathbf{N}_g)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g}\frac{\partial p^{gw}}{\partial T} (\mathbf{L}\mathbf{N}_T) \bar{\mathbf{T}} d\Omega
\end{aligned}$$

$$
\begin{aligned}
&+\int_{\Omega} \mathbf{N}_g^{\,T} \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L}\left(\mathbf{N}_u \dot{\overline{\mathbf{u}}}\right) d\Omega \\
&-\int_{\Omega} \mathbf{N}_g^{\,T} \rho^{ga} n \frac{\partial S_w}{\partial p^c} \mathbf{N}_c \dot{\overline{\mathbf{p}}}^c d\Omega \\
&-\int_{\Omega} \mathbf{N}_g^{\,T} \left[\rho^{ga} \beta_s (\alpha - n) S_g + \rho^{ga} n \frac{\partial S_w}{\partial T} \right] \mathbf{N}_T \dot{\overline{\mathbf{T}}} d\Omega \\
&-\int_{\Omega} \left(\mathbf{L}\mathbf{N}_g\right)^T \rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \rho^g \mathbf{g} d\Omega \\
&+\int_{\Gamma} \mathbf{N}_g^{\,T} q^{ga} d\Gamma = 0
\end{aligned} \qquad [3.68]
$$

We can rewrite the equation [3.68] as follow:

$$
\mathbf{I}'\overline{\mathbf{p}}^g - \mathbf{H}'\overline{\mathbf{p}}^c - \mathbf{E}'\overline{\mathbf{T}} + \mathbf{S}'\dot{\overline{\mathbf{p}}}^c - \mathbf{T}'\dot{\overline{\mathbf{T}}} + \mathbf{R}'\dot{\overline{\mathbf{u}}} = \mathbf{f}_g \qquad [3.69]
$$

where

$$
\begin{aligned}
&\mathbf{I}' = \int_{\Omega} \left(\mathbf{L}\mathbf{N}_g\right)^T \left(\rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} + \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{p^{gw}}{{p^g}^2} \right) \left(\mathbf{L}\mathbf{N}_g\right) d\Omega \\
&\mathbf{H}' = \int_{\Omega} \left(\mathbf{L}\mathbf{N}_g\right)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial p^c} \left(\mathbf{L}\mathbf{N}_c\right) d\Omega \\
&\mathbf{E}' = \int_{\Omega} \left(\mathbf{L}\mathbf{N}_g\right)^T \rho^g \frac{M_a M_w}{M_g^2} \mathbf{D}_g^{ga} \frac{1}{p^g} \frac{\partial p^{gw}}{\partial T} \left(\mathbf{L}\mathbf{N}_T\right) d\Omega \\
&\mathbf{S}' = -\int_{\Omega} \mathbf{N}_g^{\,T} \rho^{ga} n \frac{\partial S_w}{\partial p^c} \mathbf{N}_c d\Omega \\
&\mathbf{T}' = \int_{\Omega} \mathbf{N}_g^{\,T} \left[\rho^{ga} \beta_s (\alpha - n) S_g + \rho^{ga} n \frac{\partial S_w}{\partial T} \right] \mathbf{N}_T d\Omega \\
&\mathbf{R}' = \int_{\Omega} N_g^{\,T} \alpha \rho^{ga} S_g \mathbf{m}^T \mathbf{L}\mathbf{N}_u d\Omega \\
&\mathbf{f}_g = \int_{\Omega} \left(\mathbf{L}\mathbf{N}_g\right)^T \rho^{ga} \frac{k^{rg}\mathbf{k}}{\mu^g} \rho^g \mathbf{g} d\Omega - \int_{\Gamma} \mathbf{N}_g^{\,T} q^{ga} d\Gamma
\end{aligned} \qquad [3.70]
$$

3.2.6 Enthalpy balance equation of the mixture

Starting from the general equation [2.323]:

$$
\begin{aligned}
&\left(\rho C_p\right)_{eff} \frac{\partial T}{\partial t} - div\left(\chi_{eff}\, gradT\right) \\
&-\Delta H_{vap} div\left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(-gradp^w + \rho^w \mathbf{g}\right) \right]
\end{aligned}
$$

$$+\begin{pmatrix} C_p^w \rho^w n S_w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)+ \\ + nS_g\rho_g C_p^g \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g+\rho^g\mathbf{g}\right) \end{pmatrix}\cdot\nabla T$$

$$-\Delta H_{vap}\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\right]\frac{\partial p^w}{\partial t}$$

$$+\Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t}$$

$$-\Delta H_{vap}\rho^w\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^g}{\partial t}$$

$$-\Delta H_{vap}\rho^w S_w\alpha\mathbf{m}^T\mathbf{L}\frac{\partial\mathbf{u}}{\partial t}$$

$$-\Delta H_{vap}\begin{bmatrix}\rho^w\left(\dfrac{\alpha-n}{K_s}p^wS_w-\dfrac{\alpha-n}{K_s}p^gS_w+n\right)\\ -\rho^{gw}\left(\dfrac{\alpha-n}{K_s}p^cS_g+n\right)\end{bmatrix}\frac{\partial S_w}{\partial t}=0 \qquad [3.\ 71]$$

The boundary conditions for enthalpy balance equation are imposed value and fluxes:

$$T=\overline{T} \qquad \text{on } \Gamma_T \qquad [3.\ 72]$$

$$\begin{bmatrix}\rho^w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)^T\Delta H_{vap}\\ +\chi_{eff}\,grad\,T\end{bmatrix}\cdot\mathbf{n} \qquad [3.\ 73]$$

$$=q^T+\alpha_c(T-T\infty) \qquad \text{on } \Gamma_T^q$$

Applying the integral equation [3.7] to the [3.71] and the above boundary conditions we have:

$$-\int_\Omega \mathbf{W}_T^T div\left(\chi_{eff}\,gradT\right)d\Omega$$

$$-\Delta H_{vap}\int_\Omega \mathbf{W}_T^T div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]d\Omega$$

$$+\int_\Omega \mathbf{W}_T^T\begin{bmatrix} C_p^w \rho^w n S_w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)+ \\ + nS_g\rho_g C_p^g \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-gradp^g+\rho^g\mathbf{g}\right) \end{bmatrix}\cdot gradTd\Omega$$

$$-\Delta H_{vap}\int_\Omega \mathbf{W}_T^T\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\right]\frac{\partial p^w}{\partial t}d\Omega$$

$$-\Delta H_{vap}\int_\Omega \mathbf{W}_T^T\rho^w\frac{\alpha-n}{K_s}S_wS_g\frac{\partial p^g}{\partial t}d\Omega$$

$$
\begin{aligned}
&-\Delta H_{vap}\int_{\Omega}\mathbf{W}_T^T\rho^w S_w\alpha\mathbf{m}^T\mathbf{L}\frac{\partial\mathbf{u}}{\partial t}d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\mathbf{W}_T^T\beta_{sw}\frac{\partial T}{\partial t}d\Omega\\
&+\int_{\Omega}\mathbf{W}_T^T\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t}d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{W}_T^T\begin{bmatrix}\rho^w\left(\dfrac{\alpha-n}{K_s}p^wS_w-\dfrac{\alpha-n}{K_s}p^gS_w+n\right)+\\-\rho^{gw}\left(\dfrac{\alpha-n}{K_s}p^cS_g+n\right)\end{bmatrix}\frac{\partial S_w}{\partial t}d\Omega\\
&+\int_{\Gamma}\overline{\mathbf{W}}_T^T\left\{\begin{matrix}\begin{bmatrix}\rho^w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)^T\Delta H_{vap}+\\-\chi_{eff}\,grad\,T\end{bmatrix}\cdot\mathbf{n}\\-q^T-\alpha_c(T-T\infty)\end{matrix}\right\}d\Gamma=0
\end{aligned}
\qquad [3.\ 74]
$$

It is assume that the weighting functions are:

$$
\begin{aligned}
\mathbf{W}_T&=-\overline{\mathbf{W}}_T &&\text{on }\Gamma_T^q\\
\mathbf{W}_T&=0 &&\text{on }\Gamma_T
\end{aligned}
\qquad [3.\ 75]
$$

Using Green's Theorem [ZT00] the first two terms of [3.74] can be replaced by the following equality:

$$
\begin{aligned}
&-\int_{\Omega}\mathbf{W}_T^T div\left(\chi_{eff}\,grad\,T\right)d\Omega+\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{W}_T^T div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]d\Omega=\\
&=\int_{\Omega}\left(\mathbf{L}\mathbf{W}_T\right)^T\left(\chi_{eff}\,gradT\right)d\Omega+\\
&+\Delta H_{vap}\int_{\Omega}\left(\mathbf{L}\mathbf{W}_T\right)^T\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]d\Omega+\\
&-\int_{\Gamma}\mathbf{W}_T^T div\left(\chi_{eff}\,grad\,T\right)\cdot\mathbf{n}d\Gamma+\\
&-\Delta H_{vap}\int_{\Gamma}\mathbf{W}_T^T div\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]\cdot\mathbf{n}d\Gamma
\end{aligned}
\qquad [3.\ 76]
$$

So the equation [3.74] becomes:

$$
\begin{aligned}
&\int_{\Omega}\left(\mathbf{L}\mathbf{W}_T\right)^T\left(\chi_{eff}\,gradT\right)d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\left(\mathbf{L}\mathbf{W}_T\right)^T\left[\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(-gradp^w+\rho^w\mathbf{g}\right)\right]d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{W}_T^T\left[\rho^w\left(\frac{\alpha-n}{K_s}S_w^2+\frac{nS_w}{K_w}\right)\right]\frac{\partial p^w}{\partial t}d\Omega
\end{aligned}
$$

$$
\begin{aligned}
&+\int_{\Omega} \mathbf{W}_T^T \begin{bmatrix} C_p^w \rho^w n S_w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-\,gradp^w + \rho^w \mathbf{g}\right) + \\ + n S_g \rho_g C_p^g \dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\,gradp^g + \rho^g \mathbf{g}\right) \end{bmatrix} \cdot gradT d\Omega \\
&-\Delta H_{vap} \int_{\Omega} \mathbf{W}_T^T \rho^w \frac{\alpha - n}{K_s} S_w S_g \frac{\partial p^g}{\partial t} d\Omega \\
&-\Delta H_{vap} \int_{\Omega} \mathbf{W}_T^T \rho^w S_w \alpha m^T L \frac{\partial \mathbf{u}}{\partial t} d\Omega \\
&+\Delta H_{vap} \int_{\Omega} \mathbf{W}_T^T \beta_{sw} \frac{\partial T}{\partial t} d\Omega \\
&+\int_{\Omega} \mathbf{W}_T^T \left(\rho C_p\right)_{eff} \frac{\partial T}{\partial t} d\Omega \\
&-\Delta H_{vap} \int_{\Omega} \mathbf{W}_T^T \begin{bmatrix} \rho^w \left(\dfrac{\alpha - n}{K_s} p^w S_w - \dfrac{\alpha - n}{K_s} p^g S_w + n \right) + \\ -\rho^{gw} \left(\dfrac{\alpha - n}{K_s} p^c S_g + n \right) \end{bmatrix} \frac{\partial S_w}{\partial t} d\Omega \\
&+\int_{\Gamma} \mathbf{W}_T^T \left[q^T + \alpha_c (T - T_\infty) \right] d\Gamma = 0
\end{aligned}
\qquad [3.\ 77]
$$

Now the primary variables are expressed by their nodal values and the shape functions

$$
\begin{aligned}
&\mathbf{u} = \mathbf{N}_u \overline{\mathbf{u}} \\
&p^g = \mathbf{N}_g \overline{\mathbf{p}}^g \\
&p^c = \mathbf{N}_c \overline{\mathbf{p}}^c \\
&T = \mathbf{N}_T \overline{\mathbf{T}}
\end{aligned}
\qquad [3.\ 78]
$$

The standard Bubnov-Galerkin procedure [ZT00] is applied replacing the weighting functions by the corresponding shape functions.

$$
\begin{aligned}
&\mathbf{W_g} = \mathbf{N_g} \\
&\mathbf{W_w} = \mathbf{N_w} \\
&\mathbf{W_T} = \mathbf{N_T} \\
&\mathbf{W_u} = \mathbf{N_u}
\end{aligned}
\qquad [3.\ 79]
$$

Substituting the [3. 78] and [3.79] in the [3.77] we arrive at:

$$
\begin{aligned}
&\int_{\Omega} \left(\mathbf{L}\mathbf{N}_T\right)^T \left(\chi_{eff} \mathbf{L}\mathbf{N}_T \overline{\mathbf{T}}\right) d\Omega \\
&+\Delta H_{vap} \int_{\Omega} \left(\mathbf{L}\mathbf{N}_T\right)^T \left[\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w} \left(-\mathbf{L}\left(\mathbf{N}_g \overline{\mathbf{p}}^g - \mathbf{N}_c \overline{\mathbf{p}}^c\right) + \rho^w \mathbf{g} \right) \right] d\Omega \\
&-\Delta H_{vap} \int_{\Omega} \mathbf{N}_T^T \left[\rho^w \left(\frac{\alpha - n}{K_s} S_w^2 + \frac{n S_w}{K_w} \right) \right] \left(\mathbf{N}_g \dot{\overline{\mathbf{p}}}^g - \mathbf{N}_c \dot{\overline{\mathbf{p}}}^c \right) d\Omega
\end{aligned}
$$

$$
\begin{aligned}
&+\int_{\Omega}\mathbf{N}_T^T\begin{bmatrix} C_p^w\rho^w nS_w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(-\mathbf{L}\left(\mathbf{N}_g\overline{\mathbf{p}}^g-\mathbf{N}_c\overline{\mathbf{p}}^c\right)+\rho^w\mathbf{g}\right)\\ +nS_g\rho_g C_p^g\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\mathbf{L}\mathbf{N}_g\overline{\mathbf{p}}^g+\rho^g\mathbf{g}\right)\end{bmatrix}\cdot\mathbf{L}\mathbf{N}_T\overline{\mathbf{T}}d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^w\frac{\alpha-n}{K_s}S_wS_g\mathbf{N}_g\dot{\overline{\mathbf{p}}}^g d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^w S_w\alpha\mathbf{m}^T\mathbf{L}\mathbf{N}_u\dot{\overline{\mathbf{u}}}d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\beta_{sw}\mathbf{N}_T\overline{\mathbf{T}}d\Omega\\
&+\int_{\Omega}\mathbf{N}_T^T\left(\rho C_p\right)_{eff}\mathbf{N}_T\overline{\mathbf{T}}d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^w\left(-\frac{\alpha-n}{K_s}S_w\mathbf{N}_c\overline{\mathbf{p}}^c+n\right)\left(\frac{\partial S_w}{\partial T}\mathbf{N}_T\dot{\overline{\mathbf{T}}}+\frac{\partial S_w}{\partial p^c}\mathbf{N}_c\dot{\overline{\mathbf{p}}}^c\right)d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^{gw}\left(\frac{\alpha-n}{K_s}S_g\mathbf{N}_c\overline{\mathbf{p}}^c+n\right)\left(\frac{\partial S_w}{\partial T}\mathbf{N}_T\dot{\overline{\mathbf{T}}}+\frac{\partial S_w}{\partial p^c}\mathbf{N}_c\dot{\overline{\mathbf{p}}}^c\right)d\Omega\\
&+\int_{\Gamma}\mathbf{N}_T^T\left[q^T+\alpha_c(T-T\infty)\right]d\Gamma=0
\end{aligned}
\qquad [3.\ 80]
$$

With the assumption of incompressible grain at microscopic level $\left(\alpha=1,\dfrac{1}{K_s}=0\right)$, the equation [3.79] becomes:

$$
\begin{aligned}
&-\Delta H_{vap}\int_{\Omega}\left(\mathbf{L}\mathbf{N}_T\right)^T\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(\mathbf{L}\mathbf{N}_g\right)\overline{\mathbf{p}}^g d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\left(\mathbf{L}\mathbf{N}_T\right)^T\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left(\mathbf{L}\mathbf{N}_c\right)\overline{\mathbf{p}}^c d\Omega\\
&+\int_{\Omega}\left\{\begin{array}{l}\mathbf{N}_T^T\begin{bmatrix} nC_p^w\rho^w S_w\dfrac{k^{rw}\mathbf{k}}{\mu^w}\left(\mathbf{L}\mathbf{N}_c\overline{\mathbf{p}}^c-\mathbf{L}\mathbf{N}_g\overline{\mathbf{p}}^g+\mathbf{g}\right)\\ +nS_g\rho_g C_p^g\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left(-\mathbf{L}\mathbf{N}_g\overline{\mathbf{p}}^g+\mathbf{g}\right)\end{bmatrix}\\ +\left(\mathbf{L}\mathbf{N}_T\right)^T\chi_{eff}\end{array}\right\}\cdot\left(\mathbf{L}\mathbf{N}_T\right)\overline{\mathbf{T}}d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^w\frac{nS_w}{K_w}\mathbf{N}_g\dot{\overline{\mathbf{p}}}^g d\Omega\\
&-\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^w S_w\alpha\mathbf{m}^T\mathbf{L}\mathbf{N}_u\dot{\overline{\mathbf{u}}}d\Omega\\
&+\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\left[\rho^w\frac{nS_w}{K_w}+n\left(\rho^{gw}-\rho^w\right)\frac{\partial S_w}{\partial p^c}\right]\mathbf{N}_c\dot{\overline{\mathbf{p}}}^c d\Omega
\end{aligned}
\qquad [3.\ 81]
$$

$$
\begin{aligned}
&+\int_{\Omega}\mathbf{N}_T^T\begin{bmatrix}\Delta H_{vap}\left(\beta_{sw}+n\left(\rho^{gw}-\rho^{w}\right)\dfrac{\partial S_w}{\partial T}\right)\\ +\left(\rho C_p\right)_{eff}\end{bmatrix}\mathbf{N}_T\dot{\overline{\mathbf{T}}}d\Omega\\
&+\int_{\Omega}\left(\mathbf{LN}_T\right)^T\rho^{w}\frac{k^{rw}\mathbf{k}}{\mu^{w}}\rho^{w}\mathbf{g}d\Omega\\
&+\int_{\Gamma}\mathbf{N}_T^T\left[q^T+\alpha_c(T-T_\infty)\right]d\Gamma=0
\end{aligned}
$$

We can rewrite the equation [3.81] in such a way:

$$
\mathbf{K}_{TT}\overline{\mathbf{T}}-\mathbf{K}_{Tg}\overline{\mathbf{p}}^{\mathbf{g}}+\mathbf{K}_{Tc}\overline{\mathbf{p}}^{\mathbf{c}}+\mathbf{C}_{TT}\dot{\overline{\mathbf{T}}}-\mathbf{C}_{Tg}\dot{\overline{\mathbf{p}}}^{\mathbf{g}}+\mathbf{C}_{Tc}\dot{\overline{\mathbf{p}}}^{\mathbf{c}}-\mathbf{C}_{Tu}\dot{\overline{\mathbf{u}}}=\mathbf{f}_T \qquad [3.\ 82]
$$

In above

$$
\begin{aligned}
&\mathbf{C}_{TT}=\int_{\Omega}\mathbf{N}_T^T\begin{bmatrix}\Delta H_{vap}\left(\beta_{sw}+n\left(\rho^{gw}-\rho^{w}\right)\dfrac{\partial S_w}{\partial T}\right)\\ +\left(\rho C_p\right)_{eff}\end{bmatrix}\mathbf{N}_T d\Omega\\
&\mathbf{C}_{Tg}=\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^{w}\frac{nS_w}{K_w}\mathbf{N}_g d\Omega\\
&\mathbf{C}_{Tc}=\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\begin{bmatrix}\rho^{w}\dfrac{nS_w}{K_w}\\ +n\left(\rho^{gw}-\rho^{w}\right)\dfrac{\partial S_w}{\partial p^c}\end{bmatrix}\mathbf{N}_c d\Omega\\
&\mathbf{C}_{Tu}=\Delta H_{vap}\int_{\Omega}\mathbf{N}_T^T\rho^{w}S_w\alpha\mathbf{m}^T\mathbf{LN}_u d\Omega+\\
&\mathbf{K}_{TT}=\int_{\Omega}\left\{\begin{matrix}\mathbf{N}_T^T\left\{\begin{matrix}nC_p^{w}\rho^{w}S_w\dfrac{k^{rw}\mathbf{k}}{\mu^{w}}\left(\mathbf{LN}_c\overline{\mathbf{p}}^{c}-\mathbf{LN}_g\overline{\mathbf{p}}^{g}+\mathbf{g}\right)\\ +nS_g\rho_g C_p^{g}\dfrac{k^{rg}\mathbf{k}}{\mu^{g}}\left(-\mathbf{LN}_g\overline{\mathbf{p}}^{g}+\mathbf{g}\right)\end{matrix}\right\}\\ +\left(\mathbf{LN}_T\right)^T\chi_{eff}\end{matrix}\right\}\cdot\left(grad\mathbf{N}_T\right)d\Omega\\
&\mathbf{K}_{Tg}=\Delta H_{vap}\int_{\Omega}\left(\mathbf{LN}_T\right)^T\rho^{w}\frac{k^{rw}\mathbf{k}}{\mu^{w}}\left(\mathbf{LN}_g\right)d\Omega \qquad [3.\ 83]\\
&\mathbf{K}_{Tc}=\Delta H_{vap}\int_{\Omega}\left(\mathbf{LN}_T\right)^T\rho^{w}\frac{k^{rw}\mathbf{k}}{\mu^{w}}\left(\mathbf{LN}_c\right)d\Omega\\
&\mathbf{f}_T=-\int_{\Omega}\left(\mathbf{LN}_T\right)^T\rho^{w2}\frac{k^{rw}\mathbf{k}}{\mu^{w}}\mathbf{g}d\Omega-\int_{\Gamma}\mathbf{N}_T^T\left[q^T+\alpha_c(T-T_\infty)\right]d\Gamma
\end{aligned}
$$

3.3 Time domain discretization

After the spatial discretization, we obtain a system of four ordinary differential in time equations, resumed in the following system:

$$\begin{cases} \int_{\Omega} \mathbf{B}^{\mathbf{T}} \boldsymbol{\sigma}' d\Omega - \mathbf{Q}\overline{\mathbf{p}}^{g} + \mathbf{R}\overline{\mathbf{p}}^{c} + \mathbf{M}\ddot{\overline{\mathbf{u}}} = \mathbf{f}_{u} \\ \mathbf{U}\dot{\overline{\mathbf{p}}}^{g} + \mathbf{S}\dot{\overline{\mathbf{p}}}^{c} + \mathbf{T}\dot{\overline{\mathbf{T}}} + \mathbf{Q}'\dot{\overline{\mathbf{u}}} - \mathbf{I}\overline{\mathbf{p}}^{g} + \mathbf{H}\overline{\mathbf{p}}^{c} + \mathbf{E}\overline{\mathbf{T}} = \mathbf{f}_{w} \\ \mathbf{I}'\overline{\mathbf{p}}^{g} - \mathbf{H}'\overline{\mathbf{p}}^{c} - \mathbf{E}'\overline{\mathbf{T}} + \mathbf{S}'\dot{\overline{\mathbf{p}}}^{c} - \mathbf{T}'\dot{\overline{\mathbf{T}}} + \mathbf{R}'\dot{\overline{\mathbf{u}}} = \mathbf{f}_{g} \\ \mathbf{K}_{TT}\overline{\mathbf{T}} - \mathbf{K}_{Tg}\overline{\mathbf{p}}^{g} + \mathbf{K}_{Tc}\overline{\mathbf{p}}^{c} + \mathbf{C}_{TT}\dot{\overline{\mathbf{T}}} - \mathbf{C}_{Tg}\dot{\overline{\mathbf{p}}}^{g} + \mathbf{C}_{Tc}\dot{\overline{\mathbf{p}}}^{c} - \mathbf{C}_{Tu}\dot{\overline{\mathbf{u}}} = \mathbf{f}_{T} \end{cases} \qquad [3.\ 84]$$

We can notice that:

- the order of time differentiation for the variables is different: first and second order

- the equations are coupled

- the equations are non linear

We use the implicit Generalized Newmark scheme as a direct solution procedure for time discretization. The Newton's method is used to obtain iterative convergence to solve the non-linear set of algebric equations [ZT00].

Firstly it is assumed that the differential equation are to be satisfied at each discrete time station. For the equation sistem [3.84] we can write:

$$\begin{cases} \mathbf{M}^{n+1}\ddot{\overline{\mathbf{u}}}^{n+1} + \left[\int_{\Omega} \mathbf{B}^{\mathbf{T}} \boldsymbol{\sigma}' d\Omega \right]^{n+1} - \mathbf{Q}^{n+1}\overline{\mathbf{p}}^{\mathbf{g}^{n+1}} + \mathbf{R}^{n+1}\overline{\mathbf{p}}^{\mathbf{c}^{n+1}} = \mathbf{f}_{u}^{\ n+1} \\ \\ \mathbf{U}^{n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{g}^{n+1}} + \mathbf{S}^{n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{c}^{n+1}} + \mathbf{T}^{n+1}\dot{\overline{\mathbf{T}}}^{n+1} + \mathbf{Q}'^{n+1}\dot{\overline{\mathbf{u}}}^{n+1} \\ - \mathbf{I}^{n+1}\overline{\mathbf{p}}^{\mathbf{g}^{n+1}} + \mathbf{H}^{n+1}\overline{\mathbf{p}}^{\mathbf{c}^{n+1}} + \mathbf{E}^{n+1}\overline{\mathbf{T}}^{n+1} = \mathbf{f}_{w}^{\ n+1} \\ \\ \mathbf{U}'^{n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{g}^{n+1}} + \mathbf{S}'^{n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{c}^{n+1}} + \mathbf{T}'^{n+1}\dot{\overline{\mathbf{T}}}^{n+1} + \mathbf{R}'^{\mathbf{T},n+1}\dot{\overline{\mathbf{u}}}^{n+1} \\ + \mathbf{I}'^{n+1}\overline{\mathbf{p}}^{\mathbf{g}^{n+1}} - \mathbf{H}'^{n+1}\overline{\mathbf{p}}^{\mathbf{c}^{n+1}} - \mathbf{E}'^{n+1}\overline{\mathbf{T}}^{n+1} = \mathbf{f}_{g}^{\ n+1} \\ \\ \mathbf{C}_{TT}^{\ n+1}\dot{\overline{\mathbf{T}}}^{n+1} - \mathbf{C}_{Tg}^{\ n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{g}^{n+1}} - \mathbf{C}_{Tc}^{\ n+1}\dot{\overline{\mathbf{p}}}^{\mathbf{c}^{n+1}} - \mathbf{C}_{Tu}^{\ n+1}\dot{\overline{\mathbf{u}}}^{n+1} \\ - \mathbf{K}_{Tg}^{\ n+1}\overline{\mathbf{p}}^{\mathbf{g}^{n+1}} + \mathbf{K}_{Tc}^{\ n+1}\overline{\mathbf{p}}^{\mathbf{c}^{n+1}} + \mathbf{K}_{TT}^{\ n+1}\overline{\mathbf{T}}^{n+1} = \mathbf{f}_{T}^{\ n+1} \end{cases} \qquad [3.\ 85]$$

Secondly the link between the successive values at t_{n+1} and t_{n} can be established by truncated series expansions [ZT00, page 515]:

$$\begin{aligned}
&\dot{\overline{\mathbf{u}}}^{n+1} = \dot{\overline{\mathbf{u}}}^{n} + \Delta t\ddot{\overline{\mathbf{u}}}^{n} + \beta_1 \Delta t \Delta \ddot{\overline{\mathbf{u}}}^{n} \\
&\overline{\mathbf{u}}^{n+1} = \overline{\mathbf{u}}^{n} + \Delta t\dot{\overline{\mathbf{u}}}^{n} + \frac{1}{2}\Delta\Delta t^2\ddot{\overline{\mathbf{u}}}^{n} + \frac{1}{2}\beta_2 \Delta t^2 \Delta \ddot{\overline{\mathbf{u}}}^{n} \\
&\overline{\mathbf{T}}^{n+1} = \overline{\mathbf{T}}^{n} + \Delta t\dot{\overline{\mathbf{T}}}^{n} + \alpha \Delta t \Delta \dot{\overline{\mathbf{T}}}^{n} \\
&\overline{\mathbf{p}}^{c^{n+1}} = \overline{\mathbf{p}}^{c^{n}} + \Delta t\dot{\overline{\mathbf{p}}}^{c^{n}} + \vartheta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{c^{n}} \\
&\overline{\mathbf{p}}^{g^{n+1}} = \overline{\mathbf{p}}^{g^{n}} + \Delta t\dot{\overline{\mathbf{p}}}^{g^{n}} + \theta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{g^{n}}
\end{aligned} \qquad [3.\ 86]$$

where

$$\begin{aligned}
&\Delta \ddot{\overline{\mathbf{u}}}^{n} = \ddot{\overline{\mathbf{u}}}^{n+1} - \ddot{\overline{\mathbf{u}}}^{n} \\
&\Delta \dot{\overline{\mathbf{T}}}^{n} = \dot{\overline{\mathbf{T}}}^{n+1} - \dot{\overline{\mathbf{T}}}^{n} \\
&\Delta \dot{\overline{\mathbf{p}}}^{c^{n}} = \dot{\overline{\mathbf{p}}}^{c^{n+1}} - \dot{\overline{\mathbf{p}}}^{c^{n}} \\
&\Delta \dot{\overline{\mathbf{p}}}^{g^{n}} = \dot{\overline{\mathbf{p}}}^{g^{n+1}} - \dot{\overline{\mathbf{p}}}^{g^{n}}
\end{aligned} \qquad [3.\ 87]$$

are the undetermined quantities and $\beta_1, \beta_2, \alpha, \vartheta, \theta$ are parameters chosen in the range $0 \div 1$.

For the unconditional stability of the direct solution procedure it is required that:

$$\frac{1}{2} \le \beta_1 \le \beta_2 \qquad \frac{1}{2} \le \beta_1, \alpha, \vartheta, \theta \le 1 \qquad [3.\ 88]$$

see [Ch88] and [ZT00]. However, stability of the time integration does not ensure sufficent accurancy of the solution. To obtain an accurate solution Δt should be chosen corresponding to the smallest period in the loading pulse [Sl92]. The time step can be adjusted to the size of the finite elements. If the size of the elements is chosen corresponding to the wave lengths of the load a critical time step can be derived.

With the insertion of the series expansions [3.86] in the system [3.85], we obtain four general non linear equations in which only $\Delta \ddot{\overline{\mathbf{u}}}^{n}, \Delta \dot{\overline{\mathbf{T}}}^{n}, \Delta \dot{\overline{\mathbf{p}}}^{c^{n}}, \Delta \dot{\overline{\mathbf{p}}}^{g^{n}}$ remain unknowns:

$$\begin{aligned}
&\mathbf{M}^{n+1}\Delta \ddot{\overline{\mathbf{u}}}^{n} + \left[\int_{\Omega} \mathbf{B}^{\mathrm{T}}\boldsymbol{\sigma}' d\Omega\right]^{n+1} - \mathbf{Q}^{n+1}\theta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{g^{n}} + \mathbf{R}^{n+1}\vartheta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{c^{n}} = \mathbf{f}_u^{\;n+1} \\
\\
&\mathbf{U}^{n+1}\Delta \dot{\overline{\mathbf{p}}}^{g^{n}} + \mathbf{S}^{n+1}\Delta \dot{\overline{\mathbf{p}}}^{c^{n}} + \mathbf{T}^{n+1}\Delta \dot{\overline{\mathbf{T}}}^{n} + \mathbf{Q}'^{n+1}\beta_1 \Delta t \Delta \ddot{\overline{\mathbf{u}}}^{n} + \\
&- \mathbf{I}^{n+1}\theta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{g^{n}} + \mathbf{H}^{n+1}\vartheta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{c^{n}} + \mathbf{E}^{n+1}\alpha \Delta t \Delta \dot{\overline{\mathbf{T}}}^{n} = \mathbf{f}_w^{\;n+1} \\
\\
&\mathbf{U}'^{n+1}\Delta \dot{\overline{\mathbf{p}}}^{g^{n}} + \mathbf{S}'^{n+1}\Delta \dot{\overline{\mathbf{p}}}^{c^{n}} - \mathbf{T}'^{n+1}\Delta \dot{\overline{\mathbf{T}}}^{n} + \mathbf{R}'^{\mathrm{T},n+1}\beta_1 \Delta t \Delta \ddot{\overline{\mathbf{u}}}^{n} + \\
&+ \mathbf{I}'^{n+1}\theta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{g^{n}} - \mathbf{H}'^{n+1}\vartheta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{c^{n}} - \mathbf{E}'^{n+1}\alpha \Delta t \Delta \dot{\overline{\mathbf{T}}}^{n} = \mathbf{f}_g^{\;n+1} \\
\\
&- \mathbf{C}_{Tg}^{\;n+1}\Delta \dot{\overline{\mathbf{p}}}^{g^{n}} - \mathbf{C}_{Tc}^{\;n+1}\Delta \dot{\overline{\mathbf{p}}}^{c^{n}} + \mathbf{C}_{TT}^{\;n+1}\Delta \dot{\overline{\mathbf{T}}}^{n} - \mathbf{C}_{Tu}^{\;n+1}\beta_1 \Delta t \Delta \ddot{\overline{\mathbf{u}}}^{n} + \\
&+ \mathbf{K}_{Tg}^{\;n+1}\theta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{g^{n}} + \mathbf{K}_{Tc}^{\;n+1}\vartheta \Delta t \Delta \dot{\overline{\mathbf{p}}}^{c^{n}} + \mathbf{K}_{TT}^{\;n+1}\alpha \Delta t \Delta \dot{\overline{\mathbf{T}}}^{n} = \mathbf{f}_T^{\;n+1}
\end{aligned} \qquad [3.\ 89]$$

This can be written as:

$$
\begin{aligned}
&\mathbf{G}_u^{n+1} = \mathbf{M}^{n+1}\varDelta\ddot{\bar{\mathbf{u}}}^n + \left[\int_\Omega \mathbf{B}^{\mathbf{T}}\boldsymbol{\sigma}' d\varOmega\right]^{n+1} - \mathbf{Q}^{n+1}\theta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} + \mathbf{R}^{n+1}\vartheta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} - \mathbf{F}_u^{\ n+1} \\
&\mathbf{G}_w^{n+1} = \begin{pmatrix} -\mathbf{I}^{n+1}\theta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} + \mathbf{H}^{n+1}\vartheta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} + \mathbf{E}^{n+1}\alpha\varDelta t\varDelta\dot{\bar{\mathbf{T}}}^n + \mathbf{U}^{n+1}\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} + \\ + \mathbf{S}^{n+1}\vartheta\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} + \mathbf{T}^{n+1}\varDelta\dot{\bar{\mathbf{T}}}^n + \mathbf{Q}'^{n+1}\beta_1\varDelta t\varDelta\ddot{\bar{\mathbf{u}}}^n - \mathbf{F}_w^{\ n+1} \end{pmatrix} \\
&\mathbf{G}_g^{n+1} = \begin{pmatrix} \mathbf{I}'^{n+1}\theta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} - \mathbf{H}'^{n+1}\vartheta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} - \mathbf{E}'^{n+1}\alpha\varDelta t\varDelta\dot{\bar{\mathbf{T}}}^n + \mathbf{U}'^{n+1}\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} + \\ + \mathbf{S}'^{n+1}\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} - \mathbf{T}'^{n+1}\varDelta\dot{\bar{\mathbf{T}}}^n + \mathbf{R}'^{\mathbf{T},n+1}\beta_1\varDelta t\varDelta\ddot{\bar{\mathbf{u}}}^n - \mathbf{F}_g^{\ n+1} \end{pmatrix} \\
&\mathbf{G}_T^{n+1} = \begin{pmatrix} \mathbf{K}_{Tg}^{\ \ n+1}\theta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} + \mathbf{K}_{Tc}^{\ \ n+1}\vartheta\varDelta t\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} + \mathbf{K}_{TT}^{\ \ n+1}\alpha\varDelta t\varDelta\dot{\bar{\mathbf{T}}}^n + \\ - \mathbf{C}_{Tg}^{\ \ n+1}\varDelta\dot{\bar{\mathbf{p}}}^{g\,n} - \mathbf{C}_{Tc}^{\ \ n+1}\varDelta\dot{\bar{\mathbf{p}}}^{c\,n} + \mathbf{C}_{TT}^{\ \ n+1}\varDelta\dot{\bar{\mathbf{T}}}^n - \mathbf{C}_{Tu}^{\ \ n+1}\beta_1\varDelta t\varDelta\ddot{\bar{\mathbf{u}}}^n - \mathbf{F}_T^{\ n+1} \end{pmatrix}
\end{aligned}
\tag{3. 90}
$$

in above

$$
\begin{aligned}
&\mathbf{F}_{\mathbf{u}}^{\ n+1} = -\mathbf{M}^{n+1}\ddot{\bar{\mathbf{u}}}^n + \mathbf{Q}^{n+1}\left(\bar{\mathbf{p}}^{g\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{g\,n}\right) + \mathbf{R}^{n+1}\left(\bar{\mathbf{p}}^{c\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{c\,n}\right) + \mathbf{f}_u^{\ n+1} \\
&\mathbf{F}_w^{\ n+1} = \mathbf{I}^{n+1}\left(\bar{\mathbf{p}}^{g\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{g\,n}\right) - \mathbf{H}^{n+1}\left(\bar{\mathbf{p}}^{c\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{c\,n}\right) - \mathbf{E}^{n+1}\left(\bar{\mathbf{T}}^n + \varDelta t\dot{\bar{\mathbf{T}}}^n\right) + \\
&- \mathbf{U}^{n+1}\dot{\bar{\mathbf{p}}}^g - \mathbf{S}^{n+1}\dot{\bar{\mathbf{p}}}^{c\,n} - \mathbf{T}^{n+1}\dot{\bar{\mathbf{T}}}^n - \mathbf{Q}'^{n+1}\left(\dot{\bar{\mathbf{u}}}^n + \varDelta t\ddot{\bar{\mathbf{u}}}^n\right) + \mathbf{f}_w^{\ n+1} \\
&\mathbf{F}_{\mathbf{g}}^{\ n+1} = -\mathbf{I}'^{n+1}\left(\bar{\mathbf{p}}^{g\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{g\,n}\right) + \mathbf{H}'^{n+1}\left(\bar{\mathbf{p}}^{c\,n} + \Delta t\dot{\bar{\mathbf{p}}}^{c\,n}\right) + \mathbf{E}'^{n+1}\left(\bar{\mathbf{T}}^n + \Delta t\dot{\bar{\mathbf{T}}}^n\right) + \\
&- \mathbf{U}'^{n+1}\dot{\bar{\mathbf{p}}}^g - \mathbf{S}'^{n+1}\dot{\bar{\mathbf{p}}}^{c\,n} + \mathbf{T}'^{n+1}\dot{\bar{\mathbf{T}}}^n - \mathbf{R}'^{\mathbf{T},n+1}\left(\dot{\bar{\mathbf{u}}}^n + \varDelta t\ddot{\bar{\mathbf{u}}}^n\right) + \mathbf{f}_g^{\ n+1} \\
&\mathbf{F}_{\mathbf{T}}^{\ n+1} = -\mathbf{K}_{Tg}^{\ \ n+1}\left(\bar{\mathbf{p}}^{g\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{g\,n}\right) - \mathbf{K}_{Tc}^{\ \ n+1}\left(\bar{\mathbf{p}}^{c\,n} + \varDelta t\dot{\bar{\mathbf{p}}}^{c\,n}\right) - \mathbf{K}_{TT}^{\ \ n+1}\left(\bar{\mathbf{T}}^n + \varDelta t\dot{\bar{\mathbf{T}}}^n\right) + \\
&+ \mathbf{C}_{Tg}^{\ \ n+1}\dot{\bar{\mathbf{p}}}^{g\,n} + \mathbf{C}_{cg}^{\ \ n+1}\dot{\bar{\mathbf{p}}}^{c\,n} - \mathbf{C}_{TT}^{\ \ n+1}\dot{\bar{\mathbf{T}}}^n - \mathbf{C}_{cu}^{\ \ n+1}\left(\dot{\bar{\mathbf{u}}}^n + \varDelta t\ddot{\bar{\mathbf{u}}}^n\right) + \mathbf{f}_T^{\ n+1}
\end{aligned}
\tag{3. 91}
$$

and

$$
\begin{aligned}
&\mathbf{P}\left(\bar{\mathbf{u}}^{n+1}\right) = \left[\int_\Omega \mathbf{B}^{\mathbf{T}}\boldsymbol{\sigma}' d\varOmega\right]^{n+1} = \\
&= \int_\Omega \mathbf{B}^{\mathbf{T}}\boldsymbol{\sigma}'_{n+1} d\varOmega = \\
&= \int_\Omega \mathbf{B}^{\mathbf{T}}\varDelta\boldsymbol{\sigma}'_n d\varOmega + \mathbf{P}\left(\bar{\mathbf{u}}^n\right)
\end{aligned}
\tag{3. 92}
$$

where $\varDelta\boldsymbol{\sigma}'_n$ is evaluated by integrating the incremental constitutive relation.

3.4 Solution strategy for the nonlinear equation

The coupled equation system is non-linear and it requires linearising by an iterative Newton-Raphson procedure. It can be written in compact way as:

$$\mathbf{G}(\mathbf{x})=\mathbf{0} \qquad [3.\ 93]$$

with

$$\mathbf{x}=\begin{Bmatrix} \Delta\ddot{\mathbf{u}} \\ \Delta\dot{\mathbf{p}}_c \\ \Delta\dot{\mathbf{p}}_g \\ \Delta\dot{\mathbf{T}} \end{Bmatrix} \qquad [3.\ 94]$$

the vector of the unknown, and

$$\mathbf{G}=\begin{Bmatrix} \mathbf{G}^u \\ \mathbf{G}^w \\ \mathbf{G}^g \\ \mathbf{G}^T \end{Bmatrix}$$

At each time step the equations need to be solved by an iterative process until some prescribed tolerance is reached.

Assuming that the solution of i^{th} iteration $\mathbf{x}_i$ is known, we seek:

$$\mathbf{x}_{i+1}=\mathbf{x}_i+d\mathbf{x}_i \qquad [3.\ 95]$$

which satisfies

$$\mathbf{G}(\mathbf{x}_{i+1})=\mathbf{0} \qquad [3.\ 96]$$

Expanding in Taylor series and neglecting the second order terms, it gives that:

$$\mathbf{G}(\mathbf{x}_{i+1})\cong\mathbf{G}(\mathbf{x}_i)+\left.\frac{\partial\mathbf{G}}{\partial\mathbf{x}}\right|_{x=x_i} d\mathbf{x}_i\cong 0 \qquad [3.\ 97]$$

or

$$\mathbf{J}d\mathbf{x}_i=-\mathbf{G}(\mathbf{x}_i) \qquad [3.\ 98]$$

with

$$\mathbf{J}=\left.\frac{\partial\mathbf{G}}{\partial\mathbf{x}}\right|_{x=x_i} \text{ the Jacobian matrix} \qquad [3.\ 99]$$

so according to this scheme:

$$\left.\mathbf{J}\right|_{\mathbf{x}_{n+1}^{i}} d\mathbf{x}_{n+1}^{i+1}=-\mathbf{G}\left(\mathbf{x}_{n+1}^{i}\right) \qquad [3.\ 100]$$

that means:

$$[\mathbf{J}]_{n+1,i}\begin{Bmatrix} d\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}\right)_n \\ d\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}_c\right)_n \\ d\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}_g\right)_n \\ d\left(\mathit{\Delta}\dot{\bar{\mathbf{T}}}\right)_n \end{Bmatrix}_{i+1} = -\begin{Bmatrix} G^u_{n+1} \\ G^w_{n+1} \\ G^g_{n+1} \\ G^T_{n+1} \end{Bmatrix}_i \qquad [3.\ 101]$$

where the Jacobian matrix at n+1 step and i^{th} iteration is represented as:

$$\mathbf{J}^i_{n+1} = \begin{bmatrix} \frac{\partial \mathbf{G}_g}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^g\right)} & \frac{\partial \mathbf{G}_g}{\partial\left(v\dot{\bar{\mathbf{p}}}^c\right)} & \frac{\partial \mathbf{G}_g}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{T}}}\right)} & \frac{\partial \mathbf{G}_g}{\partial\left(v\ddot{\bar{\mathbf{u}}}_x\right)} & \frac{\partial \mathbf{G}_g}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_y\right)} \\ \frac{\partial \mathbf{G}_w}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^g\right)} & \frac{\partial \mathbf{G}_w}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^c\right)} & \frac{\partial \mathbf{G}_w}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{T}}}\right)} & \frac{\partial \mathbf{G}_w}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_x\right)} & \frac{\partial \mathbf{G}_w}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_y\right)} \\ \frac{\partial \mathbf{G}_T}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^g\right)} & \frac{\partial \mathbf{G}_T}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^c\right)} & \frac{\partial \mathbf{G}_T}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{T}}}\right)} & \frac{\partial \mathbf{G}_T}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_x\right)} & \frac{\partial \mathbf{G}_T}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_y\right)} \\ \frac{\partial \mathbf{G}_{u_X}}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^g\right)} & \frac{\partial \mathbf{G}_{u_X}}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^c\right)} & \frac{\partial \mathbf{G}_{u_X}}{\partial\left(\mathit{\Delta}\Delta\dot{\bar{\mathbf{T}}}\right)} & \frac{\partial \mathbf{G}_{u_X}}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_x\right)} & \frac{\partial \mathbf{G}_{u_X}}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_y\right)} \\ \frac{\partial \mathbf{G}_{u_Y}}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^g\right)} & \frac{\partial \mathbf{G}_{u_Y}}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{p}}}^c\right)} & \frac{\partial \mathbf{G}_{u_Y}}{\partial\left(\mathit{\Delta}\dot{\bar{\mathbf{T}}}\right)} & \frac{\partial \mathbf{G}_{u_Y}}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_x\right)} & \frac{\partial \mathbf{G}_{u_Y}}{\partial\left(\mathit{\Delta}\ddot{\bar{\mathbf{u}}}_y\right)} \end{bmatrix} \qquad [3.\ 102]$$

and the residual vector at n+1 step and $i+1$ iteration is:

$$-\mathbf{G}(\mathbf{x}_i) = -\begin{bmatrix} \mathbf{G}^{\;i}_{w\,n+1} \\ \mathbf{G}^{\;i}_{g\,n+1} \\ \mathbf{G}^{\;i}_{T\,n+1} \\ \mathbf{G}^{\;i}_{u_x\,n+1} \\ \mathbf{G}^{\;i}_{u_y\,n+1} \end{bmatrix} \qquad [3.\ 103]$$

In this thesis the classical Newton method [ZT00] is used so the Jacobian matrix is update at each step of the iterative process.

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NUMERICAL SOLUTIONS

4.1 Introduction

In this fourth chapter the numerical validation of the model derived in the previous chapters and implemented in the finite element code Comes-Geo [GS96], [LS98], [SPS6] is presented.

Different examples from literature are analyzed in order to consider separately the different phase and then their coupling. Some difficulties arise, since no exact solutions of simple problems are available, especially for non-isothermal problems or partially saturated problems in dynamics.

As regards the validation of the solid phase model in isothermal conditions, a wave propagation problem in a single phase solid bar [Sl92] is investigated and the finite element results are compared with the analytical solution and the numerical solution of a commercial finite element code. Another test performed is a wave propagation problem in a dry soil column subjected to a step load and the finite element results are compared with those obtained by Schrefler and Scotta [SS98].

For the validation of the isothermal water saturated model, a dynamic consolidation problem is considered, following Markert [Ma10].

For the non-isothermal water saturated model, a quasi-static fully saturated non-isothermal mechanical consolidation problem is analyzed, (Aboustit test), [Ab85].

The validation of the isothermal partially saturated model is performed by solving the Liakopoulos test [Lia65], in which a quasi-static drainage of liquid water from a initially water saturated soil column is analyzed.

Another test performed in this thesis is the simulation of an isothermal wave propagation problem in an initially unsaturated soil column subjected to a step load following Schrefler and Scotta [SS98].

4.2 Numerical validation of the model for isothermal single phase solids

4.2.1 Wave propagation in a solid bar

The aim of this test is to verify the model for isothermal single phase solids. The problem is solved with the multiphase model by setting α_{Biot}=0, for which the equations result uncoupled. A one-dimensional bar is analyzed (Poisson's coefficient ν=0), fixed at the left side [Sl92]. A uniform load, constant in time, is applied at the free right side of the bar, causing a wave load which propagates through the bar and reflects at the left boundary.

This longitudinal wave propagation problem, its geometry with the boundary and loading conditions are illustrated in Figure 4.1.

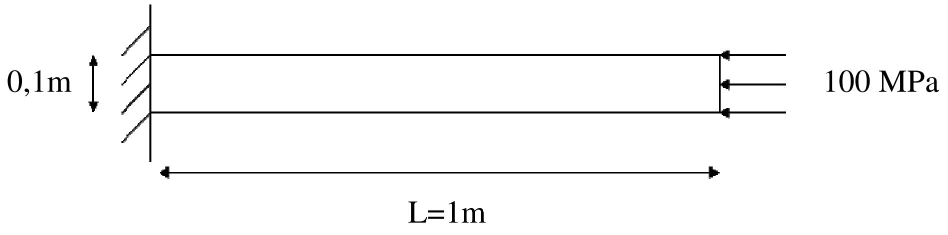

Figure 4. 1: *Geometry, boundary and loading condition.*

The material parameters of the elastic analysis used for the problem are listed in the following Table 4.1.

Parameters		Value	SI unit
Young's Modulus	E	210	GPa
Poisson's Modulus	ν	0	-
Porosiy	n	0	-
Density of the solid	ρ	7860	kg/m^3

Table 4. 1: *Material parameters for the elastic analysis used for the example problem.*

The time step used in the computation is of 1E-5 seconds and the finite element discretization, composed of ten four-node elements, is illustrated in Figure 4.2.

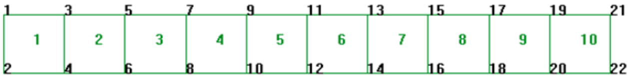

Figure 4. 2: *Finite element discretization of the bar: ten four-nodes isoparametric elements.*

This problem is described by the classical equation of plane waves (a partial differential equation of the second order, linear and homogeneous, hyperbolic type) in one dimension:

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0 \qquad [4.\ 1]$$

where c is the longitudinal wave velocity. The general solution is a linear combination of two solutions:

$$u(x,t) = u_1(x - ct) + u_2(x + ct) \qquad [4.\ 2]$$

that are two disturbances that propagate in opposite directions.

The solution is given by:

$$u(x,t) = ACos(-\frac{2\pi}{T}t) \qquad [4.\ 3]$$

where A is the amplitude and T is the period of the wave.

The following characteristics of the problem can be computed:

- Axial displacement (steady state solution)

$$\Delta L = \varepsilon_x L = \frac{\sigma_x}{E}L = \frac{100E6}{210E9}1 = 4{,}76E - 4m = 0{,}47mm \qquad [4.\ 4]$$

- Linear elastic longitudinal wave velocity

$$c = \sqrt{\frac{E}{\rho}} = \sqrt{\frac{210E9}{7860}} = 5044\frac{m}{s} \qquad [4.\ 5]$$

- Period of the wave

$$T = \frac{4L}{c} = \frac{4}{5044} = 7{,}93E - 4s \qquad [4.\ 6]$$

In Figure 4.3 is plotted the finite element solution of the horizontal displacement of the free side of the bar, where we can see that the analytical values of the deformation ΔL [4.4] and of the period T [4.6] are captured.

If the analysis continues for a longer time, the steady state solution is reached for the displacement at the free side of the bar, as plotted in Figure 4.4.

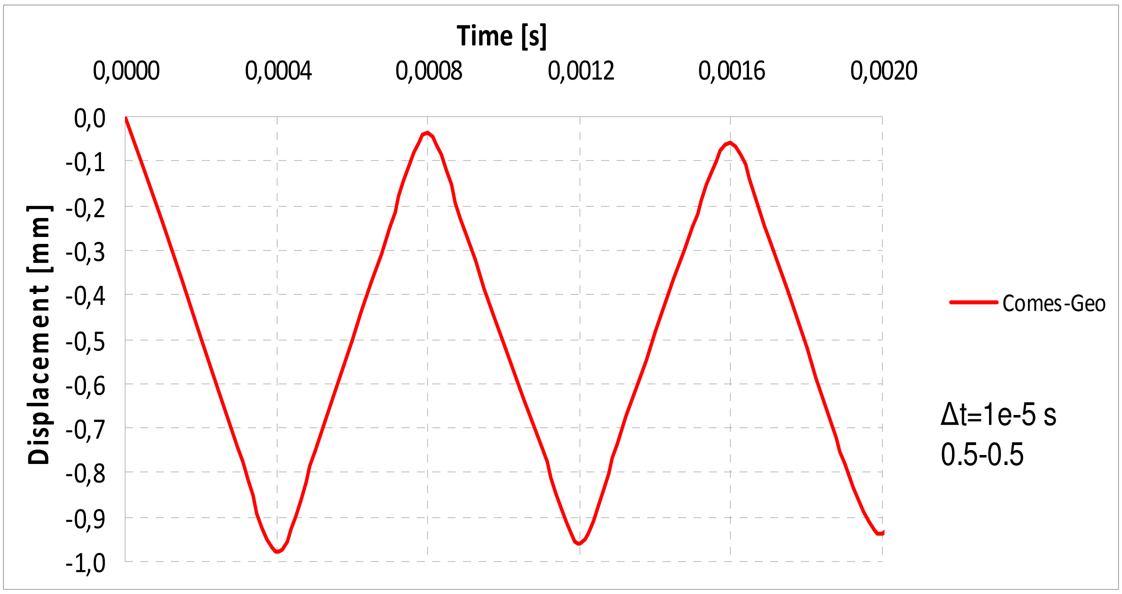

Figure 4. 3: *Displacement of the free side of the bar obtained with the dynamic model. The value of time integration parameters are:* $\beta_2, \beta_1, \alpha, \vartheta, \theta = 0{,}5$ *and the time step is* $\Delta t = 1E-5s$.

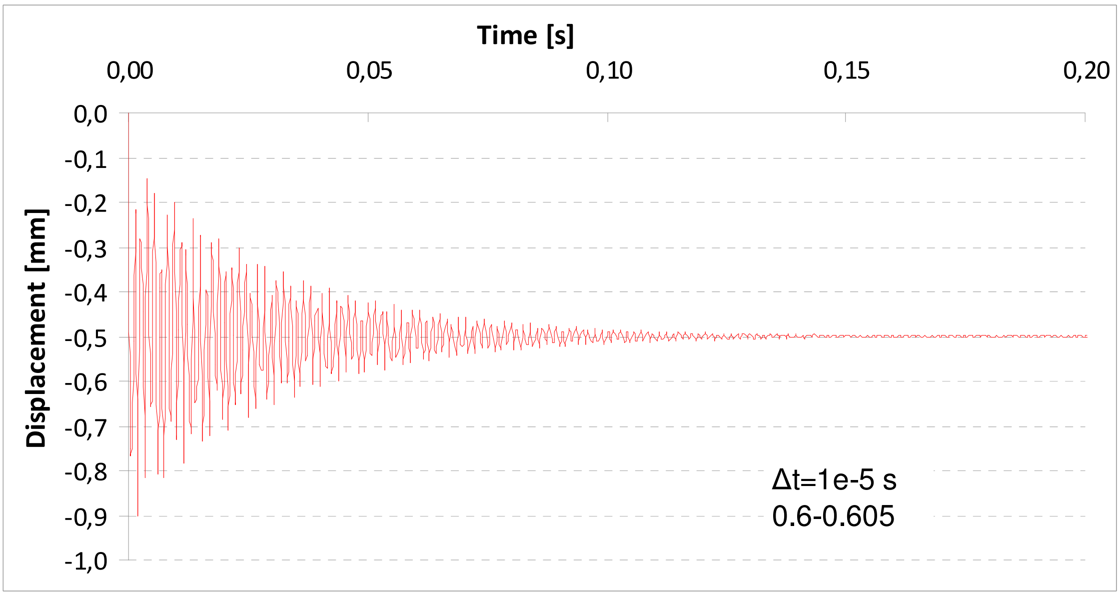

Figure 4. 4: *Displacement time history at the free side of the bar obtained with the dynamic model. The value of time integration parameters are:* $\beta_2 = 0{,}605$ *and* $\beta_1, \alpha, \vartheta, \theta = 0{,}6$ *and the time step is* $\Delta t = 1E-5s$.

The finite element solution from the dynamic formulation of Comes-Geo is compared with the analytical solution for plane waves [4.3] and the numerical solution of the commercial finite element code “Straus” [Str7]. In this case the analysis β_{Newmark}

coefficient was set to 0,5 and the dumping term in the equation of the motion was neglected. As we can see in Figure 4.5, the period T and the mean value of the displacement are equal in all the analysis, while the numerical dumping of the solution is a bit different even if the three solutions are similar.

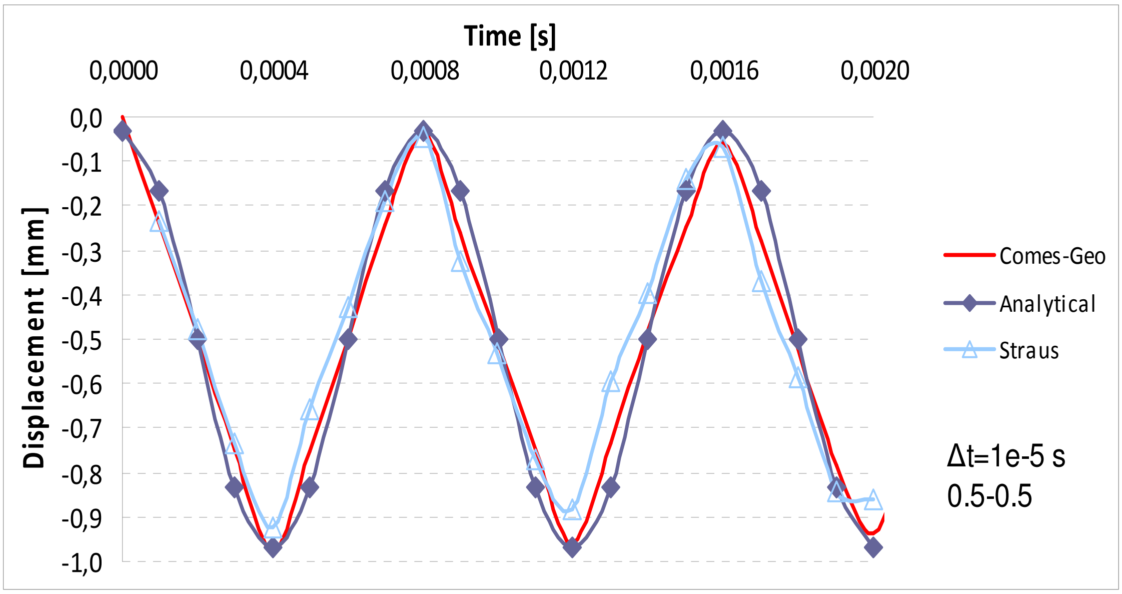

Figure 4. 5: *Comparison between Comes-Geo solution, the analytical solution and the solution of the commercial code Straus. The value of time integration parameters are:* $\beta_2, \beta_1, \alpha, \vartheta, \theta = 0.5$ *and the time step is* $\Delta t = 1E-5s$.

For the study of numerical damping, in Figure 4.6 there is the comparison between the displacement of the free side of the bar obtained with different time integration parameters. As expected, the numerical dumping is higher when time integration parameters are higher.

As regards the numerical accuracy, it is higher when the time step are smaller and we can see this in Figure 4.7, where there is the comparison between the analysis performed with different time step.

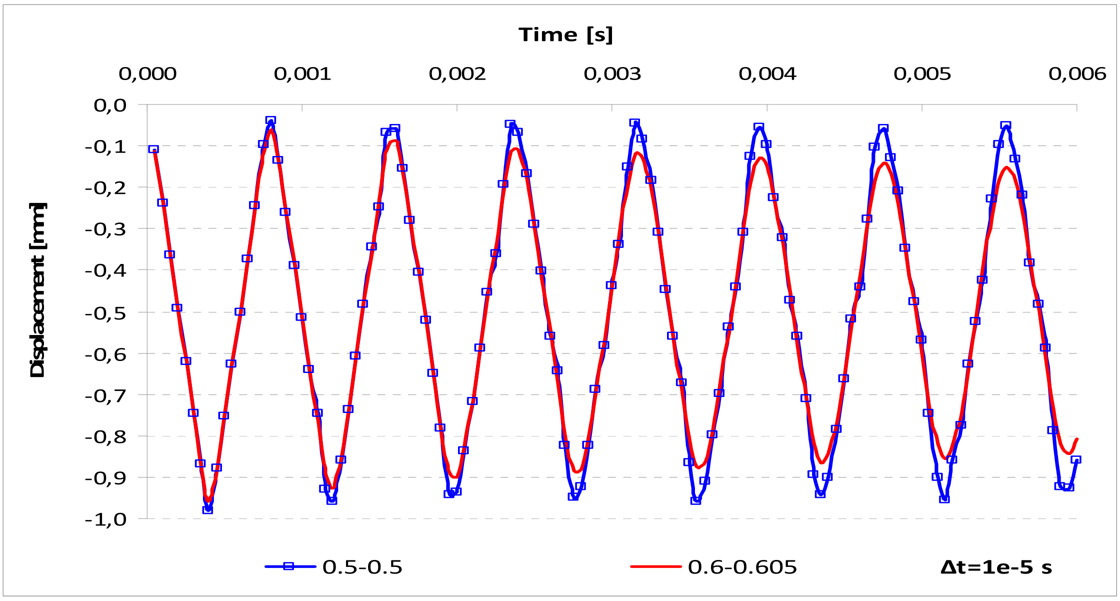

Figure 4. 6: *Displacement of the free side of the bar: comparison between analysis performed with different time integration parameters.*

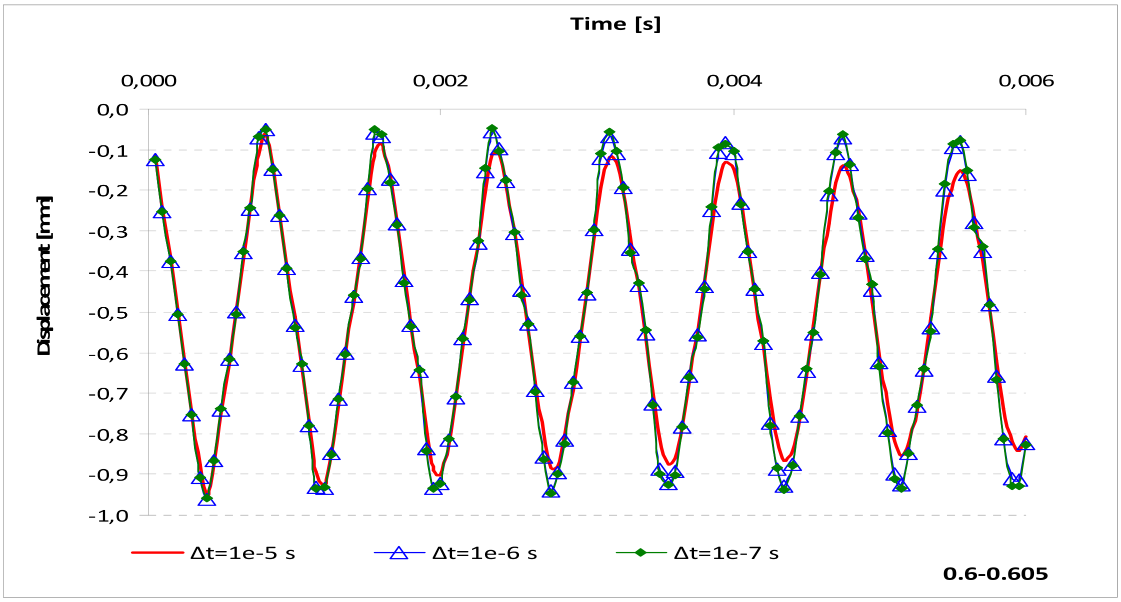

Figure 4. 7: *Displacement time history of the free side of the bar: comparison between analysis performed with different value of time step.*

4.2.2 Wave propagation problem in a dry soil column

This example deals with the dynamic behaviour of a dry sand column to which a step load is applied, as proposed by Schrefler and Scotta [SS98]. A load of 0,1 MPa is applied at the top of the column and then removed after 1 s. The column is 10m high and 1m wide and is discretized by eight-node isoparametric elements (with nine Gauss points integration) see Figure 4.8. The material parameters are summarised in Table 4.2.

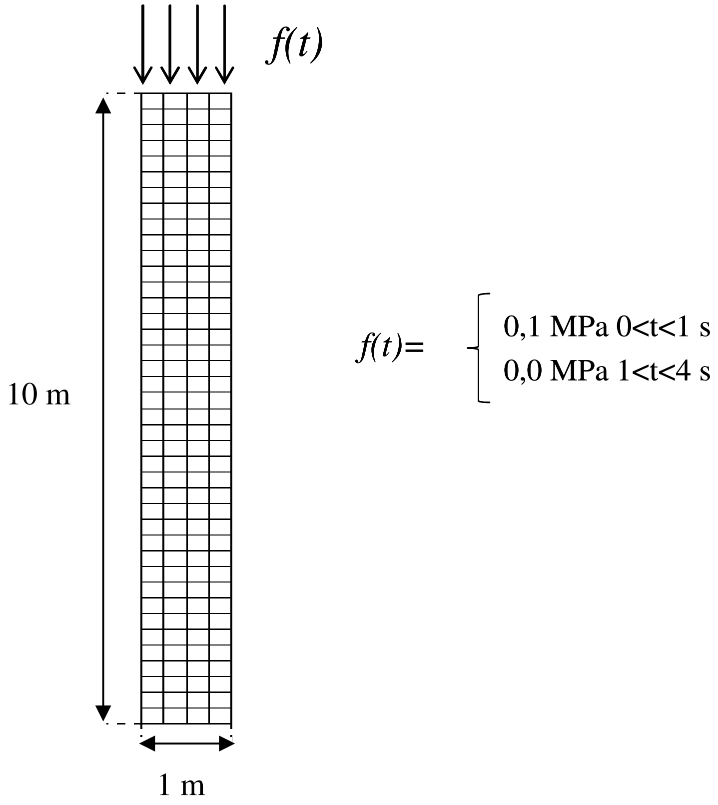

Figure 4. 8: *Geometry and loading conditions of the confined compression of a dry soil column.*

Parameters		Value	SI unit
Porosity	n	0,3	-
Solid skeleton density	ρ_s	2000	kg/m^3
Young's modulus	E	4,5 E+06	Pa
Poisson's coefficient	ν	0,8	-
Gravitational acceleration	g	9,806	m/s^2

Table 4. 2: *Material data used for the wave propagation problem in a dry soil column.*

For this problem only the solid skeleton is considered in the numerical model, with no coupling with the fluid phases. The initial and boundary conditions are summarized in Table 4.3 and Table 4.4.

Initial condition	
P^g = Patm	fixed
P^c = 0,0 MPa	fixed
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom
V_y = 0.0	on the bottom

Table 4. 3: *Initial conditions for the finite element analysis.*

Boundary condition	
P^g = Patm	on the top
P^c = 0,0 MPa	on the top
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom

Table 4. 4: *Boundary conditions for the finite element analysis.*

In Figure 4.9 we can see the comparison of the displacement time history at the top of the column with the solution presented in Schrefler and Scotta [SS98]. In the first part of the analysis $(t < 1s)$, when the load of 0,1 MPa is applied, the solution oscillates on the equilibrium position $\left(\Delta y = \varepsilon_x H = \frac{\sigma_x}{E} H = \frac{0{,}1E6Pa}{4{,}5E6Pa} 10m = 0{,}2m \right)$.

When the load is removed, the solution oscillates on the zero value $(\Delta y = 0m)$.

The velocity of propagation of the axial displacement waves is:

$$V = \sqrt{\frac{E_s}{\rho_s (1-n)}} = \sqrt{\frac{4{,}5E6}{2000(1-0{,}3)}} = 56{,}7\frac{m}{s} \qquad [4.\ 7]$$

as confirmed by the fact that the mid of the column starts to move after about

$\frac{5m}{56{,}7\frac{m}{s}} = 0{,}088s$ from the application of the load, as shown in Figure 4.10.

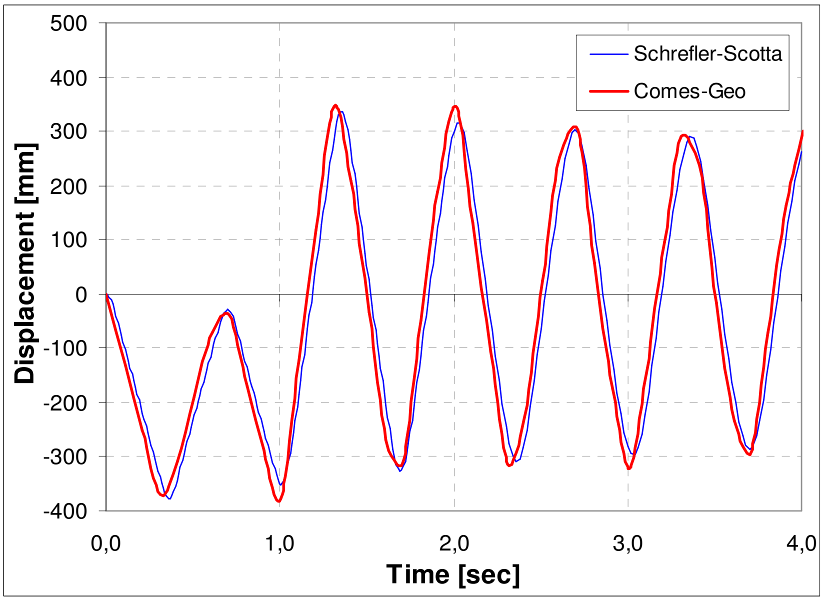

Figure 4. 9: *Displacement history at top of the column: comparison with Schrefler and Scotta* [SS98].

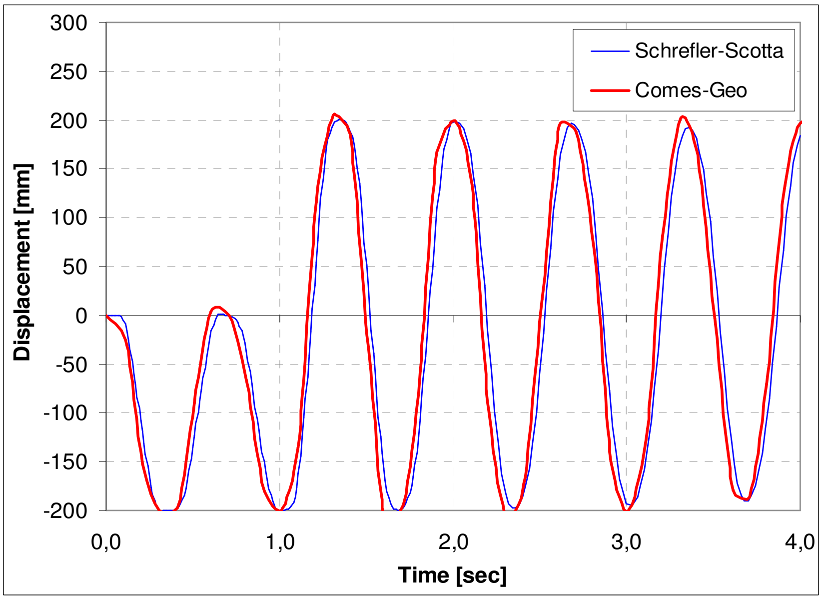

Figure 4. 10: *Displacement history at mid height of the column: comparison with Schrefler and Scotta*[SS98].

The comparison with Schrefler and Scotta [SS98] shows that the analysis give similar results.

4.3 Validation of the water saturated model in isothermal conditions

4.3.1 Dynamic consolidation of a saturated poroelastic column under harmonic load

In this example the response of a homogeneous and isotropic, water-saturated, poroelastic column (height 10m, width 2m) is analyzed under plane-strain, confined compression conditions, following [Ma10]. The domain is surrounded by impermeable, frictionless but rigid boundaries except for the loaded top side which is perfectly drained. The geometry and the spatial discretization (eight-node isoparametric elements with nine Gauss integration points) and the loading path are illustrated in Figure 4.11 and Figure 4.12, respectively.

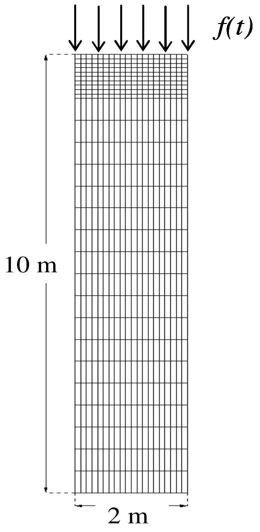

Figure 4. 11: *Geometry and spatial discretization of the dynamic confined compression of a saturated poroelastic column.*

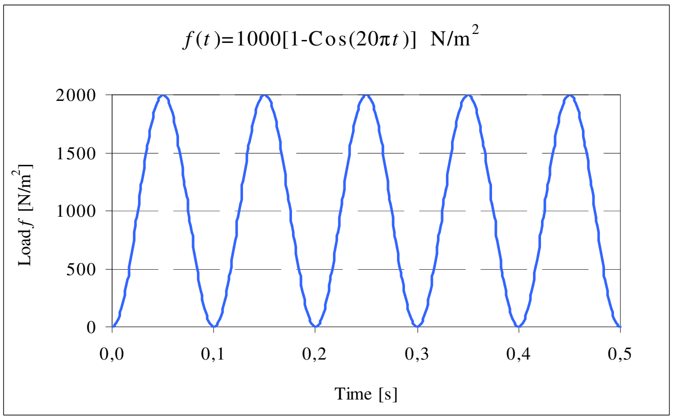

Figure 4. 12: *Loading path of the dynamic confined compression of a saturated poroelastic column.*

The material parameters are listed in Table 4.5 [Ma10], [deB93]. The initial and boundary conditions are described in Table 4.6 and Table 4.7.

Parameters		Value	SI unit
Young's Modulus	E	1,45E+07	Pa
Poisson's Modulus	ν	0,3	-
Porosiy	n	0,33	-
Density of the solid	ρ_s	2000	kg/m^3
Density of the lquid water	ρ_w	1000	kg/m^3
Gravitational acceleration	g	0	m/s^2
Darcy Permeability	K	$10^{-2};10^{-5}$	m/s

Table 4. 5: *Material parameters for the elastic analysis used for the example problems.*

Initial condition	
P^g = Patm	fixed
P^c = 0,0	
T = 293.15 °K	fixed
u_x = 0.0	on the lateral nodes
u_x = 0.0	on the lateral nodes
V_y = 0.0	on the bottom

Table 4. 6: *Initial conditions for the finite element analysis.*

Boundary condition	
P^g = Patm	fixed
P^c = 0.0	at the top
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom

Table 4. 7: *Boundary conditions for the finite element analysis.*

The objective of this benchmark problem is to compare the dynamic model solution obtained with Comes-Geo with an existing (semi-) analytical solutions for the solid displacement and the pore-fluid pressure of an infinite half-space under dynamic loading obtained via Laplace transform [deB93] as presented in [Ma10]. For this problem different integration scheme have been analyzed in [Ma10], as represented in Table 4.8, under the assumption of incompressible liquid water.

Abbr.	Prim.vars.	Governing equations	Solution algorithm	
uvp(1)	$\mathbf{u}_S, \mathbf{v}_F, p$	(4.19, 4.20, 4.21, 4.32)	monolithic implicit	(4.39)
uvp(2)	$\mathbf{u}_S, \mathbf{v}_F, p$	(4.19, 4.33, 4.21, 4.32)	monolithic implicit	(4.39)
uwp	$\mathbf{u}_S, \mathbf{w}_{FR}, p$	(4.19, 4.33, 4.21, 4.32) + $(4.4)_4$	monolithic implicit	(4.39)
uvp(α)	$\mathbf{u}_S, \mathbf{v}_F, p$	(4.19, 4.33, 4.21, 4.32) + (4.37)	monolithic implicit	(4.39)
uvp(pc)	$\mathbf{u}_S, \mathbf{v}_F, p$	(4.19, 4.20, 4.21, 4.22)	semi-explicit-implicit	(4.67)
uvp(β)	$\mathbf{u}_S, \mathbf{v}_F, p$	(4.19, 4.20, 4.21, 4.22) + (4.72)	semi-explicit-implicit	(4.67)
up	$\mathbf{u}_S, p$	(4.19) + weak forms of (4.17,4.18)	monolithic implicit	(4.39)

Abbr.	Time integration	Abbr.	Approximation of primary variables
IE	implicit Euler	QL	$\mathbf{u}_S, \mathbf{v}_S$: quadratic; $\mathbf{v}_F/\mathbf{w}_{FR}, p$: linear
TR	trapezoidal rule	LL	$\mathbf{u}_S, \mathbf{v}_S$: linear; $\mathbf{v}_F/\mathbf{w}_{FR}, p$: linear
TB2	TR-BDF2	QQ	$\mathbf{u}_S, \mathbf{v}_S$: quadratic; $\mathbf{v}_F/\mathbf{w}_{FR}, p$: quadratic

Table 4. 8: *Different integration scheme,* [Ma10].

In particular, two scenarios are tested: a high permeability case, K=10^{-2} m/s, and a moderately low permeability case, K=10^{-5} m/s, which is the lowest permeability for which the (semi-)analytical solutions are achieved by using Maple code.

Here we have to note that for the first value of the permeability the **u**-p approximation is valid just for period less then 0,5 s, whereas for the second case the **u**-p formulation can reproduce the complete frequency range, see section 2.8.1.6.

The first analysis is a static one to compute the equilibrium conditions, neglecting the gravitational load. For the subsequent dynamic analysis, an harmonic load (Figure 4.12) is applied at the top surface of the column, the time step used in the analysis is of 10^{-3} s, the gravitational load is still neglected.

We can see the displacement history at the top of the column for the two cases in Figures 4.13 and 4.14. Both the graphs have a period equal to 0,1 s, which is the period of the harmonic load. With the lowest permeability, the development of displacement of the top surface is slower than the case with higher permeability.

Figures 4.15 and 4.16 is present the comparison with the analytical solution and the different analysis of Markert [Ma10] for the displacement history of the top surface with permeability of K=10^{-2} m/s and K=10^{-5} m/s. Because the value of the permeability and of the period belong to the range of validity of **u**-p formulation, the numerical solutions obtained with the dynamic analysis are equal to the analytical one.

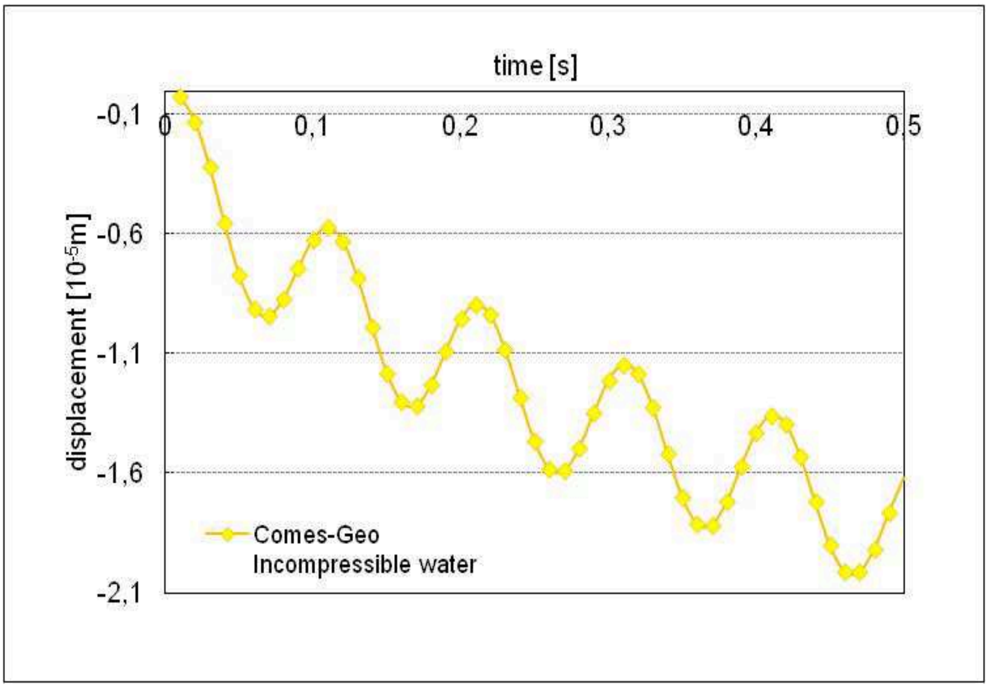

Figure 4. 13: *Top displacement history for* K =10^{-2}*m/s,*
t = [0, 0.5] *s.*

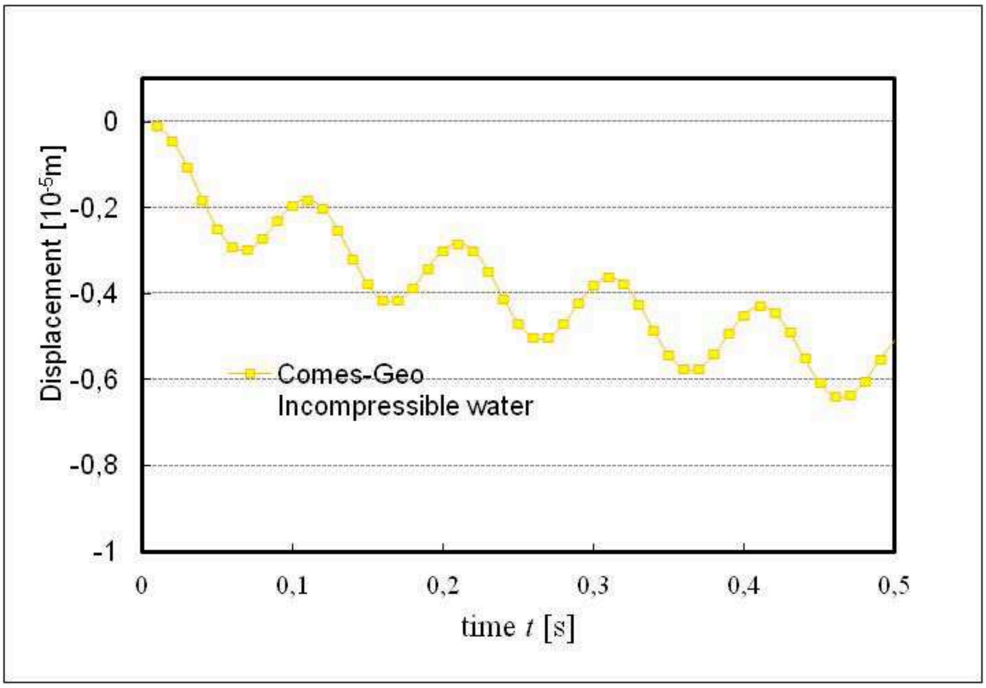

Figure 4. 14: *Top displacement history for* K =10^{-5}*m/s,*
t = [0, 0.5] *s.*

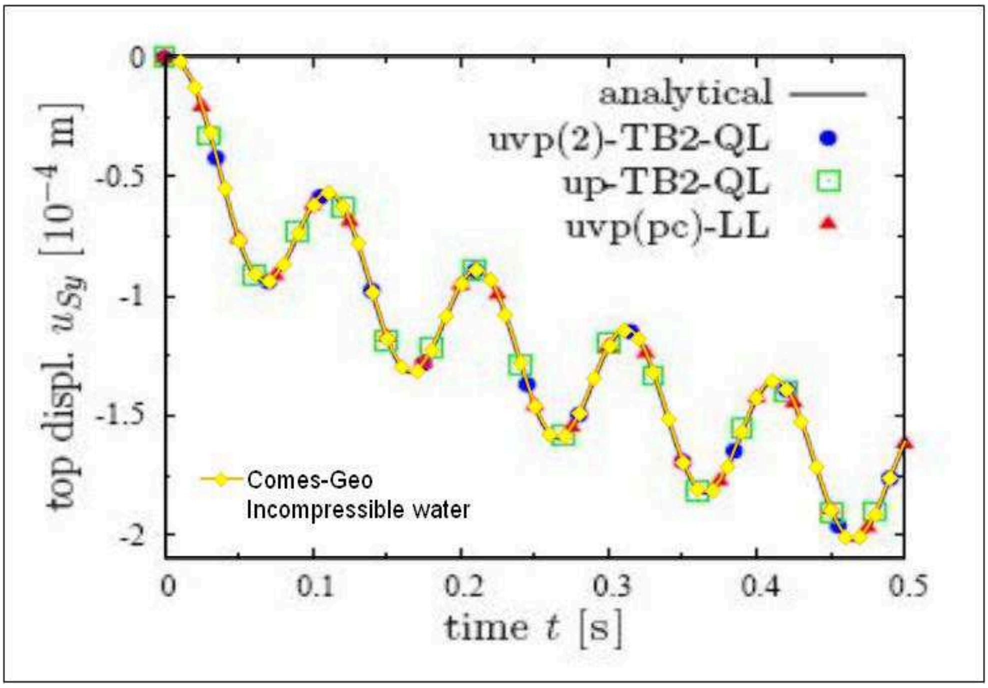

Figure 4. 15: *Top displacement history for* K =10^{-2}*m/s,*
t = [0, 0.5] s, comparison with the analytical and numerical
analysis of Markert [Ma10].

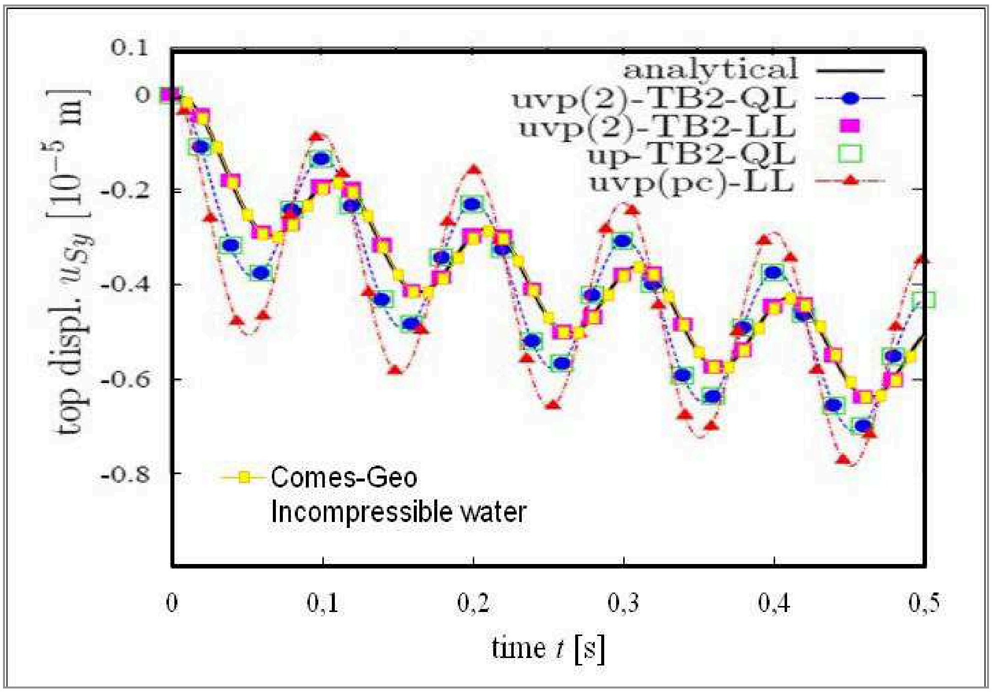

Figure 4. 16: *Top displacement history for* K =10^{-5}*m/s,*
t = [0, 0.5] *s, comparison with the analytical and numerical*
analysis of Markert [Ma10].

In Figure 4.17 and 4.18 the nodal displacement and pressure values in the first half meter below the top of the column are given for a coarse discretization (10 elements per meter). Starting form an undeformed initial state, equilibrium requires the pore fluid to bear the entire load until deformation activates the resistance of the solid skeleton (consolidation process). At the top we have p^c=0 which must be compensated by an immediate pressure increase in a small layer below the boundary.

From this figures it can be observed that the results are similar to those performed by Markert [Ma10] for both the displacement and the water pressure.

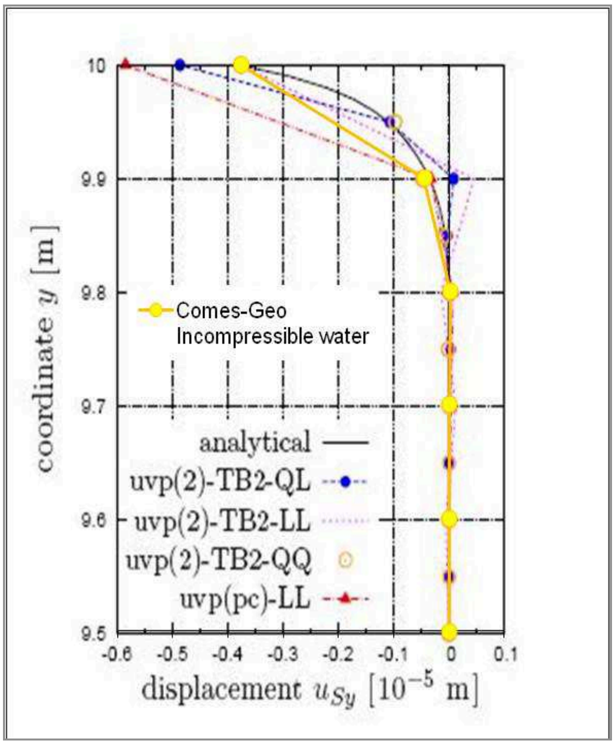

Figure 4. 17: *Solid displacement in the first half meter under the loaded top of the column for* K $=10^{-5}$*m/s,10 elements/meter at* $t = 0,1.5$ *s* [Ma10].

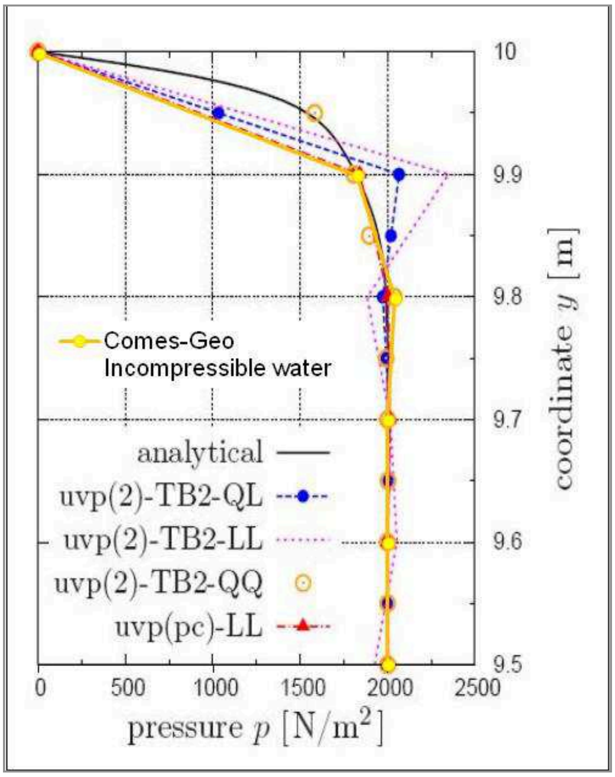

Figure 4. 18: *Water pressure in the first half meter under the loaded top of the column for* K =10^{-5}*m/s,10 elements/meter at* t = 0,1.5 *s* [Ma10].

4.4 Validation of the non-isothermal water saturated model

As mentioned at the beginning of this chapter, the numerical validation of the non-isothermal model in dynamic presents some difficulties because the exact solution of simple problems is not available, to the author knowledge. We present in the following the comparison between the solution of a quasi-static model Comes-Geo [GS96], [LS98], [SPS6] with that obtained with the dynamic model.

4.4.1 Quasi-static fully saturated non-isothermal mechanical consolidation problem (Aboustit test)

This problem deals with fully saturated thermoelastic consolidation. Following [Ab85], a column, 7 m high and 2 m wide, of a linear elastic material is subjected to an external surface load of 1000 Pa and to a surface temperature jump of 50 K above the initial temperature of 293.15 K (Figure 4.19).

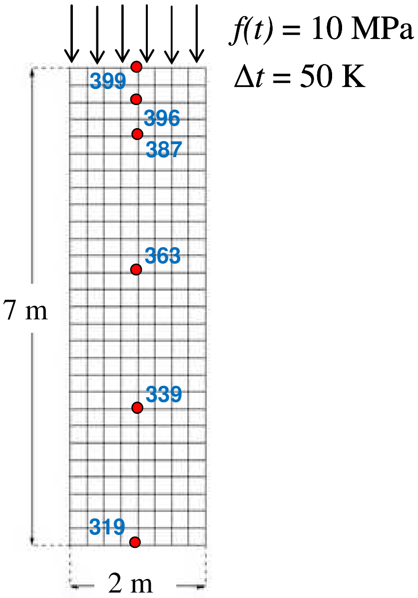

Figure 4. 19: *Geometry, loading conditions and finite element discretization of the saturated soil column.*

The material parameters are summarised in Table 4.9.

The liquid water and the solid grain are assumed incompressible for the static analysis, whereas the compressibility of the liquid water is taken into account in the dynamic analysis.

For the numerical calculation, the problem was solved as a two-dimensional problem in plane stain condition. The column is discretized with eight-node isoparametric elements (4 elements/meter) with nine Gauss points integration.

The spatial discretization used in the finite element simulation is shown in Figure 4.19.

Parameters		Value	SI unit
Porosity	n	0,39	-
Intrinsic permeability	k	2,0 E-19	m^2
Solid skeleton density	ρ_s	2670	kg/m^3
Tortuosity factor	T	0,5	-
Irreducible saturation point	S_{irr}	0,05	-
Solid thermal conductivity		0,42	W/(m K)
Solid matrix heat conductivity		1,9 E-16	W/(m K)
Solid specific heat		732	J/(kg K)
Cubic thermal expansion coefficient		1,3 E-5	K^{-1}
Biot's constant	α_B	1	-

Table 4. 9: *Material parameters.*

The initial and boundary conditions are described in Table 4.10 and Table 4.11.

Initial condition	
P^g = Patm	fixed
P^c = idrostatic	
T = 293.15 K	fixed
$u_x = 0.0$	on the lateral nodes
$u_y = 0.0$	on the bottom

Table 4. 10: *Initial conditions.*

Boundary condition	
P^g = Patm	fixed
$P^c = 0.0$	at the top
T	not fixed
$u_x = 0.0$	on the lateral nodes
$u_y = 0.0$	on the bottom

Table 4. 11: *Boundary conditions.*

During computations the saturation-capillary pressure and relative permeability of water-capillary pressure relationships of the following form:

$$S_w = S_{ir} + (1 - S_{ir}) \cdot \left(\frac{p_b}{p^c} \right)^{\lambda} \qquad [4.\ 8]$$

$$k^{rw} = S_e^{\frac{2+3\lambda}{\lambda}} \qquad [4.\ 9]$$

$$S_e = (S_w - S_{ir})/(1 - S_{ir}) \qquad [4.\ 10]$$

were applied, where S_{ir} is the irreducible saturation point (S_{ir}=0.2), p_b is the bubbling pressure (p_b=1680 Pa), λ is the pore size distribution index (λ=3), S_e is the effective saturation. Furthermore the water saturation is fixed to unit value when $p_c < p_b$ and to irreducible saturation point when $p_c > 1E8$, the water relative permeability is fixed to 0 for $S_w \le S_{ir}$ and to unit value for S_w=1. The relative permeability of gas phase k^{rg} was assumed according to the relationship of Brooks and Corey [BC92]:

$$k^{rg} = (1 - S_e)^2 \left(1 - S_e^{(2+\lambda)/\lambda} \right) \qquad [4.\ 11]$$

During the computations, the value of the tolerance for the global iterative Newton-Rapson procedure is fixed to 1.0E-04 and the maximum number of iteration inside a time step is fixed to 30.

In the following graphs there is the comparison between the solution of the quasi-static and of the dynamic model. We plotted, for each variable, the value in the six nodes highlighted in Figure 4.19.

From Figure 4.20 to Figure 2.26 there is the profile of the temperature history.

We can see that at the beginning of the analysis the dynamic solution is faster than the static one, while at the end of the analysis the dynamic solution reaches the static one.

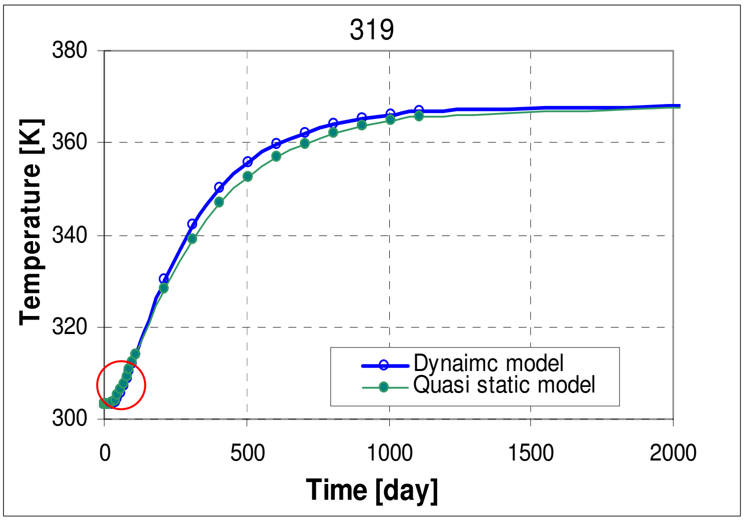

Figure 4. 20: *Temperature time history of node 319.*

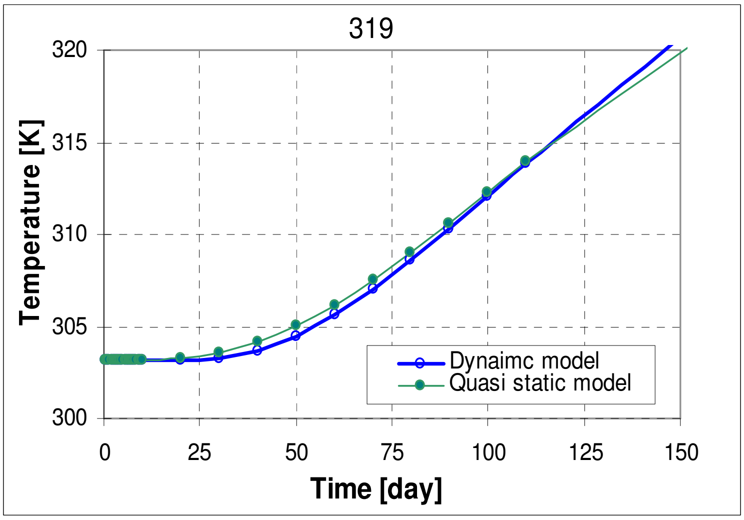

Figure 4. 21: *Zoom of the first part of the previous graph. Temperature history.*

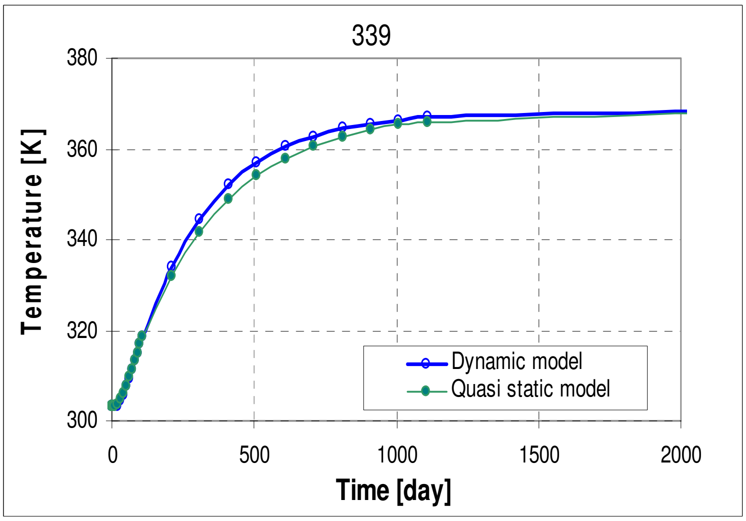

Figure 4. 22: *Temperature time history of node 339.*

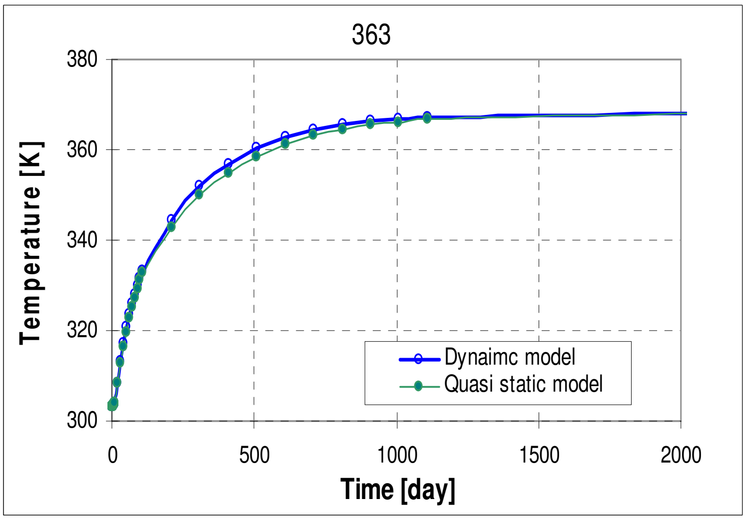

Figure 4. 23: *Temperature time history of node 363.*

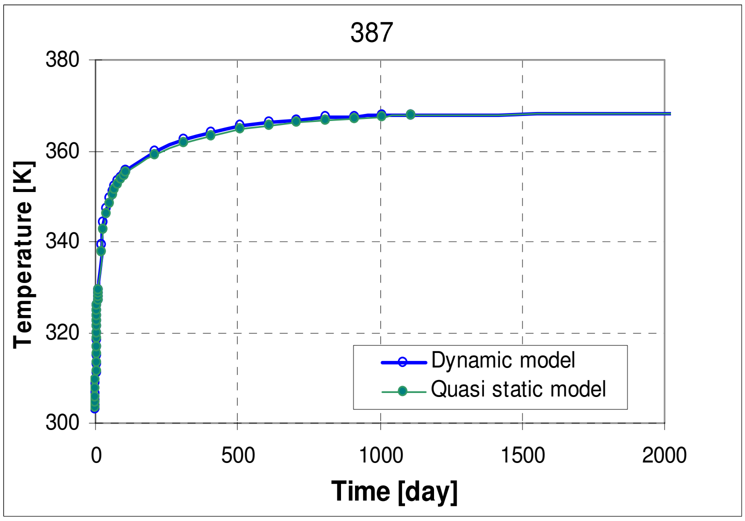

Figure 4. 24: *Temperature time history of node 387.*

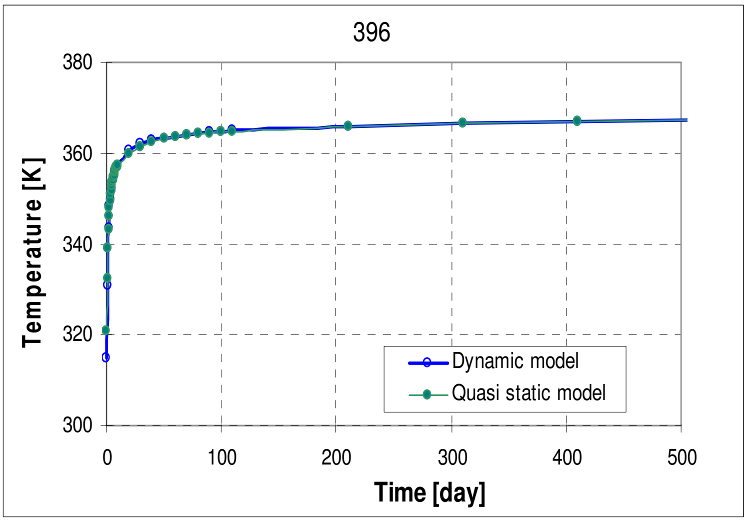

Figure 4. 25: *Temperature time history of node 396.*

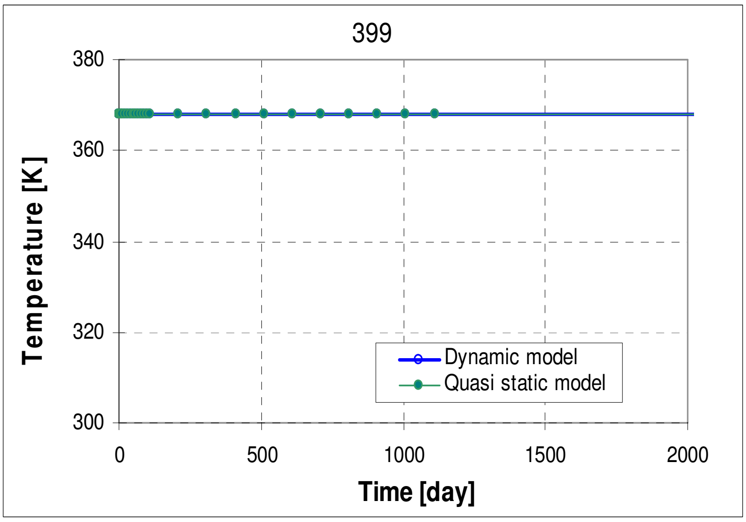

Figure 4. 26: *Temperature time history of node 399.*

From Figure 4.27 to Figure 4.33 the profile of the capillary pressure history is represented. At the beginning the profile of the solution obtained with the dynamic model is faster than the quasi static one, while, after the transitory, the solution of the dynamic model reach the steady static solution.

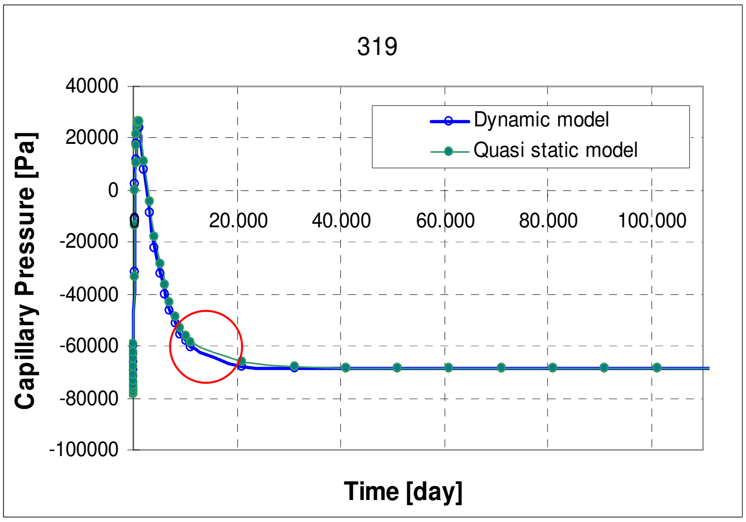

Figure 4. 27: *Capillary pressure time history of node 319.*

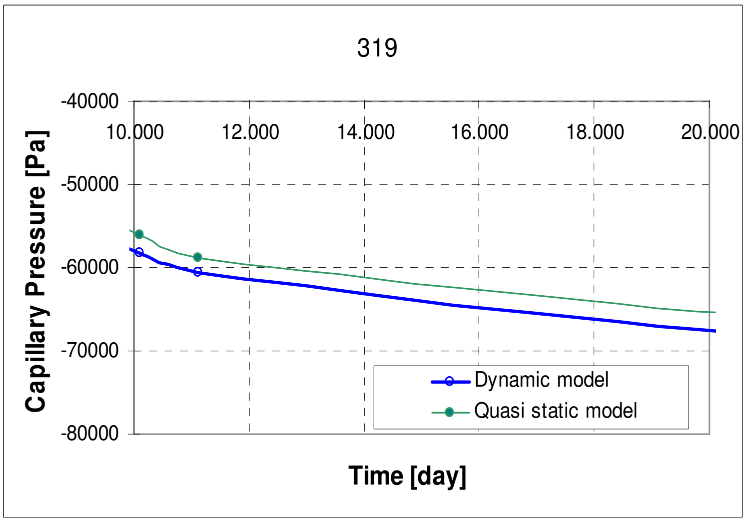

Figure 4. 28: *Zoom of the highlighted zone of the previous graph. Capillary pressure history.*

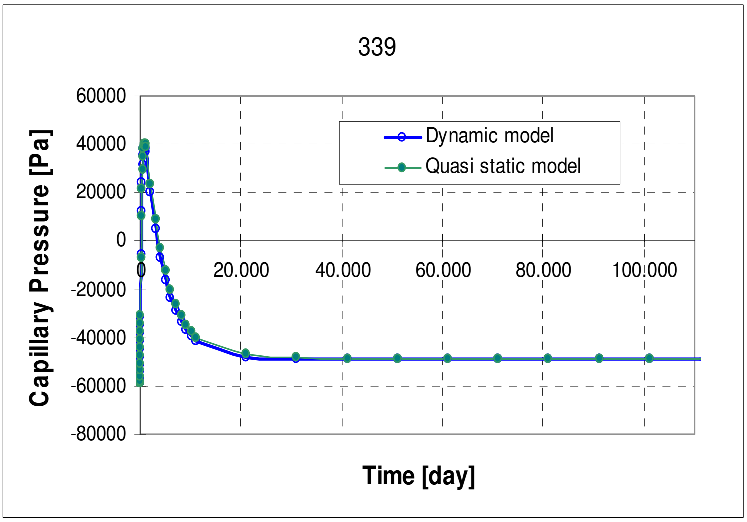

Figure 4. 29: *Capillary pressure time history of node 339.*

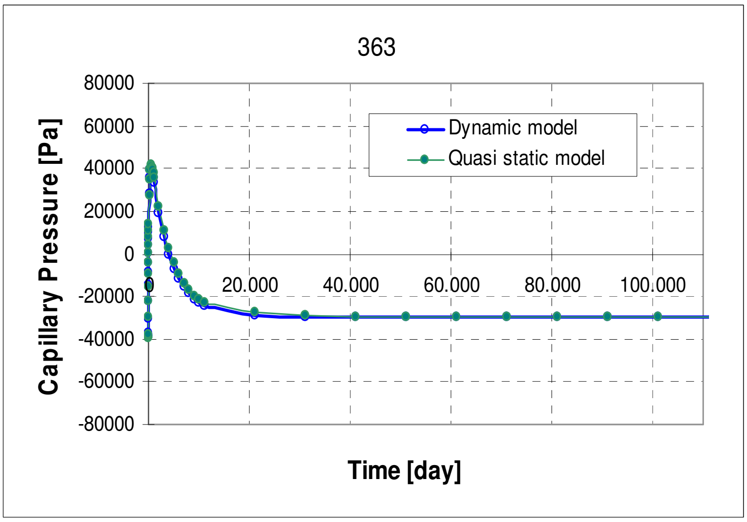

Figure 4. 30: *Capillary pressure time history of node 363.*

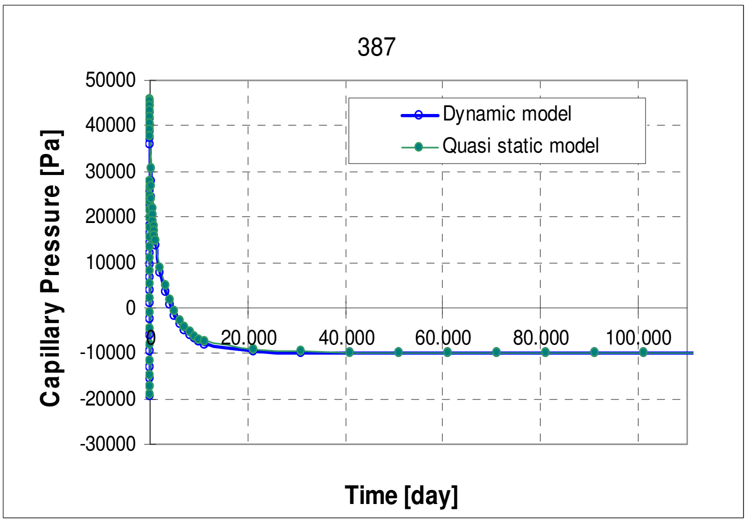

Figure 4. 31: *Capillary pressure time history of node 387.*

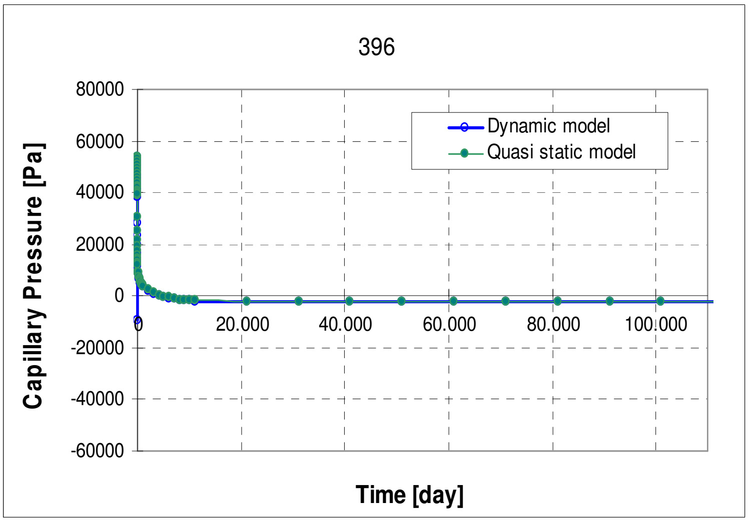

Figure 4. 32: *Capillary pressuretime history of node 396.*

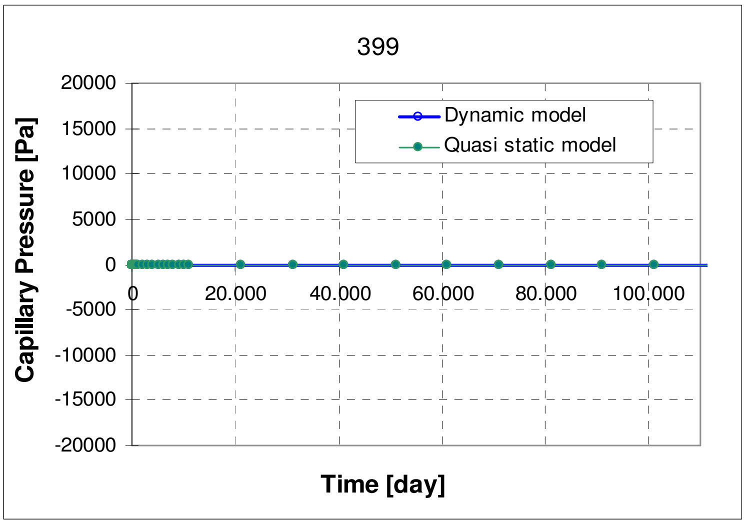

Figure 4. 33: *Capillary pressur etime history of node 399.*

From Figure 4.34 to Figure 4.40 is represented the profile of the displacement time history in the six nodes chosen for the comparison. It follows the same considerations as before: at the beginning of the simulation the profile of the solution obtained with the dynamic model is faster than the quasi static one, while, after the transitory, the solution of the dynamic model reaches the steady state (static) solution.

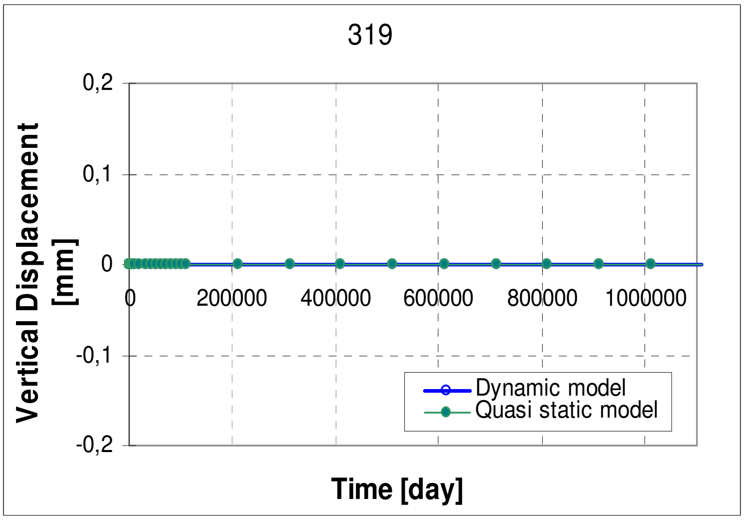

Figure 4. 34: *Vertical displacement time history of node 319.*

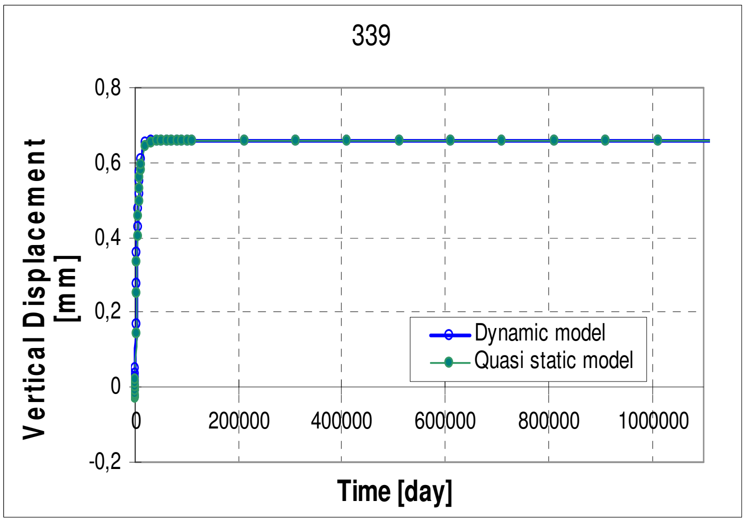

Figure 4. 35: *Vertical displacement time history of node 339.*

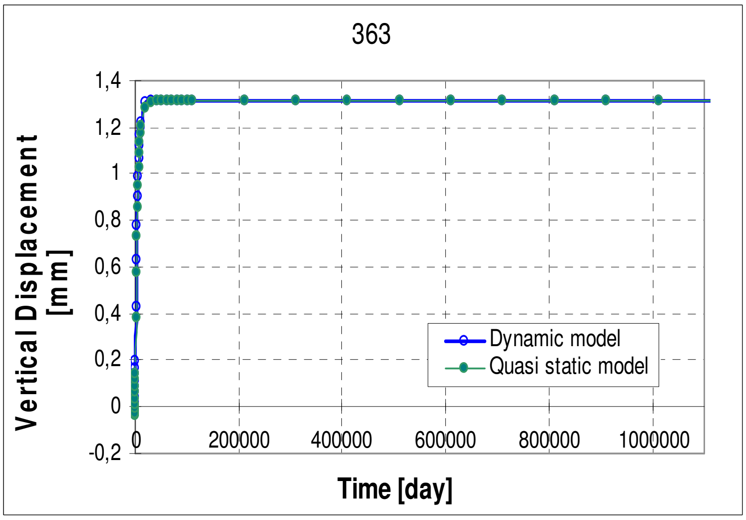

Figure 4. 36: *Vertical displacement time history of node 363.*

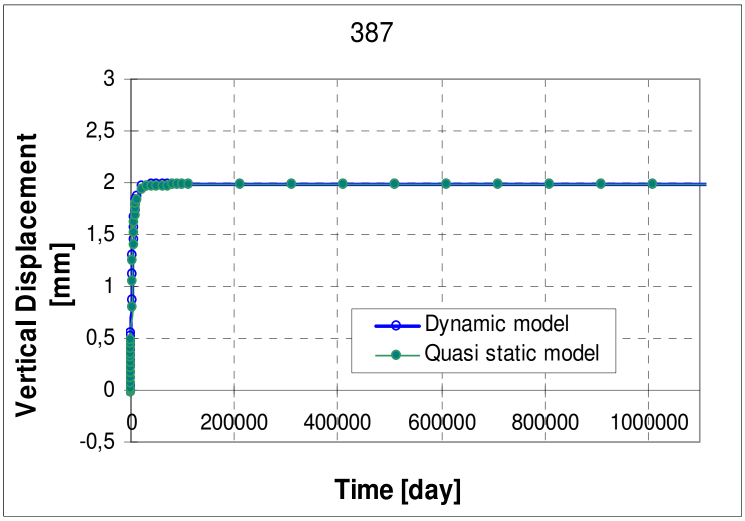

Figure 4. 37: *Vertical displacement time history of node 387.*

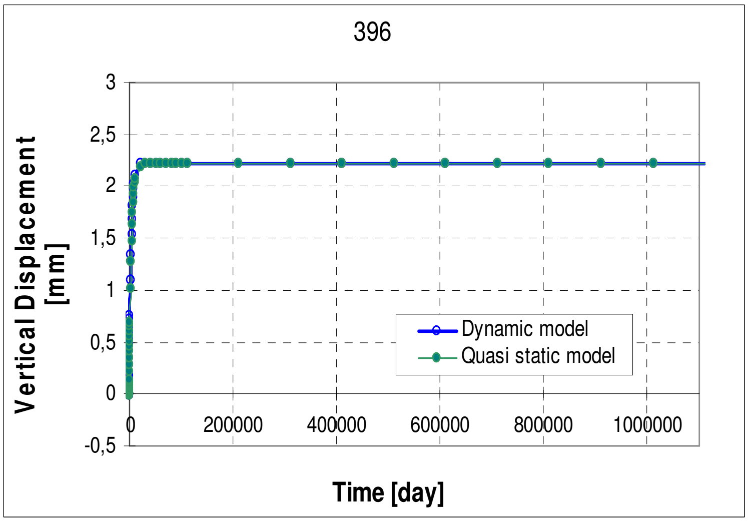

Figure 4. 38: *Vertical displacement time history of node 396.*

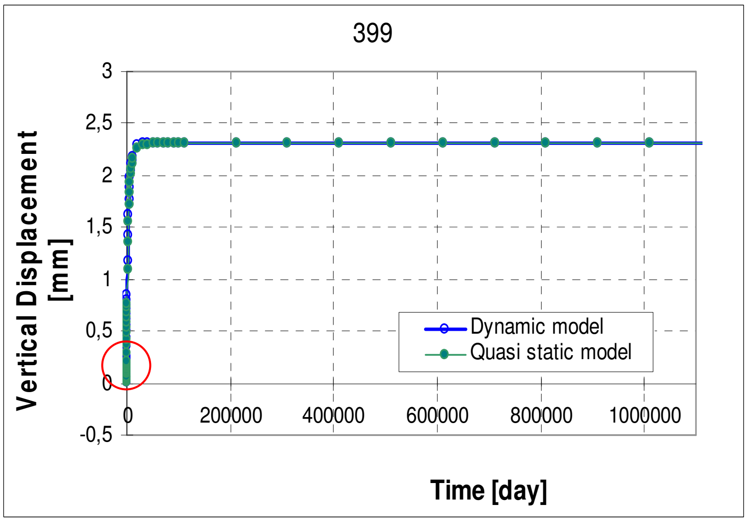

Figure 4. 39: *Vertical displacement time history of node 399.*

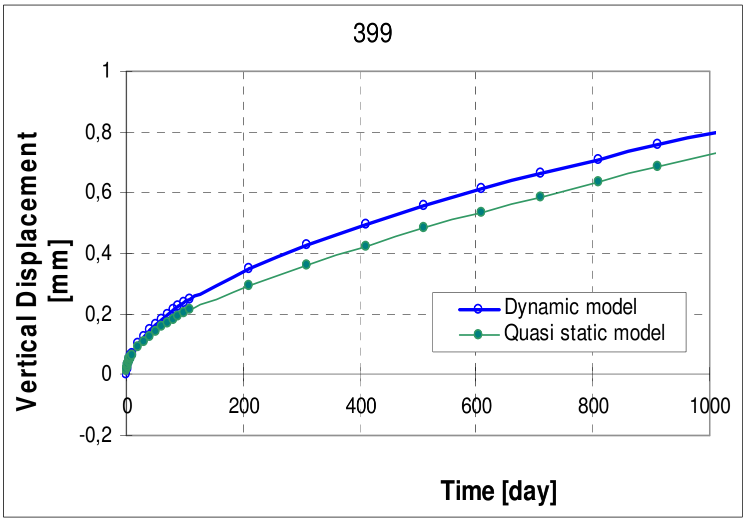

Figure 4. 40: *Zoom of the highlighted zone of the previous graph. Vertical displacement time history.*

4.4 Validation of the isothermal two phase flow model

As for the non-isothermal case, no exact solutions of simple problems are available for partially saturated porous media in dynamics. In the following section we present the comparison between the solution of a quasi static model with the solution obtained with the dynamic model of a drainage of liquid water from a soil column [Lia65].

4.4.1 Quasi-static drainage of liquid water from an initially water saturated soil column (Liakopoulos test)

The proposed benchmark is based on an experiment performed by Liakopoulos [Lia65] on a column, 1 meter high, of Del Monte sand and instrumented to measure the moisture tension at several points along the column during its desaturation due to gravitational effects. Before the start of the experiment, water was continuosly added from the top and was allowed to drain freely at the bottom through a filter, until uniform flow conditions were established. Then the water supply was ceased and the tensiometer readings were recorded.

The finite element simulation is performed with the two-phase flow model in isothermal conditions, with switching between saturated and unsaturated solution performed at p^c= 2000 Pa (S_w= 0,998), which corresponds to bubbling pressure of the analyzed sand, and an additional lower limit for the gas relative permeability of 0,0001.

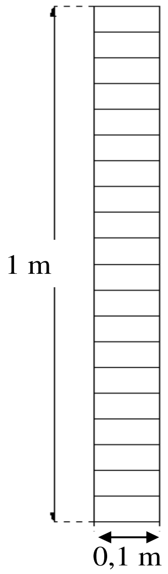

Figure 4. 41: *Geometry and finite element discretization of the sand column.*

For the numerical calculation, the problem is solved as a two-dimensional problem in plane strain conditions; the spatial domain of the column is divided into 20 eight-node isoparametric finite elements of equal size (Figure 4.41). Furthermore, nine Gauss integration points was used.

The material parameters are listed in Table 4.12. The missing data for the mechanical behaviour of the Del Monte sand, have been obtained numerically in previous work [GS96].

Parameters		Value	SI unit
Porosity	n	0,2975	-
Intrinsic permeability	k	4,5 E-13	m^2
Solid grain density	ρ_s	2000	kg/m^3
Tortuosity factor	T	1	-
Irreducible saturation point	S_{irr}	0,2	-
Critical saturation point	S_{cri}	0,909	-
Young's modulus	E	1,3 E+06	Pa
Poisson's coefficient	ν	0,4	-
Biot's constant	α_B	1	-

Table 4. 12: *Material parameters for the elastic analysis used for the Liakopoulos test.*

During computations, the equations for the saturation-capillary pressure and the relative permeability of water-capillary pressure relationships of the following form:

$$S_w = 1 - 1.9722 \cdot 10^{-11} p_c^{\ 2.4279} \qquad [4.\ 12]$$

$$k^{rw} = 1 - 2.207(1 - S_w)^{0.9529} \qquad [4.\ 13]$$

were applied [GS96]. Furthermore the water saturation is fixed to unit value when $p_c < 1E - 20$, the water relative permeability is fixed to 0 for $S_w \leq S_{irr}$ and to unit value for $S_w = 1$, where S_{irr} is the irreducible saturation point.

The relative permeability of gas phase, k^{rg}, was assumed according to the relationship of Brooks and Corey [BC92]:

$$k^{rg} = (1 - S_e)^2 \left(1 - S_e^{\ (2+\lambda)/\lambda}\right) \qquad [4.\ 14]$$

$$S_e = (S_w - S_{ir})/(1 - S_{ir}) \qquad [4.\ 15]$$

with the additional lower limit $k^{rg} \geq 0{,}0001$, where S_e is the effective saturation and λ is the pore size distribution index.

This problem has been solved considering single or two-phase flow, always in quasi-static condition by many authors, for instance [Zi90], [LS98] or [GS96]. Schrefler and Scotta solved this problem for the first time with a dynamic model [SS98].

As specified by Gawin et al.[GS97], initial conditions for this numerical test are slightly different from the experimental ones. The initial mechanical equilibrium state and fluxes have been obtained by a preliminary static solution (hydrostatic water and imposed air pressure). For the dynamic initial and boundary condition see Table 4.13 and Table 4.14.

Initial condition	
P^g = Patm	fixed
P^c = idrostatic	
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom
V_y = 0.0	on the bottom

Table 4. 13: *Initial conditions.*

Boundary condition	
P^g = Patm	on the top, on the bottom
P^c = 0.0	on the bottom
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom

Table 4. 14: *Boundary conditions.*

Since in the experiment the inertial loads are negligible, the quasi-static solutions give almost the same results of the dynamic one.

In the following are reported the evolution in time for water pressure, saturation and vertical displacement versus the height of the column and also a comparison with the quasi-static finite element solution.

In Figure 4.42 is plotted the evolution of the water pressure obtained with the dynamic model; it can be observed that at the beginning of the analysis it increase rapidly, then the curves are closer.

In Figure 4.43 the comparison with the quasi-static solution shows that the dynamic solution is faster at the beginning, while continuing with the analysis they are closer.

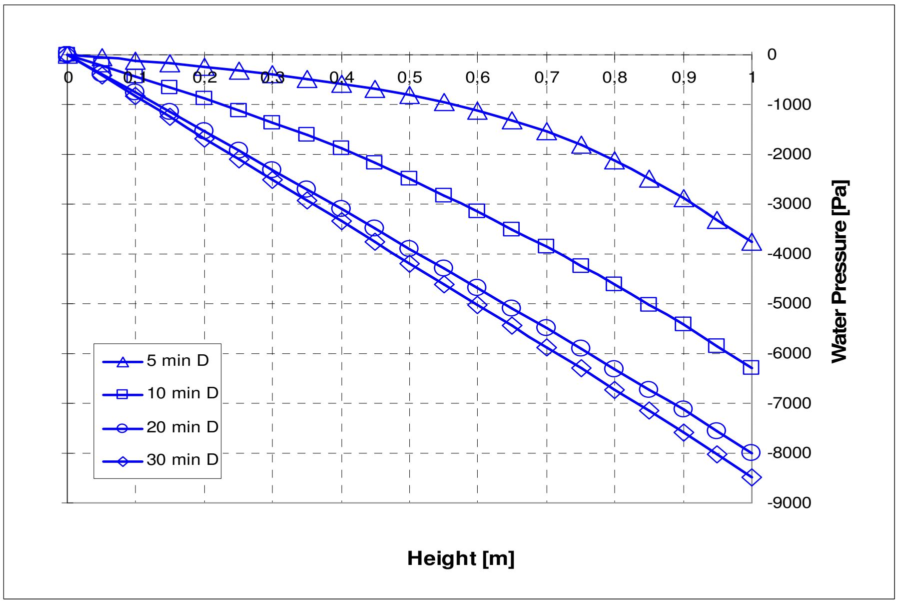

Figure 4. 42: P*rofiles of water pressure versus height (lines with different symbols are plotted at different time stations)*

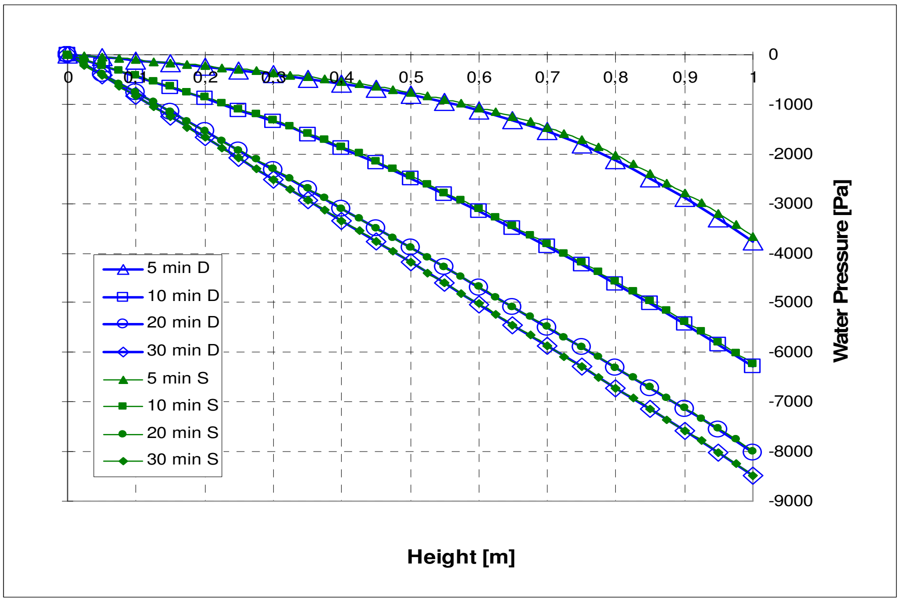

Figure 4. 43: *Profiles of water pressure versus height: comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes.*

In Figure 4.44 is plotted the evolution of the vertical displacement; it can be observed that at the beginning of the analysis it increase rapidly, then the curves are closer.

In Figure 4.45 the comparison with the quasi-static solution shows that fot this variable the dynamic solution is slower.

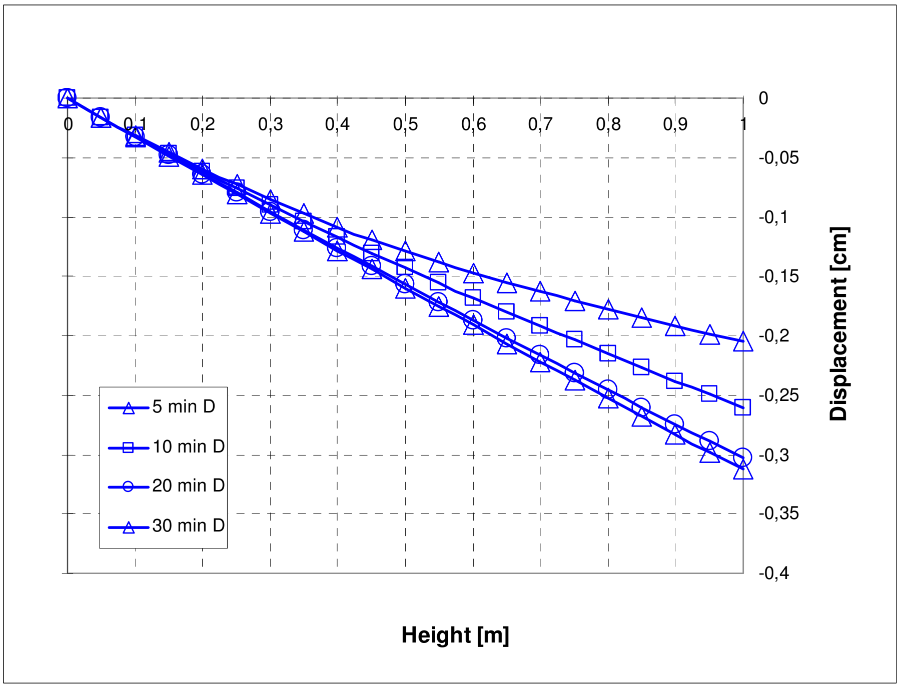

Figure 4. 44: *The resulting profiles of water pressure versus height (lines with different symbols are plotted at different time stations)*

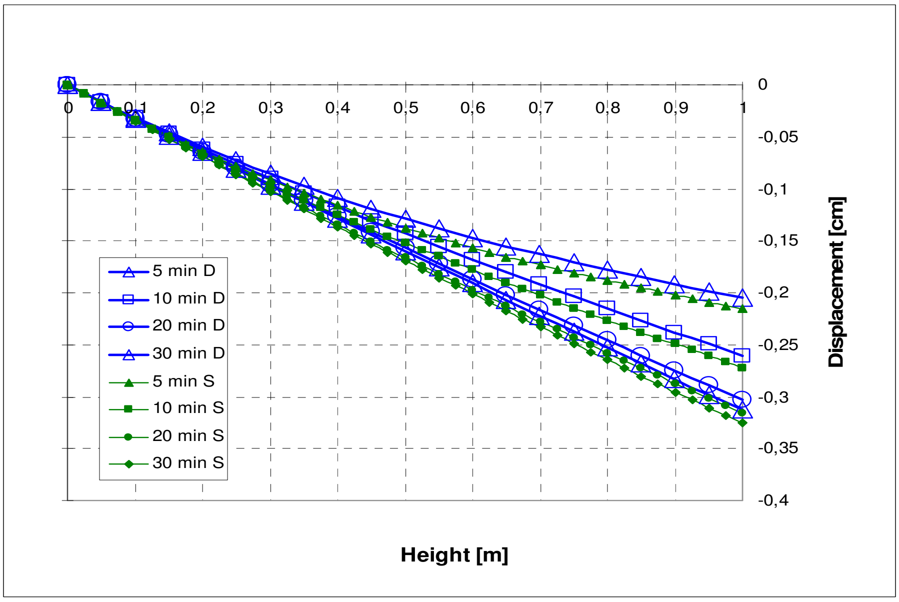

Figure 4. 45: *Profiles of vertical displacement versus height: comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes.*

In Figure 4.46 is plotted the evolution of the degree of water saturation.

In Figure 4.47 the comparison with the quasi-static solution shows that the dynamic solution faster in the first five minutes of analysis, while then the curves are similar.

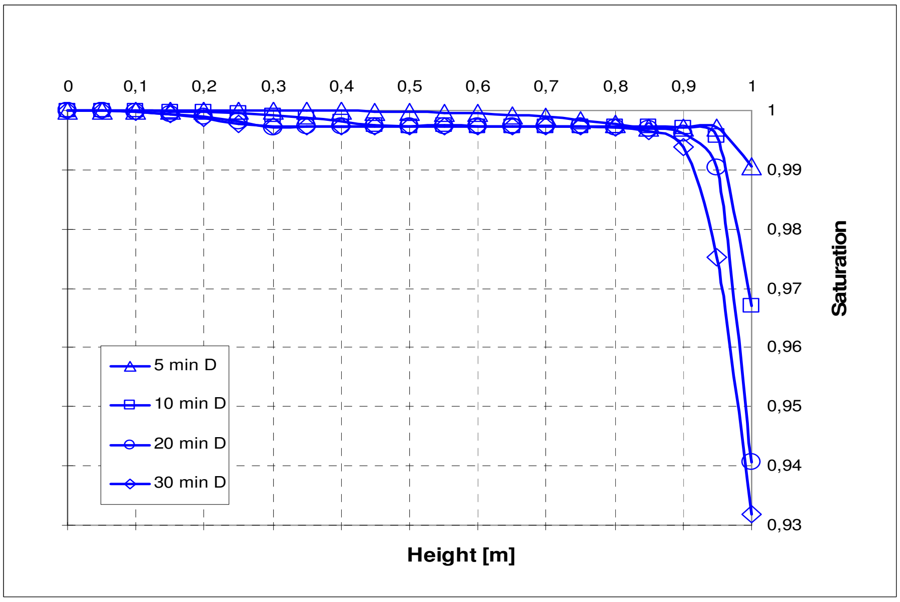

Figure 4. 46: *The resulting profiles of saturation versus height (lines with different symbols are plotted at different time stations)*

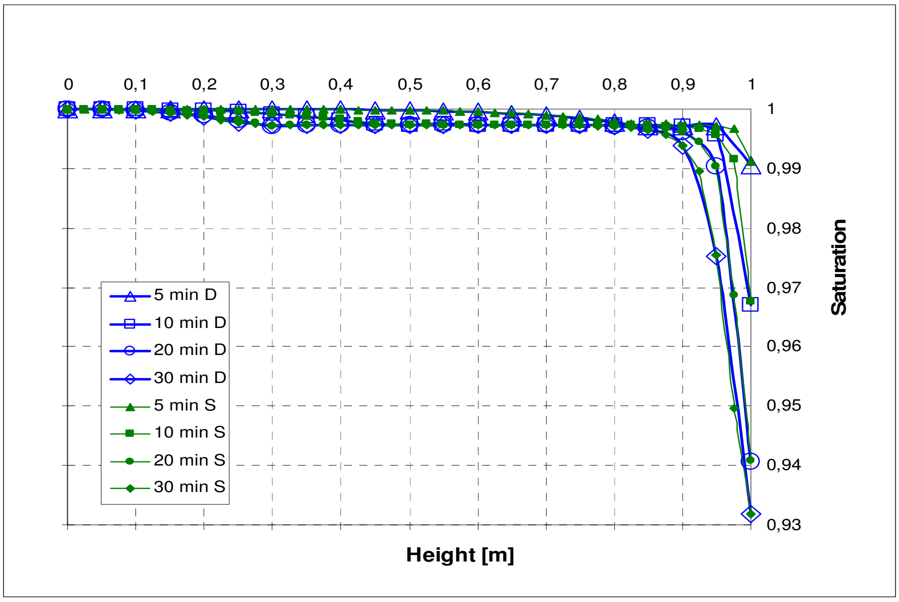

Figure 4. 47: *Profiles of saturation versus height: comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes.*

4.4.2 Sand column subjected to a step load: wave propagation problem in an initially unsaturated soil column

The dynamic behaviour of an initially partially saturated sand column subjected to a step load inducing a longitudinal wave is analyzed following [SS98].

The column is 10 m high and 1 m wide, see Figure 4.48. The material parameters are summarised in Table 4.15.

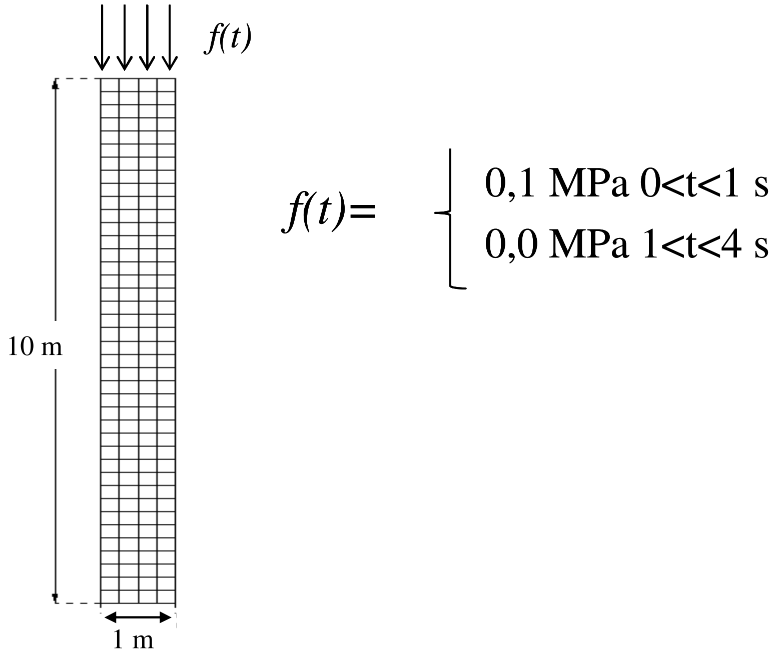

Figure 4. 48: *Geometry, loading conditions and spatial discretization of the confined compression of a initially partially saturated sand column.*

Parameters		Value	SI unit
Porosity	n	0,3	-
Intrinsic permeability	k	5,0 E-13	m^2
Solid skeleton density	ρ_s	2000	kg/m^3
Young's modulus	E	4,5 E+06	Pa
Poisson's coefficient	ν	0,8	-
Water density	ρ_w	1000	kg/m^3
Bulk modulus of water	K_w	2,0 E+08	Pa
Gravitational acceleration	g	9,806	m/s^2
Biot's constant	α_B	1	-

Table 4. 15: *Material parameters*

Initially the material and the fluids are in static equilibrium with the gravitational load and we assume p^c=0,1 MPa at the top surface to obtain the initial partially saturated condition in the column.

In Table 4.16 and Table 4.17 are summarized the initial and boundary conditions.

Initial condition	
P^g = Patm	on the top
P^c = idrostatic; 0,1 MPa on the top	
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom
V_y = 0.0	on the bottom

Table 4. 16: *Initial conditions.*

Boundary condition	
P^g	not fixed
P^c = 0,1 MPa	on the top
T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom

Table 4. 17: *Boundary conditions.*

At time 0 a vertical compressive step surface load of 0,1 MPa is applied at the top of the column and is removed after 1 s.

In Figure 4.49 is plotted the displacement time history: the behaviour is similar to that of the solid skeleton for dry material (see section 4.2.2), the oscillation frequency is increased and the maximum displacement is reduced because part of the applied load is carried out by an increase of the fluids pressure.

In Figure 4.50 is plotted the comparison of the displacement time history at top of the column with the results of Schrefler and Scotta [Bas 98]. During the loading phase the graphs are similar, whereas when the load is removed they are slightly different.
Similar consideration can be done for the displacement time history at mid height of the column, see Figure 4.51.

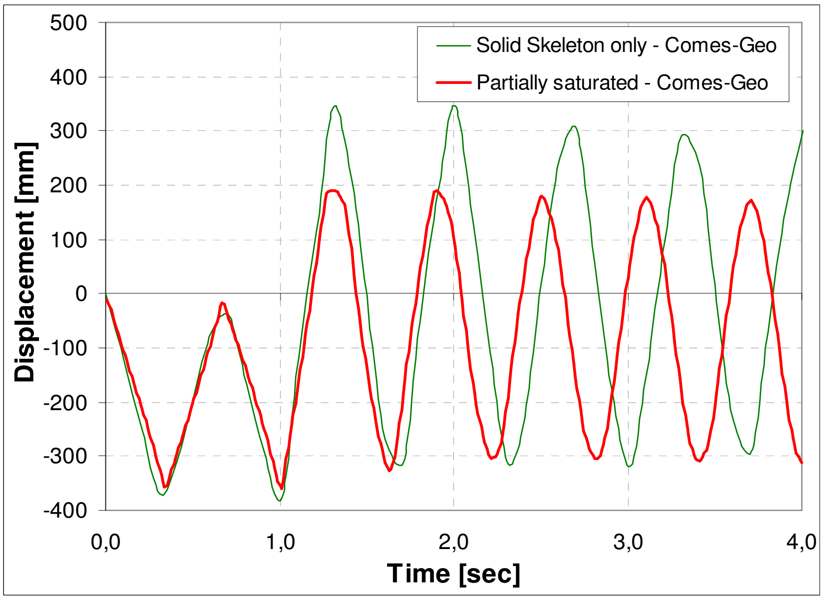

Figure 4. 49: *Comparison of the time history displacement at top of the column between the single solid phase case and the partially saturated case.*

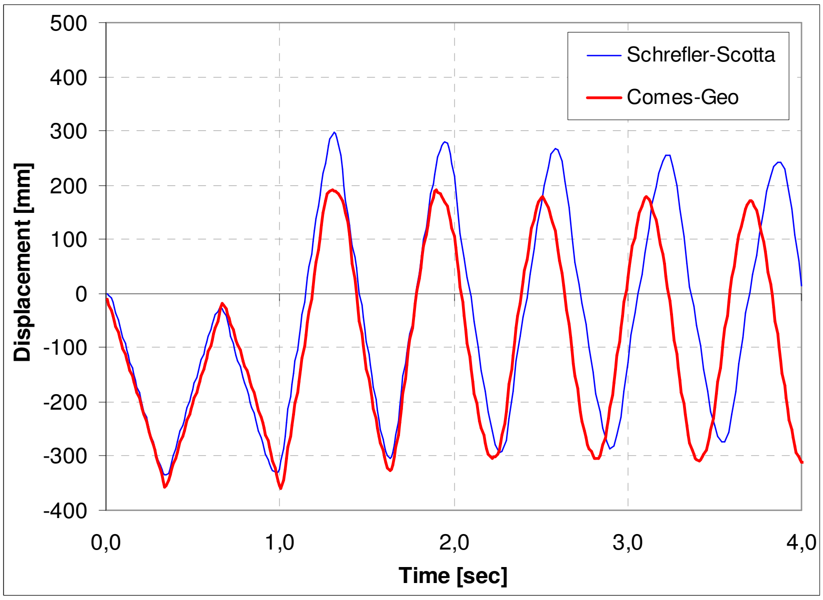

Figure 4. 50: *Displacement time history at top of the column: comparison with the results of Schrefler and Scotta* [SS98].

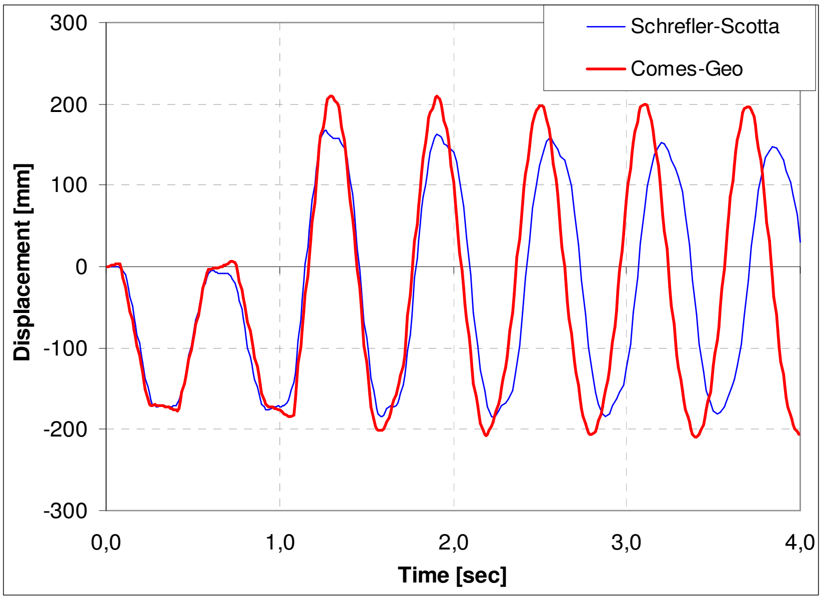

Figure 4. 51: *Displacement time history at mid height of the column: comparison with Schrefler and Scotta*[SS98].

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CONCLUSIONS

In this thesis the development of a model for the analysis of the thermo-hydro-mechanical behaviour of porous media in dynamics has been developed.

Starting from the generalized mathematical model developed for deforming porous media in non-isothermal conditions in dynamics by Lewis and Schrefler [LS98], as original contribution of this thesis, the **u**-p(-T) formulation has been derived following [Z99]. The validity of such an approximation is limited to low frequencies problems [Z99], which is the case of earthquake engineering. In this formulation the relative accelerations of the fluids and the convective terms related to this accelerations have been neglected.

Moreover the compressibility of the solid grain at microscopic level and the dynamic seepage forcing terms (in the mass and enthalpy balance equations) have been neglected.

The numerical model has been derived within the finite element method. In particular for the discretization in space the standard Bubnov-Galerkin procedure [ZT00] was adopted, for the discretization in time the implicit and unconditionally stable Newmark procedure was applied [ZT00].

The independent variables chosen are: the displacement of the solid skeleton **u**, the capillary pressure p^c, the gas pressure p^g and the temperature T.

The model has been implemented in the finite element code Comes-Geo [GS96], [LS98], [SPS6].

The formulation and the implemented solution procedure are validated through the comparison with literature benchmarks, finite element solutions or analytical solutions when available. The numerical validation of the non-isothermal model and partially saturated model in dynamic presents some difficulties because the exact solution of simple problems is not available, to the author knowledge. The comparison between the solution of the quasi-static model Comes-Geo [GS96], [LS98], [SPS6] with that obtained with the dynamic model has been presented.

As further step the application of the model developed in this thesis to real cases as the simulation of the failure of San Fernando dam, 1971, [Z99] or the analysis of the onset of catastrophic landslides [Va02], will be performed.

Other further step will be the dynamics of strain localization in multiphase geomaterials following [SM95], [SS96], [GS98], [ZS99], [SZ99], [ZS01], [SP05] and thermo-elasto-plastic problems (e.g.) [SF08].

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