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An Overview of models for Porous Media of Biomechanical Interest

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Thesis Submitted for the degree of
PhilosophiæDoctor (PhD)

2011 December

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Preface

We study a biological tissue as a biphasic material composed of several constituents allowed to be transferred from one phase to the other .

Our porpuse in the following chapters is to give an overview of the most fundamental problems of biomechanical and biophysical interest, retracing the state of the art in term of contents and results.

We start recalling the basic concepts of the Kinematics of Continua and Differential Geometry (Chapter 1) giving an overview on some fundamental concepts of Continuum Physics and introducing the mathematical framework that we are going to use, i.e., Piola transformation, First and the Second Principle of Thermo-dynamics in terms of generalised balance laws, thermo-mechanic constraint's concept (Chapter 2).

All these considerations allowed us to describe macroscopically the growth and mass transfer in a biological tissue.

Next step (Chapter 3) is to assume the solid phase comprised of two sub-phases, i.e. matrix and fibre-like inclusion $\phi_S = \phi_M + \phi_I$, moving with the common phase velocity $\mathbf{v}_S$. Each phase will be modelled as a mixture on its own with several constituents. Because of mass exchanges between phases, the solid-phase experiences growth (or resorption). Growth, and the material inhomogeneities related to it, will be described through the multiplicative decomposition of the solid-phase deformation gradient tensor, and the introduction of the growth velocity gradient.

It's time now to discuss possible evolution laws for both mass transfer and growth, and to characterize the equilibrium of the system (Chapter 4). In order to do that we will use the Kröner's decomposition to find an elastic, $\mathbf{F}_e$, and inelastic, $\mathbf{F}_a$, part of the deformation gradient tensor, $\mathbf{F} = \mathbf{F}_e\mathbf{F}_a$. This approch has origin in the Theory of Plasticity and it is one of the milestones of the mathematical modelling of volumetric growth. After the introduction, in the previous chapters, of many important concepts such as the Mixture Theory, the mass balances and the kinematics of anelastic processes, we will obtain in Chater 5, the expression of residual dissipation as shown by Grillo *et al.* (136) and we will study the residual dissipation inequality improving some of the results presented in (2, 58, 112).

We will adapt the model of fiber reorientation put forward by Olsson and Klarbring (126) to the case of a multi-constituent solid with statistical distribution of fibers. Morever the latter model in the presence of chemical agents will also prepresent the starting point for the next and last chapter (Chapter 6).

CONTENTS

Chapter 1

Elements of Continuum Kinematics and Differential Geometry

1.1 Introduction

This Chapter is devoted to recall the basic concepts of the Kinematics of Continua and Differential Geometry which are employed throughout this Thesis.

Will be exploited the Lagrangian and Eulerian Descriptions of the Kinematics of Continuum media with attention on their differences and analogies and presented some geometric aspects of Continuum Kinematics related to the Theory of Differentiable Manifolds (Marsden and Hughes, 1983; Felsager, 1998).

1.2 Preliminary Definitions

The mathematical description of the behaviour of deformable media under the action of external agents of various nature is called **Continuum Mechanics**. In this context a body is said to be *continuum* if the smallest characteristic length established by a certain interaction is much greater than the molecular, or atomic, characteristic distances (Eringen, 1980) and its elementary constituent is referred to as *particle* or *material point*.

In this Chapter, we shall be concerned with the study "*simple*" continua, i.e., those media which can be naturally studied in the three-dimensional Euclidean space, or in manifolds of the same dimensions (Marsden and Hughes, 1983). Therefore, generalized continua, i.e. those media which may require higher order dimensional spaces (for example, liquid crystals) will not be treated throughout this Chapter.

In the *Configuration Space* (Lanczos, 1970; Landau and Lifshitz, 1976), a particle (as elementary constituent of a continuum body) can be defined as *curve* parameterised by time, t. If curves are admitted to be twice differentiable functions of time, then each curve, ℓ, belongs to the functional space $C^2(\mathbb{R}_0^+;\mathbb{R}^3)$. Consequently, the body, B, can be identified with a subset of $C^2(\mathbb{R}_0^+;\mathbb{R}^3)$, i.e. $\mathrm{B} \subset C^2(\mathbb{R}_0^+;\mathbb{R}^3)$. For every $t \in \mathbb{R}_0^+$, the point $\ell(t)$ and the set $\mathrm{B}_t \subset \mathbb{R}^3$ represent the *configuration* of particle, ℓ, and of the body, B, respectively, at time t.

If we disregard the occurrence bifurcations, the curves of B never intersect each other, i.e. for every $\ell_1, \ell_2 \in \mathrm{B}$, the inequality $\ell_1(t) \neq \ell_2(t)$ is respected for every $t \in \mathbb{R}_0^+$.

The configuration of the body at time t, B_t, can be found by introducing a *localization map*, i.e. a map $\phi_t : \mathrm{B} \to \mathrm{B}_t$ such that $\phi_t(\mathrm{B}) = \mathrm{B}_t$. For every $\ell \in \mathrm{B}$, the map ϕ_t is such that $\phi_t(\ell) = \ell(t) \in \mathrm{B}_t$. Localization maps are bijective functions and, for every $t_1, t_2 \in \mathbb{R}_0^+$, the *diffeomorphism* $\phi_{t_2} \circ \phi_{t_1}^{-1} : \mathrm{B}_{t_1} \to \mathrm{B}_{t_2}$ represents the *motion* of the body, i.e. its time evolution from time t_1 to time t_2, B_{t_1} and B_{t_2} being two different configurations of the body.

Given a body, $\mathrm{B} \subset C^2(\mathbb{R}_0^+;\mathbb{R}^3)$, and a normed space, Y, a generic physical quantity related to the body, f, can be expressed as a function, $f : \mathrm{I} \times \mathrm{B} \to Y$, I being an interval of time, such that $y = f(t, \ell)$ for every $y \in Y$, and $(t, \ell) \in \mathrm{I} \times B$. Moreover, for every $\tau, t \in \mathrm{I}$ such that $\tau < t$, we may define a map, $\hat{f} : \mathrm{I} \times \mathrm{B}_\tau \to Y$, such that

$$y = f(t, \ell) = \hat{f}(t, \ell(\tau)) = \hat{f}(t, \phi_\tau(\ell)), \tag{1.1}$$

where $\hat{f}(t, \cdot) = f(t, \cdot) \circ \phi_\tau^{-1}$.

1.3 Lagrangian Formulation of the Kinematics of Continua

The Lagrangian Formulation of the Kinematics of Continua is based on the definition of a *reference configuration*, B_R, associated with the body, B. Although the configuration B_R simply represents an arbitrarily chosen coordinate patch, and it may never be attained by the body, it is sometimes *naturally* identified with the subset of $\mathbb{R}^3$ occupied by the body at time $t = 0$, i.e. $\mathrm{B}_R = \mathrm{B}_0 = \phi_0(\mathrm{B})$.

Coordinates in B_R are usually referred to as *material coordinates*, or *referential coordinates*.

1.3.1 Manifolds and Coordinate Systems

In general, the configuration of a body at time t can be regarded as a *smooth manifold* in $\mathbb{R}^3$. A set $\mathrm{M} \subset \mathbb{R}^3$ is said to be a manifold if, and only if, for each point $P \in \mathrm{M}$, there exists a subset $\mathrm{U} \subset \mathrm{M}$ containing P, an open subset $\mathrm{V} \subset \mathbb{R}^3$, and a smooth one-to-one mapping, called *chart* or *coordinate system*, $(s^a)_{a=1}^3$, such that $s : \mathrm{U} \to \mathrm{V}$ (Marsden and Hughes, 1983).

Given a subset $\mathrm{U} \subset \mathrm{M}$, and two coordinate systems, $s_{(1)} : \mathrm{U} \to \mathrm{V}_{(1)}$ and $s_{(2)} : \mathrm{U} \to \mathrm{V}_{(2)}$, the map $\xi_{(1,2)} : \mathrm{V}_{(1)} \to \mathrm{V}_{(2)}$, such that $\xi_{(1,2)} \in C^\infty(\mathrm{V}_{(1)}, \mathrm{V}_{(2)})$, is said to be a *change of coordinate*. The change of coordinate is characterized by the property of being invertible, i.e. there exists a smooth function $\xi_{(2,1)}$ such that $\xi^{-1}_{(1,2)} = \xi_{(2,1)}$.

Let $\mathrm{C}_t \subset \mathrm{B}_t$ be an open subset of the B_t. The coordinate system $s_{(E)} : \mathrm{C}_t \to C_t^{(E)} \subset \mathbb{R}^3$ is assumed to map C_t onto the three dimensional Euclidean space, and it is therefore said to be the *Euclidean* representation of the manifold. Let $s : \mathrm{C}_t \to C_t \subset \mathbb{R}^3$ denote another arbitrary coordinate system. In the following, we shall write $s_{(E)}(P) = z$ and $s(P) = x$, respectively, and we shall consider the change of coordinate $\xi : \mathrm{V}_{(E)} \to \mathrm{V}$ such that $x = \xi(z)$, and $\zeta = \xi^{-1} : \mathrm{V} \to \mathrm{V}_{(E)}$ such that $z = \zeta(x)$.

By regarding time t as a parameter, and introducing a map $c : \mathrm{I} \to \mathrm{V}$ such that $c(t) = x = s(P)$, and a map $c_{(E)} : \mathrm{I} \to \mathrm{V}_{(E)}$ such that $c_{(E)}(t) = z = s_{(E)}(P)$, we may write $x = \xi(c_{(E)}(t))$, and $z = \zeta(c(t))$. The maps c and $c_{(E)}$ are the parameterizations of curves in V and $\mathrm{V}_{(E)}$, respectively. On account of the decomposition $\zeta \circ c = [\zeta^i \circ c]\boldsymbol{e_i}$ (where $\{\boldsymbol{e_i}\}_{i=1}^3$ is the Euclidean orthonormal basis in $\mathbb{R}^3$) we note that the derivative of $\zeta \circ c$ with respect to time yields

$$\frac{d(\zeta \circ c)}{dt}(t) = \left[\frac{d(\zeta^i \circ c)}{dt}(t)\right]\boldsymbol{e_i} = \left[\frac{\partial \zeta^i}{\partial x^a}(x)\dot{c}^a(t)\right]\boldsymbol{e_i}. \tag{1.2}$$

By introducing the notation

$$\boldsymbol{b}_a(x) = \frac{\partial \zeta^i}{\partial x^a}(x)], \tag{1.3}$$

Eq. (1.2) becomes

$$\frac{d(\zeta \circ c)}{dt}(t) = \dot{c}^a(t)\boldsymbol{b}_a(x) = \dot{c}^a(t)\boldsymbol{b}_a(c(t)). \tag{1.4}$$

Equation (1.4) defines the *tangent vector* at point x to the line parameterized by the map $c : \mathrm{I} \to \mathrm{V}$, while Eq. (1.3) defines the three independent vectors, $\{\boldsymbol{b}_a(x)\}_{a=1}^3$, which form a basis of the *tangent space*, $\boldsymbol{T_x}\mathrm{C}_t$, at point x to the subset C_t of the manifold B_t. On the other hand, by inverting Eq. (1.3), we obtain

$$\boldsymbol{e_i} = \frac{\partial \xi^a}{\partial z^i}(z)\boldsymbol{b}_a(x) = \frac{\partial \xi^a}{\partial z^i}(\zeta(x))\boldsymbol{b}_a(x) = \frac{\partial \xi^a}{\partial z^i}(z)\boldsymbol{b}_a(\xi(z)). \tag{1.5}$$

From here on, we shall denote by $\boldsymbol{V}^i_{(E)}$ and $\boldsymbol{V}^a$ the Euclidean and arbitrary coordinates, respectively of an arbitrary vector $\boldsymbol{V}$. Moreover, coordinate systems on the ambient space $\mathbb{R}^3$ and B_R will be denoted with $\{x^a\}_{a=1}^3$ and $\{X^A\}_{A=1}^3$, respectively, while the corresponding Euclidean coordinates will be represented by $\{z^i\}_{i=1}^3$ and $\{Z^I\}_{I=1}^3$, respectively. In the following, where there is no danger of confusion, we shall identify the body manifolds, B_R and B_t, with their corresponding coordinate patches, i.e. B_R and B_t, respectively.

1.3.2 Configuration Field

The *configuration field* is defined as a map $\chi : \mathrm{I} \times \mathrm{B}_R \to \mathbb{R}^3$ such that, for every $(t, X) \in \mathrm{I} \times \mathrm{B}_R$, there exists a point $x \in \mathbb{R}^3$ such that $\chi(t, X) = x$. It should be noted that, when the reference configuration is assumed to coincide with the configuration occupied by the body at time $t = 0$ (i.e. $\mathrm{B}_R = \mathrm{B}_0$), and the map $\chi(t, \cdot)$ is restricted to $[\chi(t, \cdot)]_{\mathrm{B}_0 \to \mathrm{B}_t}$, the configuration field satisfies the identity

$$[\chi(t, \cdot)]_{\mathrm{B}_0 \to \mathrm{B}_t} = \phi_t \circ \phi_0^{-1}, \tag{1.6}$$

where B_t is said to be the current configuration of the body. In this case, the map $\chi(\cdot, X)$ associates to each material point the corresponding trajectory, ℓ, i.e. $\chi(\cdot, X) = \ell$.

1.3.3 Lagrangian Velocity

Velocity is the map $\hat{\boldsymbol{v}} : \mathrm{I} \times \mathrm{B}_R \to \mathbb{R}^3$ such that $\hat{\boldsymbol{v}}(t, X) = \partial_t \chi(t, X)$. The vector $\hat{\boldsymbol{v}}(t, X)$ is tangent to ℓ at the point $x = \ell(t) = \chi(t, X)$. By denoting with $\{\boldsymbol{b}_a(x)\}_{a=1}^3$ an orthonormal basis attached to the point $x \in \mathrm{B}_t$, velocity can be decomposed as (Marsden and Hughes, 1983)

$$\hat{\boldsymbol{v}}(t, X) = \hat{\boldsymbol{v}}^a(t, X)\boldsymbol{b}_a(x), \tag{1.7}$$

where each component coincides with the time derivative of the corresponding component of the configuration field, i.e.

$$\hat{\boldsymbol{v}}^a = \partial_t \chi^a, \forall a = 1, 2, 3. \tag{1.8}$$

In order to prove Eq. (1.8), we evaluate the quantity $[\partial_t \chi^a(t, X)]\boldsymbol{b}_a(x)$. By applying the transformation rules

$$\chi^a(t, X) = \frac{\partial \xi^a}{\partial z^i}(z)\chi^i_{(E)}(t, X), \tag{1.9}$$

and

$$\boldsymbol{b}_a(x)\frac{\partial \xi^a}{\partial z^i}(z) = \boldsymbol{e}_i, \tag{1.10}$$

and noting that

$$\partial_t \chi^a(t,X) = \partial_t \left(\frac{\partial \xi^a}{\partial z^i}(z) \chi^i_{(E)}(t,X) \right) = \frac{\partial \xi^a}{\partial z^i}(z)[\partial_t \chi^i_{(E)}(t,X)], \tag{1.11}$$

we may write

$$\begin{aligned} [\partial_t \chi^a(t,X)]\boldsymbol{b}_a(x) \quad &= \partial_t \chi^i_{(E)}(t,X) \left[\boldsymbol{b}_a(x) \tfrac{\partial \xi^a}{\partial z^i}(z) \right] = \\ &= [\partial_t \chi^i_{(E)}(t,X)]\boldsymbol{e_i} = [\hat{\boldsymbol{v}}^i_{(E)}(t,X)]\boldsymbol{e_i}. \end{aligned} \tag{1.12}$$

Since the identity

$$[\hat{\boldsymbol{v}}^i_{(E)}(t,X)]\boldsymbol{e_i} = [\hat{\boldsymbol{v}}^a(t,X)]\boldsymbol{b}_a(x) \tag{1.13}$$

must hold true, we conclude that $\partial_t \chi^a(t,X) = \hat{\boldsymbol{v}}^a(t,X)$.

1.3.4 Lagrangian Acceleration

Acceleration, $\hat{\boldsymbol{a}}$, is the partial time derivative of the configuration field, i.e.

$$\hat{\boldsymbol{a}}(t,X) = \partial_t \hat{\boldsymbol{v}}(t,X) = \partial_t^2 \chi(t,X). \tag{1.14}$$

The components of $\hat{\boldsymbol{a}}(t,X)$ are given by

$$\hat{\boldsymbol{a}}^a(t,X) = \partial_t \hat{\boldsymbol{v}}^a(t,X) + \gamma^a_{bc}(x) \hat{\boldsymbol{v}}^b(t,X) \hat{\boldsymbol{v}}^c(t,X), \tag{1.15}$$

where the terms

$$\gamma^a_{bc}(x) = \frac{\partial (\xi^{-1})^i}{\partial x^b \partial x^c}(x) \frac{\partial \xi^a}{\partial z^i}(z) \tag{1.16}$$

are said to be the Christoffel symbols.

In order to prove Eq. (1.15), we note that $\boldsymbol{b}_a(x) = \hat{\boldsymbol{b}}_a(t,X)$ and we differentiate $\hat{\boldsymbol{v}}(t,X) = \hat{\boldsymbol{v}}^a(t,X)\hat{\boldsymbol{b}}_a(t,X)$ with respect to time, i.e.

$$\partial_t \hat{\boldsymbol{v}}(t,X) \quad = [\partial_t \hat{\boldsymbol{v}}^a(t,X)]\hat{\boldsymbol{b}}_a(t,X) + \hat{\boldsymbol{v}}^a(t,X) \partial_t \hat{\boldsymbol{b}}_a(t,X) \ . \tag{1.17}$$

Since $\hat{\boldsymbol{b}}_a = \boldsymbol{b}_a \circ \chi$, we obtain the identity

$$\partial_t \hat{\boldsymbol{b}}_a(t,X) = \frac{\partial \boldsymbol{b}_a}{\partial x^b}(x) \partial_t \chi^b(t,X) = \frac{\partial \boldsymbol{b}_a}{\partial x^b}(x) \hat{\boldsymbol{v}}^b(t,X). \tag{1.18}$$

Substituting Eq. (1.18) into Eq. (1.17) yields

$$\partial_t \hat{\boldsymbol{v}}(t,X) = [\partial_t \hat{\boldsymbol{v}}^a(t,X)]\boldsymbol{b}_a(x) + \hat{\boldsymbol{v}}^a(t,X) \hat{\boldsymbol{v}}^b(t,X) \frac{\partial \boldsymbol{b}_a}{\partial x^b}(x). \tag{1.19}$$

By noting that

$$\frac{\partial \boldsymbol{b}_a}{\partial x^b}(x) = \left[\frac{\partial}{\partial x^b} \left(\frac{\partial \zeta^i}{\partial x^a} \right) \right](x) \boldsymbol{e_i} = \frac{\partial^2 \zeta^i}{\partial x^b \partial x^a}(x) \boldsymbol{e_i}, \tag{1.20}$$

and applying the inverse of Eq. (1.10), we obtain the identity

$$\frac{\partial \boldsymbol{b}_a}{\partial x^b}(x) = \frac{\partial^2 \zeta^i}{\partial x^b \partial x^a}(x)\boldsymbol{e_i} = \frac{\partial^2 \zeta^i}{\partial x^b \partial x^a}(x)\frac{\partial \xi^c}{\partial z^i}(z)b_c(x), \tag{1.21}$$

i.e., $\frac{\partial \boldsymbol{b}_a}{\partial x^b}(x) = \gamma^c_{ab}(x)\boldsymbol{b}_c(x)$, where the definition (1.16) has been used.
Finally, Eq. (1.15) is retrieved by substituting Eq. (1.21) into Eq. (1.17),

$$\partial_t \hat{\boldsymbol{v}}(t, X) = [\partial_t \hat{\boldsymbol{v}}^a(t, X) + \gamma^a_{bc}(x)\hat{\boldsymbol{v}}^b(t, X)\hat{\boldsymbol{v}}^c(t, X)]\boldsymbol{b}_a(x), \tag{1.22}$$

and noting that $\partial_t \hat{\boldsymbol{v}}(t, X) = \hat{\boldsymbol{a}}(t, X) = \hat{\boldsymbol{a}}^a(t, X)\boldsymbol{b}_a(x)$.

1.3.5 Covariant Derivative

Let $\boldsymbol{u}, \boldsymbol{v} : \Omega \to \mathbb{R}^3$ be two vector fields, and $\Omega \subset \mathbb{R}^3$ an open set. The *covariant derivative* of $\boldsymbol{v}$ along $\boldsymbol{u}$ is defined as the linear map, $D\boldsymbol{v}(x) : \mathbb{R}^3 \to \mathbb{R}^3$, such that the quantity $D\boldsymbol{v}(x) \cdot \boldsymbol{u}(x)$ is a vector field on $\mathbb{R}^3$. Covariant derivative may also be denoted with $\nabla_u \boldsymbol{v}(x)$. Moreover, the *a-th* component of $\nabla_u \boldsymbol{v}(x)$ is given by

$$(\nabla_u \boldsymbol{v}(x))^a = \frac{\partial \boldsymbol{v}^a}{\partial x^b}(x)u^b(x) + \gamma^a_{bc}(x)\boldsymbol{v}^b(x)\boldsymbol{u}^c(x). \tag{1.23}$$

In order to prove Eq. (1.23) we note that, in Euclidean coordinates, the covariant derivative reads

$$\nabla_u \boldsymbol{v}(x) = \left[\frac{\partial \boldsymbol{v}^i_{(E)}}{\partial z^j}(z)\boldsymbol{u}^j_{(E)}(z)\right]\boldsymbol{e_i} \tag{1.24}$$

By applying the transformation formulae

$$\begin{aligned} &\boldsymbol{v}^i_{(E)}(z) = \tfrac{\partial \zeta^i}{\partial x^c}(x)\boldsymbol{v}^c(x), \quad \boldsymbol{u}^j_{(E)}(z) = \tfrac{\partial \zeta^j}{\partial x^d}(x)\boldsymbol{u}^d(x), \\ &\boldsymbol{e_i} = \tfrac{\partial \xi^a}{\partial z^i}(z)\boldsymbol{b}_a(x), \end{aligned} \tag{1.25}$$

and substituting Eqs. (1.25) into Eq. (1.24), we obtain

$$\begin{aligned} \nabla_u \boldsymbol{v} \quad &= \left\{\left[\tfrac{\partial}{\partial z^j}\left(\tfrac{\partial \zeta^i}{\partial x^c}\boldsymbol{v}^c\right)\right]\left[\tfrac{\partial \zeta^j}{\partial x^d}\boldsymbol{u}^d(x)\right]\right\}\tfrac{\partial \xi^a}{\partial z^i}\boldsymbol{b}_a = \\ &= \left\{\left[\tfrac{\partial^2 \zeta^i}{\partial x^f \partial x^c}\tfrac{\partial \xi^f}{\partial z^j}\boldsymbol{v}^c + \tfrac{\partial \zeta^i}{\partial x^c}\tfrac{\partial \boldsymbol{v}^c}{\partial x^f}\tfrac{\partial \xi^f}{\partial z^j}\right]\tfrac{\partial \zeta^j}{\partial x^d}\boldsymbol{u}^d\right\}\tfrac{\partial \xi^a}{\partial z^i}\boldsymbol{b}_a = \\ &= \tfrac{\partial^2 \zeta^i}{\partial x^f \partial x^c}\tfrac{\partial \xi^f}{\partial z^j}\boldsymbol{v}^c\tfrac{\partial \zeta^j}{\partial x^d}\boldsymbol{u}^d\tfrac{\partial \xi^a}{\partial z^i}\boldsymbol{b}_a + \\ &+ \tfrac{\partial \zeta^i}{\partial x^c}\tfrac{\partial \boldsymbol{v}^c}{\partial x^f}\tfrac{\partial \xi^f}{\partial z^j}\tfrac{\partial \zeta^j}{\partial x^d}\boldsymbol{u}^d\tfrac{\partial \xi^a}{\partial z^i}\boldsymbol{b}_a. \end{aligned} \tag{1.26}$$

After noting that

$$\tfrac{\partial^2 \zeta^i}{\partial x^f \partial x^c}\tfrac{\partial \xi^a}{\partial z^i} = \gamma^a_{fc}, \quad \tfrac{\partial \xi^f}{\partial z^j}\tfrac{\partial \zeta^j}{\partial x^d} = \delta^f_d \ , \tag{1.27}$$

we rewrite Eq. (1.26) as

$$\begin{aligned}\nabla_u v &= \gamma^a_{fc}\delta^f_d \boldsymbol{v}^c \boldsymbol{u}^d \boldsymbol{b}_a + \delta^a_c \delta^f_d \tfrac{\partial \boldsymbol{v}^c}{\partial x^f} \boldsymbol{u}^d \boldsymbol{b}_a = \\ &= \left[\tfrac{\partial v^a}{\partial x^d} \boldsymbol{u}^d + \gamma^a_{dc} \boldsymbol{v}^c \boldsymbol{u}^d\right] \boldsymbol{b}_a.\end{aligned} \tag{1.28}$$

Finally, by introducing the notation

$$v^a{}_{|b} = \frac{\partial v^a}{\partial x^b} + \gamma^a_{bd} v^d, \tag{1.29}$$

covariant derivative can be given the compact form

$$\nabla_u v = (v^a{}_{|b} u^b) \boldsymbol{b}_a, \quad (\nabla_u v)^a = v^a{}_{|b} u^b \ . \tag{1.30}$$

1.3.6 Tangent Space and Tangent Bundle

Let $\mathrm{M} \subset \mathbb{R}^3$ be a manifold, and $P \in \mathrm{M}$. The *tangent space* to M at P coincides with the vector space $\mathbb{R}^3$ attached at P, and is denoted with $T_P\mathrm{M}$. The *tangent bundle* of M is defined by $T\mathrm{M} = \mathrm{M} \times T_P\mathrm{M}$, and consists of pairs $y_P = (P, y) \in \mathrm{M} \times T_P\mathrm{M}$.

Let B_R be the reference configuration of a body. For each $X \in \mathrm{B}_R$, the six-dimensional manifold $T\mathrm{B}_R = \mathrm{B}_R \times T_X\mathrm{B}_R$ is the tangent bundle of B_R.
The elements of $T\mathrm{B}_R$ are $Y_X = (X, Y(X))$, where $\{X^A\}^3_{A=1} = \{\Xi^A(Z)\}^3_{A=1}$ is an arbitrarily chosen coordinate system on B_R, $\{Z^I\}^3_{I=1}$ is the Euclidean coordinate system, and the components of the vector $\boldsymbol{Y}$ transforms as $Y^A = \frac{\partial \Xi^A}{\partial Z^I} Y^I_{(E)}$. Analogously, if B_t is the current configuration of the body, for each $x \in \mathrm{B}_t \subset \mathbb{R}^3$, the six-dimensional manifold $T\mathrm{B}_t = \mathrm{B}_t \times T_x\mathrm{B}_t$ is the tangent bundle of B_t. The elements of $T\mathrm{B}_t$ are $y_x = (x, y(x))$, where $\{x^a\}^3_{A=1} = \{\xi^a(z)\}^3_{a=1}$ in the coordinate system such that $x^a = \chi^a(t, X)$, and the components of $\boldsymbol{y}$ transform as $y^a = \frac{\partial \xi^a}{\partial z^i} y^i_{(E)}$.

By introducing a function $f : \mathrm{B}_R \to \mathbb{R}$, such that $f \in C^1(\mathrm{B}_R)$, we define the derivative of f along $\boldsymbol{Y}$ at $X \in \mathrm{B}_R$ as

$$Y_X[f] = Df(X) \cdot Y(X) = \frac{\partial f}{\partial X^A}(X) Y^A(X). \tag{1.31}$$

1.3.7 Tangent Map and Push Forward

Let $\chi_t = \chi(t, \cdot) : \mathrm{B}_R \to \mathbb{R}^3$ be a $C^1(\mathrm{B}_R)$ configuration field. The *tangent map* of χ_t is defined as the map

$$T\chi_t : T\mathrm{B}_R \to T\mathbb{R}^3, \tag{1.32}$$

such that

$$(X, Y) \to T\chi_t(X, Y) = (\chi_t(X), \nabla_Y \chi_t(X)). \tag{1.33}$$

Therefore, the tangent map, $T\chi_t$, associates to each point $X \in \mathrm{B}_R$ a point $x = \chi_t(X) \in \mathbb{R}^3$, and *transforms* each tangent vector $\boldsymbol{Y} \in T_X\mathrm{B}_R$ into the tangent vector $\boldsymbol{y} \in T_x\mathbb{R}^3$, such that $\boldsymbol{y} = \nabla_Y \chi_t$. In particular, the map $T\chi_t(X, \cdot)$ is said to be the *push forward* of the tangent vector $\boldsymbol{Y}$, and is defined by

$$(T\chi_t(X, \cdot))^a = (T\chi_t.Y_X)^a = (\chi_{t*}Y_X)^a = \frac{\partial \chi_t^a}{\partial X^A}(X)Y^A(X) \tag{1.34}$$

1.3.8 Tilt of a Vector Field

Let $\chi_t = \chi(t, \cdot) : \mathrm{B}_R \to \mathbb{R}^3$ be a $C^1(\mathrm{B}_R)$ configuration field and let $\boldsymbol{Y}$ be a vector field on B_R such that $Y_X = (X, Y(X)) \in T\mathrm{B}_R$. The map $V = T\chi_t \circ Y : \mathrm{B}_R \to T\mathbb{R}^3$ is said to be the *tilt* of $\boldsymbol{Y}$ by χ_t.

If χ_t is regular, the *push forward* of $\boldsymbol{Y}$ by χ_t is defined by

$$\chi_{t*}Y = T\chi_t.V_X = T\chi_t \circ Y \circ \chi_t^{-1}. \tag{1.35}$$

Moreover, the components of the push forward are given by

$$(\chi_{t*}Y(X))^a = \frac{\partial \chi_t^a}{\partial X^A}(X)Y^A(X). \tag{1.36}$$

Conversely, if $\boldsymbol{v}$ is a vector field on $\chi_t(\mathrm{B}_R) \subset \mathbb{R}^3$, and χ_t is regular, the *pull back* of $\boldsymbol{v}$ by χ_t is defined by

$$\chi_t{}^* v = T\chi_t^{-1} \circ v \circ \chi_t. \tag{1.37}$$

1.3.9 The Deformation Gradient

Let $\chi_t : \mathrm{B}_R \to \mathbb{R}^3$ be a $C^1(\mathrm{B}_R)$ configuration field. The tangent map of χ_t, $T\chi_t$, is also called *deformation gradient*, and is denoted by $\boldsymbol{F}$, thus $F(t, \cdot) = T\chi_t$. For each $X \in \mathrm{B}_R$, the linear map $F(t, X)$ represents the *restriction* of $\boldsymbol{F}$ to $T_X\mathrm{B}_R$. Consequently, the map $F(t, X) : T_X\mathrm{B}_R \to T_x\mathrm{B}_t$ (where $x = \chi(t, X)$, and $\mathrm{B}_t = \chi(t, \mathrm{B}_R)$) is a linear transformation for every pair $(t, X) \in \mathrm{I} \times \mathrm{B}_R$.

If $\{x^a\}_{a=1}^3 = \{\xi^a(z)\}_{a=1}^3$ and $\{X^A\}_{A=1}^3 = \{\Xi^A(Z)\}_{A=1}^3$ represent the coordinate systems on B_t and B_R, respectively, then the matrix of $F(t, X)$ with respect to the bases $\{\boldsymbol{b}_a(x)\}_{a=1}^3 \subset \mathrm{B}_t$ and $\{B_A(X)\}_{A=1}^3 \subset \mathrm{B}_R$ reads

$$F^a_A(t, X) = \frac{\partial \chi^a}{\partial X^A}(t, X). \tag{1.38}$$

1.3.10 Inner Product and Transpose of a Linear Application

Let M be a manifold, and $\boldsymbol{u}, \boldsymbol{v} \in T_x\mathrm{M}$ two vectors belonging to the tangent space to M at x. The inner product between $\boldsymbol{u}$ and $\boldsymbol{v}$ is defined as the *bilinear application*,

$$g_x(\cdot,\cdot) := \langle\cdot|\cdot\rangle_x : T_xM \times T_xM \to R \tag{1.39}$$

such that

$$g_x(u, v) = \langle u \mid v\rangle_x. \tag{1.40}$$

Since the tangent vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ can be decomposed as $\boldsymbol{u} = \boldsymbol{u}^a\boldsymbol{b}_a$ and $\boldsymbol{v} = \boldsymbol{v}^b\boldsymbol{b}_b$, respectively, Eq. (1.40) becomes

$$g_x(u, v) = g_x(\boldsymbol{u}^a\boldsymbol{b}_a, \boldsymbol{v}^b\boldsymbol{b}_b) = \boldsymbol{u}^a\boldsymbol{v}^b g_x(\boldsymbol{b}_a, \boldsymbol{b}_b). \tag{1.41}$$

Moreover, by introducing the notation $g_x(\boldsymbol{b}_a, b_b) = g_{ab}(x)$, we obtain

$$g_x(u, v) = u^a v^b g_{ab}(x). \tag{1.42}$$

By rewriting Eq. (1.41) as

$$g_x(u, v) = u^a v^b \frac{\partial\zeta^i}{\partial x^a}(x)\frac{\partial\zeta^j}{\partial x^b}(x) g(\boldsymbol{e_i}, e_j), \tag{1.43}$$

we conclude that

$$g_{ab}(x) = \frac{\partial\zeta^i}{\partial x^a}(x)\frac{\partial\zeta^j}{\partial x^b}(x)\delta_{ij}, \tag{1.44}$$

where $g(\boldsymbol{e_i}, e_j) = \delta_{ij}$. By applying the transformation formulae

$$u^i_{(E)}(x) = u^a \tfrac{\partial\zeta^i}{\partial x^a}(x), \quad v^j_{(E)}(x) = v^b \frac{\partial\zeta^j}{\partial x^b}(x), \tag{1.45}$$

Eq. (1.43) can be given the expression

$$g_x(u, v) = u^i_{(E)}(x) v^j_{(E)}(x)\delta_{ij}, \tag{1.46}$$

which coincides with the “standard” scalar product in $\mathbb{R}^3$.

Let $\mathrm{L}(X) : T_X\mathrm{B}_R \to T_x\mathbb{R}^3$ be a linear transformation, $U \in T_X\mathrm{B}_R$ and $v \in T_x\mathbb{R}^3$. The *transpose* of $\mathrm{L}(X)$ is the linear map, $\mathrm{L}^T(X) : T_x\mathbb{R}^3 \to T_X\mathrm{B}_R$, such that

$$\langle AU \mid v\rangle_x = \left\langle U \mid A^T v\right\rangle_X. \tag{1.47}$$

In components, Eq. (1.47) reads

$$\mathrm{L}^a_A U^A v^b g_{ab}(x) = U^A (\mathrm{L}^T)^B{}_b v^b G_{AB}(X), \tag{1.48}$$

where $G_{AB}(X) = G_X(B_A, B_B) = \frac{\partial Z^I}{\partial X^A}(X)\frac{\partial Z^J}{\partial X^B}(X)\delta_{IJ}$.

Equation (1.47) can be applied to calculate the components of the matrix of $F^T(t, X)$. By virtue of the definition of transpose of a linear application, the $F^T(t, X)$ must be such that

$$\langle FU \mid v\rangle_x = \left\langle U \mid F^T v\right\rangle_X. \tag{1.49}$$

In components, Eq. (1.49) reads

$$(F^t)^a{}_A U^A v^b \hat{g}_{ab} = U^A (F^T)^B{}_b v^b G_{AB}, \tag{1.50}$$

where $\hat{g}_{ab} = g_{ab} \circ \chi$.

Since Eq. (1.49) holds true for all U and v, Eq. (1.50) is equivalent to write

$$(F^t)^a{}_A \hat{g}_{ab} = G_{AB}(F^T)^B{}_b. \tag{1.51}$$

Finally, by multiplying Eq. (1.51) by G^{BC}, and noting that $G_{AB}G^{BC} = \delta^C_A$, we obtain

$$(F^T)^B{}_b = G^{AB}(F^t)^a{}_A \hat{g}_{ab}. \tag{1.52}$$

1.3.11 Green Stretch Tensor

The Green deformation tensor (also called Right Cauchy-Green deformation tensor, or *stretch tensor*) is a map $\mathbf{C}(t, X) : T_X\mathrm{B}_R \to T_X\mathrm{B}_R$ defined by

$$\mathbf{C}(t, X) = \mathbf{F}^T(t, X)\mathbf{F}(t, X). \tag{1.53}$$

In components, Eq. (1.53) reads

$$\mathbf{C}^A{}_B(t, X) = [(\mathbf{F}^T)^A{}_a \mathbf{F}^a{}_B](t, X) = (\mathbf{G}^{AC}(\mathbf{F}^t)^b{}_C \hat{g}_{ab} \mathbf{F}^a{}_B)(t, X). \tag{1.54}$$

The stretch tensor, $\mathbf{C}$, is symmetric and positive-semidefinite, i.e. $\langle \mathbf{C}\boldsymbol{U} \mid \boldsymbol{U}\rangle_X \geq 0$ for all $\boldsymbol{U}$. In particular, if $\mathbf{F}(t, X)$ is a one-to-one linear map (this condition holds true if χ_t is regular), then $\mathbf{C}(t, X)$ is invertible and positive-definite, i.e. $\langle \mathbf{C}\boldsymbol{U} \mid \boldsymbol{U}\rangle_X > 0$ for all $\boldsymbol{U}$ different from the zero vector.

1.3.12 Piola Deformation Tensor

The Piola transformation tensor (also called Left Cauchy-Green deformation tensor) is a map $\mathbf{B}(t,x) : T_x\mathrm{B}_t \to T_x\mathrm{B}_t$ defined by

$$\hat{\mathbf{B}}(t,X) = \mathbf{F}(t,X)\mathbf{F}^T(t,X), \tag{1.55}$$

where $\hat{\mathbf{B}}(t,\cdot) = \mathbf{B}(t,\cdot) \circ \chi_t$, and χ_t is a $C^1(\mathrm{B}_R)$ regular, and invertible configuration field such that $X = \chi_t^{-1}(x)$.

In components, Eq. (1.55) reads

$$\hat{\mathbf{B}}^a{}_b(t,X) = [\mathbf{F}^a{}_A(\mathbf{F}^t)^A{}_b](t,X) = (\mathbf{F}^a{}_A\hat{g}_{bc}\mathbf{F}^c{}_C\mathbf{G}^{AC})(t,X). \tag{1.56}$$

The tensor $\mathbf{B}$ is invertible and positive-definite, i.e. $\langle \mathbf{B}\boldsymbol{v} \mid \boldsymbol{v}\rangle > 0$ for all $\boldsymbol{v}$ different from the zero vector.

1.3.13 Polar Decomposition of the Deformation Gradient

The deformation gradient, $\mathbf{F}$, describes the entire deformation experienced by the body during its evolution from the reference configuration, B_R, to the current configuration, $\mathrm{B}_t = \chi(t,\mathrm{B}_R)$. The most general motion performed by the body is the superposition of a rigid motion and a deformation. Since rigid translations can always be eliminated without compromising the body description by a suitable redefinition of the configuration field (i.e. $\bar{\chi}(t,X) \to \chi(t,X) = \bar{\chi}(t,X) - \varphi(t)$, where $\varphi(t)$ denotes the rigid translation), the configuration field must take into account both rigid rotations and genuine deformations. Therefore, if we assume that the final (current) configuration of the body is given by the superposition of deformation, $\tilde{\chi}_t$, and a rigid rotation, r_t, we can describe the body motion by introducing an *intermediate* configuration, $\tilde{\mathrm{B}}_t$, such that

$$\tilde{\mathrm{B}}_t = \tilde{\chi}(t,\mathrm{B}_R), \quad \mathrm{B}_t = r(t,\tilde{\mathrm{B}}_t)\ , \tag{1.57}$$

and

$$x = \chi(t,X) = r(t,\tilde{x}) = r(t,\tilde{\chi}(t,X)) \Rightarrow \chi_t = r_t \circ \tilde{\chi}_t, \tag{1.58}$$

where $X \in \mathrm{B}_R$, $\tilde{x} \in \tilde{\mathrm{B}}_t$, and $x \in \mathrm{B}_t$. By virtue of Eq. (1.58) the deformation gradient turns out to be

$$\mathbf{F}^a{}_A = \frac{\partial\chi^a}{\partial X^A} = \frac{\partial r^a}{\partial\tilde{x}^B}\frac{\partial\tilde{\chi}^B}{\partial X^A} = R^a{}_B\boldsymbol{U}^B{}_A \Rightarrow \mathbf{F} = \mathbf{R}\boldsymbol{U}. \tag{1.59}$$

Equation (1.59) is said to be the *right polar decomposition* of the deformation gradient. It should be noted that $\mathbf{R}$ is a *orthogonal* tensor (i.e. $\mathbf{R}^T\mathbf{R} = I_{\tilde{\mathrm{B}}_t}$, and $\mathbf{R}\mathbf{R}^T = I_{\mathrm{B}_t}$), while $\boldsymbol{U}$ is a *symmetric* second order tensor.

Analogously, if we assume that the final configuration is given by superimposing a deformation, $\breve{\chi}_t$, to a rigid rotation, r_t, we can introduce an intermediate configuration, $\breve{\mathrm{B}}_t$, such that

$$\breve{\mathrm{B}}_t = r_t(\mathrm{B}_R), \quad \mathrm{B}_t = \breve{\chi}_t(\breve{\mathrm{B}}_t) \ , \tag{1.60}$$

and

$$x = \chi(t, X) = \breve{\chi}(t, \breve{x}) = \breve{\chi}(t, r(t, X)) \Rightarrow \chi_t = \breve{\chi}_t \circ r_t. \tag{1.61}$$

where $X \in \mathrm{B}_R$, $\breve{x} \in \breve{\mathrm{B}}_t$, and $x \in \mathrm{B}_t$. By virtue of Eq. (1.61), $\mathbf{F}$ can be written as the product of a symmetric tensor, $\mathbf{V}$, and the orthogonal tensor, $\mathbf{R}$, i.e.

$$\mathbf{F}^a{}_A = \frac{\partial \chi^a}{\partial X^A} = \frac{\partial \breve{\chi}^a}{\partial \breve{x}^b}\frac{\partial r^b}{\partial X^A} = \mathbf{V}^a{}_b \mathbf{R}^b{}_A \Rightarrow \mathbf{F} = \mathbf{V}\mathbf{R}. \tag{1.62}$$

Equation (1.62) is said to be the *left polar decomposition* of the deformation gradient. Equations (1.59) and (1.62) imply the identities $\boldsymbol{C} = \boldsymbol{U}^2$ and $\mathbf{B} = \mathbf{V}^2$.

1.3.14 Geometric Interpretation of the Stretch Tensor

Let $C_R \subset \mathrm{B}_R$ be a regular curve in the reference configuration, and let $\eta : [a, b] \to C_R$ be its parameterization, i.e. $\forall X \in C_R$, $\exists \lambda \in [a, b]$ such that $\eta(\lambda) = X$. On account of the configuration field, $\chi_t : \mathrm{B}_R \to \mathrm{B}_t$, the curve C_R is transformed into the curve $C_t = \chi(t, C_R)$ parameterized by the map $\tilde{\eta} = \chi_t \circ \eta$. In the current configuration, the length of the curve is given by

$$\tilde{\ell}(C_t) = \int_a^b \sqrt{\left\langle \tilde{\eta}'(\lambda) \,\middle|\, \tilde{\eta}'(\lambda) \right\rangle} d\lambda. \tag{1.63}$$

Since $\tilde{\eta}'(\lambda) = F(t, \eta(\lambda))\eta'(\lambda)$, Eq. (1.63) can be rewritten as

$$\tilde{\ell}(C_t) = \int_a^b \sqrt{\left\langle F(t, \eta(\lambda))\eta'(\lambda) \,\middle|\, F(t, \eta(\lambda))\eta'(\lambda) \right\rangle} d\lambda. \tag{1.64}$$

By applying the definition of transpose of a linear application (Eq. (1.47)), and the definition of the stretch tensor (Eq. (1.53)), Eq. (1.64) becomes

$$\tilde{\ell}(C_t) = \int_a^b \sqrt{\left\langle \eta'(\lambda) \,\middle|\, C(t, \eta(\lambda))\eta'(\lambda) \right\rangle} d\lambda. \tag{1.65}$$

In components, Eq. (1.65) reads

$$\begin{aligned} \tilde{\ell}(C_t) &= \int_a^b \sqrt{\eta'^A(\lambda) C^B_D(t,\eta(\lambda))\eta'^D(\lambda) G_{AB}(\eta(\lambda))}\, d\lambda = \\ &= \int_a^b \sqrt{C_{AD}(t,\eta(\lambda))\eta'^A(\lambda)\eta'^D(\lambda)}\, d\lambda\ . \end{aligned} \tag{1.66}$$

Equation (1.66) shows how the stretch tensor represents the *metric tensor* associated with the *deformation*.

1.3.15 Lagrange Strain Tensor

The Lagrange strain tensor is a map $\varepsilon : T\mathrm{B}_R \to T\mathrm{B}_R$ defined by

$$\varepsilon = \frac{1}{2}(\mathbf{C} - \mathbf{I}_{\mathrm{B}_R}). \tag{1.67}$$

In components, Eq. (1.67) reads

$$\varepsilon^A_B = \frac{1}{2}(\mathbf{C}^A_B - \delta^A_B). \tag{1.68}$$

By introducing the *displacement vector field*, $\boldsymbol{u}(t,X) = \chi(t,X) - X$, the gradient of $\boldsymbol{u}$ with respect to referential coordinates can be written as

$$\nabla_R \boldsymbol{u} = \nabla_R \chi - \mathbf{I}_{\mathrm{B}_R} = \mathbf{F} - \mathbf{I}_{\mathrm{B}_R} \Rightarrow \mathbf{F} = \nabla_R \boldsymbol{u} + \mathbf{I}_{\mathrm{B}_R}. \tag{1.69}$$

Consequently, Eq. (1.67) becomes

$$\begin{aligned} \varepsilon &= \frac{1}{2}\{[(\nabla_R \boldsymbol{u})^T + \mathbf{I}_{\mathrm{B}_R}][\nabla_R \boldsymbol{u} + \mathbf{I}_{\mathrm{B}_R}] - \mathbf{I}_{\mathrm{B}_R}\} = \\ &= \frac{1}{2}(\nabla_R \boldsymbol{u})^T \nabla_R \boldsymbol{u} + \frac{1}{2}\{(\nabla_R \boldsymbol{u})^T + \nabla_R \boldsymbol{u}\}. \end{aligned} \tag{1.70}$$

In the limit of *small strains*, the quadratic part of the strain tensor is negligible compared with the linear term. Thus, in this case, we can define a *linear strain tensor*, ε^{lin}, given by

$$\varepsilon^{lin} = \frac{1}{2}\{(\nabla_R \boldsymbol{u})^T + \nabla_R \boldsymbol{u}\}. \tag{1.71}$$

1.3.16 Covariant Derivative of the Velocity Field in the Reference Configuration

The deformation gradient enables us to determine the covariant derivative of the velocity field in the reference configuration. The gradient of the velocity field, $\hat{\boldsymbol{v}}(t,\cdot) : \mathrm{B}_R \to T\mathbb{R}^3$, with respect to referential coordinates is given by

$$\nabla_R \hat{\boldsymbol{v}} = (\nabla_R \hat{v}^a)\hat{\boldsymbol{b}}_{\boldsymbol{a}} + \hat{v}^a \nabla_R \hat{\boldsymbol{b}}_{\boldsymbol{a}}, \tag{1.72}$$

or

$$\frac{\partial \hat{\boldsymbol{v}}}{\partial X^A} = \frac{\partial \hat{v}^a}{\partial X^A}\hat{\boldsymbol{b}}_{\boldsymbol{a}} + \hat{v}^a \frac{\partial \hat{\boldsymbol{b}}_{\boldsymbol{a}}}{\partial X^A}. \tag{1.73}$$

Since $\hat{\boldsymbol{b}}_{\boldsymbol{a}} = \boldsymbol{b}_a \circ \chi_t$, we note that $\nabla_R \hat{\boldsymbol{b}}_{\boldsymbol{a}} = [(\nabla \boldsymbol{b}_a) \circ \chi_t]\mathbf{F}_t$. Therefore, Eq. (1.73) can be rewritten as

$$\frac{\partial \hat{\boldsymbol{v}}}{\partial X^A}(t, X) = \frac{\partial \hat{\boldsymbol{v}}^a}{\partial X^A}(t, X)\boldsymbol{b}_a(x) + \hat{\boldsymbol{v}}^a(t, X)\frac{\partial \boldsymbol{b}_a}{\partial x^b}(x)\mathbf{F}^b{}_A(t, X). \tag{1.74}$$

Moreover, by taking into account the identity

$$\frac{\partial \boldsymbol{b}_a}{\partial x^b} = \gamma^c_{ba}\boldsymbol{b}_c, \tag{1.75}$$

Eq. (1.74) can be rearranged as

$$\begin{aligned} \tfrac{\partial \hat{\boldsymbol{v}}}{\partial X^A}(t, X) \quad &= \left[\tfrac{\partial \hat{\boldsymbol{v}}^a}{\partial X^A}(t, X) + \hat{\boldsymbol{v}}^c(t, X)\gamma^a_{bc}(x)\mathbf{F}^b{}_A(t, X)\right]\boldsymbol{b}_a(x) = \\ &= \hat{\boldsymbol{v}}^a{}_{|A}(t, X)\boldsymbol{b}_a(x) \end{aligned} \tag{1.76}$$

and we may write $(\nabla_R \hat{\boldsymbol{v}})^a{}_A = \hat{\boldsymbol{v}}^a{}_{|A}$, where

$$(\nabla_R \hat{\boldsymbol{v}})^a{}_{|A} = \hat{\boldsymbol{v}}^a{}_{|A} = \frac{\partial \hat{\boldsymbol{v}}^a}{\partial X^A} + \hat{\gamma}^a_{bc}\hat{\boldsymbol{v}}^c\mathbf{F}^b{}_A \tag{1.77}$$

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1.4 Eulerian Formulation of the Kinematics of Continua

Let $\mathrm{B} \subset C^2(\mathbb{R}^+_0, \mathbb{R}^3)$ be a body, $\Omega \subset \mathbb{R}^3$ an open set, and $\mathrm{I} \subset \mathbb{R}^+_0$ an interval of time. We define *Eulerian pair* the subset $(\mathrm{I}, \Omega) \subset (\mathbb{R}^+_0, \mathbb{R}^3)$ such that $\Omega \subset \bigcap_{t \in \mathrm{I}} \mathrm{B}_t$. The set W, which does not vary with time, is called *Eulerian Control Volume*. The portion of the body "*controlled*" by the Eulerian pair, (I, Ω), is defined by the set

$$\mathrm{B}^{(\mathrm{I},\Omega)} = \{\ell \in \mathrm{B} | \ell(t) \in \Omega \forall t \in \mathrm{I}\}. \tag{1.78}$$

The set $\mathrm{B}^{(\mathrm{I},\Omega)} \subseteq \mathrm{B}$ contains all the trajectories which "pass" through the control volume, W, within the time interval I. The Lagrangian from of $\mathrm{B}^{(\mathrm{I},\Omega)}$ is given by

$$\mathrm{B}^{(\mathrm{I},\Omega)}_R = \{X \in \mathrm{B}_R | \chi(t, X) = \ell(t) \in \Omega \forall t \in \mathrm{I}\}. \tag{1.79}$$

The set $\mathrm{B}^{(\mathrm{I},\Omega)}_R$ contains the points of the reference configuration which reach the points of the control volume, Ω, at time t.

In principle, any physical quantity can be expressed either in the Lagrangian or Eulerian formalism. If we let ${}^E f : \mathrm{I} \times \Omega \to Y$ denote a physical quantity defined on the Eulerian pair (I, Ω), Y being a generic normed space, the Lagrangian form of the same quantity is given by

$\hat{f} : \mathrm{I} \times \mathrm{B}_R^{(\mathrm{I},\Omega)} \to Y$. In order to pass from the Eulerian to the Lagrangian description we introduce a map, $\tau : \mathrm{I} \times \mathrm{B}_R \to \mathrm{I}$, such that $\tau(t, X) = t$. This auxiliary map is called *time map* (Federico, 2000). This enables us to write

$$ {}^E f(t, x) = \hat{f}(t, X) = [{}^E f \circ (\tau, \chi)](t, X) \Rightarrow \hat{f} = {}^E f \circ (\tau, \chi). \tag{1.80}$$

In the following, we shall replace ${}^E f$ with f for the sake of simplicity.

1.4.1 Eulerian Velocity

In the Eulerian framework, velocity is given *a priori*. It is defined as a vector field on the Eulerian pair (I, Ω) which associates a velocity vector to any pair $(t, x) \in (\mathrm{I}, \Omega)$, i.e. $\boldsymbol{v} : \mathrm{I} \times \Omega \to \mathbb{R}^3$. Since this definition must be consistent with the Lagrangian definition of velocity, we obtain the identity

$$\boldsymbol{v}(t, x) = \hat{\boldsymbol{v}}(t, X) \Rightarrow \hat{\boldsymbol{v}} = \partial_t \chi = \boldsymbol{v} \circ (\tau, \chi), \tag{1.81}$$

where $\hat{\boldsymbol{v}} : \mathrm{I} \times \mathrm{B}_R^{(\mathrm{I},\Omega)} \to \mathbb{R}^3$.

1.4.2 Eulerian Acceleration

The Eulerian acceleration is a vector field, $\boldsymbol{a} : \mathrm{I} \times \Omega \to \mathbb{R}^3$, which associates an acceleration, $\boldsymbol{a}(t, x)$, to each pair $(t, x) \in \mathrm{I} \times \Omega$. In analogy, with Eq. (1.81), we write

$$\boldsymbol{a}(t, x) = \hat{\boldsymbol{a}}(t, X) \Rightarrow \hat{\boldsymbol{a}} = \partial_t \hat{\boldsymbol{v}} = \partial_t^2 \chi = \boldsymbol{a} \circ (\tau, \chi). \tag{1.82}$$

By virtue of Eq.(1.82) we note that

$$\begin{aligned} \hat{\boldsymbol{a}} &= \partial_t \hat{\boldsymbol{v}} = \partial_t [\boldsymbol{v} \circ (\tau, \chi)] = \\ &= \partial_t \boldsymbol{v} \circ (\tau, \chi) + [\nabla \boldsymbol{v} \circ (\tau, \chi)] \cdot [\boldsymbol{v} \circ (\tau, \chi)] = \\ &= \{\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}\} \circ (\tau, \chi). \end{aligned} \tag{1.83}$$

By introducing the *substantial derivative operator*, $D_t = \partial_t + \boldsymbol{v} \cdot \nabla \boldsymbol{v}$, we can rewrite Eq. (1.83) as

$$\hat{\boldsymbol{a}}(t, X) = \boldsymbol{a}(t, x) = D_t \boldsymbol{v}(t, x). \tag{1.84}$$

In components, we obtain

$$\hat{\boldsymbol{a}} = \partial_t (\hat{v}^a \hat{\boldsymbol{b}}_a) = (\partial_t \hat{v}^a) \hat{\boldsymbol{b}}_a + \hat{v}^a \partial_t \hat{\boldsymbol{b}}_a. \tag{1.85}$$

By noting that

$$\begin{aligned}\partial_t\hat{\boldsymbol{v}}^a &= \partial_t[\boldsymbol{v}^a \circ (\tau,\chi)] = \left\{\tfrac{\partial \boldsymbol{v}^a}{\partial t} + \tfrac{\partial bolds^a}{\partial x^b} v^b\right\} \circ (\tau,\chi),\\ \partial_t\hat{\boldsymbol{b}}_a &= \partial_t[\boldsymbol{b}_a \circ \chi] = \left\{\tfrac{\partial \boldsymbol{b}_a}{\partial x^b}\boldsymbol{v}^b\right\} \circ (\tau,\chi) = \{\gamma^c_{ab}\boldsymbol{b}_c\boldsymbol{v}^b\} \circ (\tau,\chi),\end{aligned} \tag{1.86}$$

Eq. (1.85) becomes

$$\boldsymbol{a}^a = \frac{\partial \boldsymbol{v}^a}{\partial t} + \boldsymbol{v}^b\frac{\partial \boldsymbol{v}^a}{\partial x^b} + \gamma^a_{bc}\boldsymbol{v}^b\boldsymbol{v}^c. \tag{1.87}$$

1.4.3 Decomposition of the Velocity Gradient, Rate of Deformation Tensor and Spin Tensor

In the Eulerian formalism, the velocity gradient is the second-order tensor $\mathbf{L} = \nabla\boldsymbol{v}$, and its components are given by

$$\mathbf{L}^a{}_b(t,x) = \frac{\partial \boldsymbol{v}^a}{\partial x^b}(t,x) + \gamma^a_{bc}(x)\boldsymbol{v}^c(t,x) = \mathbf{v}^a{}_{|b}(t,x). \tag{1.88}$$

Differentiation of $\mathbf{F}$ with respect to time may be written as

$$\begin{aligned}\partial_t\mathbf{F} &= \tfrac{\partial \mathbf{F}^i_{(E)\,I}}{\partial t}\boldsymbol{e_i}\otimes\mathbf{E}^I = \tfrac{\partial\hat{\boldsymbol{v}}^i_{(E)}}{\partial Z^I}\boldsymbol{e_i}\otimes\mathbf{E}^I =\\ &= \left(\tfrac{\partial \boldsymbol{v}^i_{(E)}}{\partial z^j}\mathbf{F}^j_{(E)\,I}\right)\boldsymbol{e_i}\otimes\mathbf{E}^I,\end{aligned} \tag{1.89}$$

where $\mathbf{F} = \mathbf{F}^i_{(E)\,I}e_i \otimes \mathbf{E}^I$ is the Euclidean decomposition of $\mathbf{F}$. Equation (1.89) enables us to state that

$$(\partial_t\mathbf{F})^i_{(E)\,I} = \partial_t\mathbf{F}^i_{(E)\,I} = \hat{\mathbf{L}}^i_{(E)\,j}\mathbf{F}^j_{(E)\,I}, \tag{1.90}$$

where $\hat{\mathbf{L}} = \mathbf{L}\circ(\tau,\chi)$. Equation (1.90) can be rearranged for generalized coordinates by noting that

$$\begin{aligned}\tfrac{\partial\hat{\boldsymbol{v}}^i_{(E)}}{\partial Z^I}\boldsymbol{e_i}\otimes E^I &= \tfrac{\partial}{\partial Z^I}\left(\tfrac{\partial\zeta^i}{\partial x^a}\hat{\boldsymbol{v}}^a\right)\boldsymbol{e_i}\otimes\mathbf{E}^I =\\ &= \left[\tfrac{\partial^2\zeta^i}{\partial x^b\partial x^a}\tfrac{\partial\xi^b}{\partial z^k}\mathbf{F}^k_{(E)\,I}\hat{\boldsymbol{v}}^a + \tfrac{\partial\zeta^i}{\partial x^a}\tfrac{\partial\hat{\boldsymbol{v}}^a}{\partial X^A}\tfrac{\partial\Xi^A}{\partial Z^I}\right]\boldsymbol{e_i}\otimes\mathbf{E}^I =\\ &= \tfrac{\partial^2\zeta^i}{\partial x^b\partial x^a}\tfrac{\partial\xi^b}{\partial z^k}\mathbf{F}^k_{(E)\,I}\hat{\boldsymbol{v}}^a\tfrac{\partial\xi^d}{\partial z^i}\tfrac{\partial Z^I}{\partial X^D}\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D+\\ &+\tfrac{\partial\zeta^i}{\partial x^a}\tfrac{\partial\hat{\boldsymbol{v}}^a}{\partial X^A}\tfrac{\partial\Xi^A}{\partial Z^I}\tfrac{\partial\xi^d}{\partial z^i}\tfrac{\partial Z^I}{\partial X^D}\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D =\\ &= \left(\hat{\gamma}^d_{ba}\hat{\boldsymbol{v}}^a\mathbf{F}^b{}_D + \tfrac{\partial\hat{\boldsymbol{v}}^d}{\partial X^D}\right)\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D.\end{aligned} \tag{1.91}$$

Therefore, we obtain that

$$\begin{aligned}\tfrac{\partial\hat{\boldsymbol{v}}^i_{(E)}}{\partial Z^I}\boldsymbol{e_i}\otimes\mathbf{E}^I &= \left(\hat{\gamma}^d_{ba}\hat{\boldsymbol{v}}^a\mathbf{F}^b{}_D + \tfrac{\partial\hat{\boldsymbol{v}}^d}{\partial X^D}\right)\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D =\\ &= \hat{\boldsymbol{v}}^d{}_{|D}\,\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D = [\boldsymbol{v}^d{}_{|b}\circ(\tau,\chi)]\mathbf{F}^b{}_D\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D.\end{aligned} \tag{1.92}$$

This result implies that

$$\partial_t\mathbf{F} = (\hat{\mathbf{L}}^d_b\mathbf{F}^b_D)\hat{\boldsymbol{b}}_d\otimes\hat{\mathbf{B}}^D \Rightarrow (\partial_t\mathbf{F})^d_D = \hat{\mathbf{L}}^d_b\mathbf{F}^b{}_D. \tag{1.93}$$

By virtue of Eq. (1.93), we conclude that the Lagrangian form of the velocity gradient is given by

$$\hat{\mathbf{L}}^a{}_b = (\partial_t\mathbf{F})^a{}_A(\mathbf{F}^{-1})^A{}_b \Rightarrow \hat{\mathbf{L}} = (\partial_t\mathbf{F})\mathbf{F}^{-1}. \tag{1.94}$$

Equation (1.94) is used to define the *rate of deformation tensor*. This tensor is found by differentiating the stretch tensor, $\mathbf{C}$, with respect to time, i.e.

$$\begin{aligned} \partial_t\mathbf{C} &= \partial_t(\mathbf{F}^T\mathbf{F}) = (\partial_t\mathbf{F}^T)\mathbf{F} + \mathbf{F}^T\partial_t\mathbf{F} = \\ &= \mathbf{F}^T\hat{\mathbf{L}}^T\mathbf{F} + \mathbf{F}^T\hat{\mathbf{L}}\mathbf{F} = 2\mathbf{F}^T\hat{\mathbf{D}}\mathbf{F}, \end{aligned} \tag{1.95}$$

where

$$\mathbf{D} = \tfrac{1}{2}(\mathbf{L}^T + \mathbf{L}), \hat{\mathbf{D}} = \mathbf{D} \circ (\tau, \chi), \tag{1.96}$$

is said to be the *rate of deformation tensor*, and coincides with the symmetric part of the velocity gradient.

By invoking the relation $\mathbf{C} = 2\varepsilon + \mathbf{I}_{\mathrm{B}_R}$, Eq. (1.96) can also be written as

$$\hat{\mathbf{D}} = \tfrac{1}{2}\mathbf{F}^{-T}(\partial_t\mathbf{C})\mathbf{F}^{-1}, \tag{1.97}$$

or

$$\hat{\mathbf{D}} = \mathbf{F}{-}T(\partial_t\varepsilon)\mathbf{F}^{-1}. \tag{1.98}$$

It is worthwhile to note that the tensor $\mathbf{D}$ represents the "part" of the velocity gradient related to the deformation process undergone by the body. Hence, the condition $\mathbf{D} = 0$ holds true if, and only if, the body experiences a rigid motion. This statement is known as Killing's Theorem (Marsden and Hughes, 1983; Liu, 2002). On the other hand, the "part" of the velocity gradient related to rigid motion, i.e. *pure rotation*, is given by the skew-symmetric part of $\mathbf{L}$, i.e.

$$\mathbf{W} = skew(\mathbf{L}) = \tfrac{1}{2}\{\mathbf{L} - \mathbf{L}^T\}. \tag{1.99}$$

The tensor $\mathbf{W}$ is the describes the *vorticity* field which is present within the body, and is usually called *spin tensor*. Therefore, the condition $\mathbf{W}(t, x) = 0$ means that the motion is *irrotational* at time t and location x. In particular, if this condition holds true for any $(t, x) \in (\mathrm{I}, \Omega)$, then the motion is said to be *irrotational* within the whole control volume. In this case, and assuming that W is a connected domain (Smirnov, 1964), the velocity field is a *potential field*, i.e. there exists a scalar field, F, such that $\boldsymbol{v} = -\nabla\Phi$. By introducing the permutation symbols, $\in^{ijk}$, the components of the vorticity field, $\boldsymbol{\omega} = \nabla \times \boldsymbol{v}$, associated with the velocity vector, $\boldsymbol{v}$, can be expressed by

$$\omega^i = \in^{ijk} W_{jk} = \in^{ijk} g_{jl} W^l{}_k. \tag{1.100}$$

Chapter 2

Balance and Constitutive Laws in Continuum Physics

2.1 Introduction

In this Chapter will be presented the “classical” formulation of Dynamics and Thermodynamics of Continua (cfr. Truesdell e Toupin, 1960; Truesdell e Noll, 1965; Marsden and Hughes, 1983; ilhavι, 1997), giving an overview on some fundamental concepts of Continuum Physics.

Using some tools of Differential Geometry and Functional Analysis, we will present the Theory of Constitutive Law (Day, 1972; Liu, 2002; Eringen, 2002). In order to do that we need to introduce the mathematical framework that we are going to use, i.e., Piola transformation, First and the Second Principle of Thermo-dynamics in terms of generalised balance laws, thermo-mechanic constraint’s concept .

2.2 Balance Laws

Balance principles can be expressed either in integral (global) form or in differential (local) form (the Reader is referred to Eringen (2002) for the details related to the generalization of balance laws to non-local continua). In regions of space where physical quantities vary sufficiently smoothly, balance laws are equivalent to *differential field equations*; on the other hand, in the presence of surfaces of discontinuity, they are to be expressed by means of *jump conditions* (Truesdell and Toupin, 1960; ilhav, 1997). In the following, we will consider as hypothesis the *saturation condition*, i.e. the sum of solid- and fluid-phase volume fractions, denoted by ϕ_S and ϕ_F, respectively, is equal the unity at all times and all points of the mixture , $\phi_S + \phi_F = 1$. Volume fraction of phase $\mathscr{F}_j$, ϕ_j $(j = S, F)$, is defined by the ratio $\phi_j = |\Omega_j|/|\Omega|$, where Ω and Ω_j are the volumes of the Representative Volume Element (RVE), and the j-th phase contained in the RVE, respectively.

If we denote by ψ a generic macroscopic physical quantity, the notation $\psi_{\alpha j}$ means that quantity ψ refers to the α-th constituent in the j-phase, $\mathscr{C}_{\alpha j}$. Index α ranges between 0 and N. The notation $\psi^p_{\alpha j}$ represents a physical quantity defined at the pore-scale, whose macroscopic counterpart is $\psi_{\alpha j}$.

Following (19), we define the intrinsic mass density of phase $\mathscr{F}_j$ as the sum of mass densities of all constituents $\mathscr{C}_{\alpha j}$, i.e. [1]

$$\rho_j := \sum_{\alpha=0}^{N} \rho_{\alpha j}. \tag{2.1}$$

Mass fractions, $C_{\alpha j}$ (with $\alpha \in \{0, \ldots, N\}$ and $j = S, F$), are defined by the ratios $C_{\alpha j} := \rho_{\alpha j}/\rho_j$ and constrained to satisfy the condition

$$\sum_{\alpha=0}^{N} C_{\alpha j} = 1. \tag{2.2}$$

Such that they are not independent on each other. With respect to each constituent $\mathscr{C}_{\alpha j}$ *inphase* $\mathscr{F}_j$ *(with$\alpha \in \{0, \ldots, N\}$ and$j \in \{F, S\}$* , the macroscopic balance laws can be written in the following general form:

$$\frac{\partial(\varphi_j \rho_j C_{\alpha j} \psi_{\alpha j})}{\partial t} + \nabla \cdot (\varphi_j \rho_j C_{\alpha j} \psi_{\alpha j} \mathbf{v}_{\alpha j}) + \nabla \cdot \Phi_{\alpha j} - \varphi_j \rho_j C_{\alpha j} \mathrm{F}_{\alpha j} = \varphi_j \rho_j C_{\alpha j} \mathrm{G}_{\alpha j} \tag{2.3}$$

Here, $\boldsymbol{v}_{\alpha j}$ is the velocity, $\Phi_{\alpha j}$ denote *flux*, $F_{\alpha j}$ net production (or decay) and $G_{\alpha j}$ the source (or sink) of the generic thermodynamic quantity $\psi_{\alpha j}$ associated with constituent $\mathscr{C}_{\alpha j}$. Eq. (2.3) is a compact way of writing balance of mass, momentum, energy, entropy and balance laws are obtained in specific form by substituting the quantities in Tables 2.1 and 2.2 into eq. (2.3). Quantity $\psi_{\alpha j}$ may represent either a scalar or a vector field. In the case of balance of momentum, $\psi_{\alpha j}$ is identified with $\mathbf{v}_{\alpha j}$, quantities $\mathrm{F}_{\alpha j}$ and $\mathrm{G}_{\alpha j}$ are vector fields, flux $\boldsymbol{\Phi}_{\alpha j}$ is a

---

[1] Since a given density $\rho_{\alpha j}$ measures the amount of mass of α-th constituent in the portion of RVE occupied by the j-th phase, it is not truly intrinsic. The true intrinsic mass density of the α-th constituents in the j-th phase, denoted by $\rho^*_{\alpha j}$, is determined by $\rho_{\alpha j} = \varphi_{\alpha j} \rho^*_{\alpha j}$, where $\varphi_{\alpha j}$ is the volume fraction of the α-th constituent in the subregion Ω_j of the RVE. Multiplication of Equation (2.1) by ϕ_j allows for re-defining the intrinsic mass density of the j-th phase by $\phi_j \rho_j := \sum_{\alpha=0}^{N} \varphi^*_{\alpha j} \rho^*_{\alpha j}$, where $\varphi^*_{\alpha j} := \phi_j \varphi_{\alpha j}$ is the volume fraction of the α-th constituent referred to the volume of the RVE. In this case, mass fraction $C_{\alpha j}$ should be understood by the ratio $C_{\alpha j} := (\varphi^*_{\alpha j} \rho^*_{\alpha j})/(\phi_j \rho_j)$.

Table 2.1: Thermodynamic quantities and related fluxes to be substituted in eq. *(2.3)*

Quantity	$\psi_{\alpha j}$	$\mathbf{\Phi}_{\alpha j}$
Mass	1	$\mathbf{0}$
Momentum	$\mathbf{v}_{\alpha j}$	$-\boldsymbol{\sigma}_{\alpha j}$
Energy	$E_{\alpha j} + \frac{1}{2}\mathrm{v}_{\alpha j}^2$	$-(\boldsymbol{\sigma}_{\alpha j}.\mathbf{v}_{\alpha j} + \mathbf{q}_{\alpha j})$
Entropy	$S_{\alpha j}$	$-\Theta^{-1}\mathbf{q}_{\alpha j}$

Table 2.2: Net production (decay) and source (sink) terms to be substituted in eq. *(2.3)*

Quantity	$\mathrm{F}_{\alpha j}$	$\mathrm{G}_{\alpha j}$
Mass	0	$R_{\alpha j}$
Momentum	$\mathbf{g}$	$R_{\alpha j}\mathbf{v}_{\alpha j} + \mathbf{T}_{\alpha j}$
Energy	$\mathbf{g} \cdot \mathbf{v}_{\alpha j} + h_{\alpha j}$	$R_{\alpha j}(E_{\alpha j} + \frac{1}{2}\mathrm{v}_{\alpha j}^2) + \mathbf{T}_{\alpha j} \cdot \mathbf{v}_{\alpha j} + Q_{\alpha j} + Q_{\alpha j}^*$
Entropy	$\Theta^{-1}h_{\alpha j}$	$\Gamma_{\alpha j} + R_{\alpha j}S_{\alpha j} + \eta_{\alpha j} + \eta_{\alpha j}^*$

second-order tensor, and the product $\psi_{\alpha j}\mathbf{v}_{\alpha j}$ on the LHS of eq. (2.3) is understood as the dyadic product $\psi_{\alpha j}\mathbf{v}_{\alpha j} = \mathbf{v}_{\alpha j} \otimes \mathbf{v}_{\alpha j}$.

In Table 2.1 and 2.2, $E_{\alpha j}$ is internal energy density, $\boldsymbol{\sigma}_{\alpha j}$ is the Cauchy stress tensor, $\mathbf{q}_{\alpha j}$ is the heat flux vector, Θ is absolute temperature, $S_{\alpha j}$ is entropy density, $\mathbf{g}$ is gravity acceleration vector, and $R_{\alpha j}$, $\mathbf{T}_{\alpha j}$, $Q_{\alpha j}$, and $\eta_{\alpha j}$ are sources (or sinks) of mass, momentum, energy, and entropy due to exchange interactions among constituents. Finally, in Table 2.2, $Q_{\alpha j}^*$ and $\eta_{\alpha j}^*$ represent a source of internal energy, and entropy related to remodelling and growth. Although here a rather general formalism has been used, these last two quantities are referred only to the solid-phase. Therefore, it is understood that $Q_{\alpha F}^* = 0$, and $\eta_{\alpha F}^* = 0$ for all fluid-phase constituents $\mathscr{C}_{\alpha F}$ ($\alpha \in \{0, \ldots, N\}$).

2.2.1 Mass Balance Law

The mass balance of constituent $\mathscr{C}_{\alpha j}$ ($\alpha \in \{0, ..., N\}$, $j = S, F$) can be written as

$$\frac{\partial(\phi_j\rho_j C_{\alpha j})}{\partial t} + \nabla \cdot (\phi_j\rho_j C_{\alpha j}\boldsymbol{v}_{\alpha j}) = \phi_j\rho_j C_{\alpha j} r_{\alpha j}, \tag{2.4}$$

where $\boldsymbol{v}_{\alpha j}$ is velocity of constituent $\mathscr{C}_{\alpha j}$, and $r_{\alpha j}$ represents the rate at which mass is gained or lost by constituent $\mathscr{C}_{\alpha j}$.

Summing Equation (2.4) over all $N + 1$ constituents of phase $\mathscr{F}_j$ leads to the mass balance of phase $\mathscr{F}_j$, i.e.

$$\frac{\partial(\phi_j\rho_j)}{\partial t} + \nabla\cdot(\phi_j\rho_j\boldsymbol{v}_j) = \phi_j\rho_jR_j, \tag{2.5}$$

where $\boldsymbol{v}_j$ and R_j are defined by the relations

$$\phi_j\rho_j\boldsymbol{v}_j := \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}\boldsymbol{v}_{\alpha j}, \tag{2.6}$$

$$\phi_j\rho_jR_j := \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}r_{\alpha j}. \tag{2.7}$$

Quantity $\boldsymbol{v}_j$ is the average velocity of phase $\mathscr{F}_j$, i.e. the velocity of the center of mass of phase $\mathscr{F}_j$, and the term $\phi_j\rho_jR_j$ measures the rate at which mass increases, or decreases, in phase $\mathscr{F}_j$.

Since the mass of the mixture cannot be conserved in the presence of growth, the sum of Equation (2.5) over all phases yields

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) = \rho R, \tag{2.8}$$

where mixture mass density, ρ, mixture velocity, $\boldsymbol{v}$, and overall mass source, R, are defined by

$$\rho = \sum_{j=S,F}\phi_j\rho_j, \tag{2.9}$$

$$\rho\boldsymbol{v} = \sum_{j=S,F}\phi_j\rho_j\boldsymbol{v}_j, \tag{2.10}$$

$$\rho R = \sum_{j=S,F}\phi_j\rho_jR_j. \tag{2.11}$$

2.2.2 Linear Momentum Balance Law

The balance of momentum of constituent $\mathscr{C}_{\alpha j}$ ($\alpha \in \{0, ..., N\}$, $j = S, F$) reads

$$\frac{\partial(\phi_j\rho_jC_{\alpha j}\boldsymbol{v}_{\alpha j})}{\partial t} + \nabla\cdot(\phi_j\rho_jC_{\alpha j}\boldsymbol{v}_{\alpha j}\otimes\boldsymbol{v}_{\alpha j}) - \nabla\cdot\boldsymbol{\sigma}_{\alpha j} - \phi_j\rho_jC_{\alpha j}\boldsymbol{g} = \phi_j\rho_jC_{\alpha j}(r_{\alpha j}\boldsymbol{v}_{\alpha j} + \boldsymbol{t}_{\alpha j}), \tag{2.12}$$

where $\boldsymbol{\sigma}_{\alpha j}$ is Cauchy stress tensor, $\boldsymbol{g}$ is the gravity acceleration vector, and terms $\phi_j\rho_jC_{\alpha j}r_{\alpha j}\boldsymbol{v}_{\alpha j}$ and $\phi_j\rho_jC_{\alpha j}\boldsymbol{t}_{\alpha j}$ are sources of momentum due to both increase, or decrease, of mass of constituent $\mathscr{C}_{\alpha j}$, and interactions among constituent $\mathscr{C}_{\alpha j}$ and all other constituents.

Summing Equation (2.12) over all $N + 1$ constituents within phase $\mathscr{F}_j$ leads to the balance of momentum for phase $\mathscr{F}_j$, i.e.

$$\frac{\partial(\phi_j\rho_j\boldsymbol{v}_j)}{\partial t} + \nabla\cdot(\phi_j\rho_j\boldsymbol{v}_j\otimes\boldsymbol{v}_j) - \nabla\cdot\boldsymbol{\sigma}_j - \phi_j\rho_j\boldsymbol{g} = \phi_j\rho_j(R_j\boldsymbol{v}_j + \boldsymbol{T}_j). \tag{2.13}$$

Here, $\boldsymbol{\sigma_j}$ is the overall Cauchy stress tensor of phase $\mathscr{F}_j$, and $\phi_j\rho_j\boldsymbol{T}_j$ is the source of momentum accounting for both mass production, and macroscale interactions among phase constituents. Quantities $\boldsymbol{\sigma_j}$ and $\phi_j\rho_j\boldsymbol{T}_j$ are defined by

$$
\begin{aligned}
\boldsymbol{\sigma_j} &= \sum_{\alpha=0}^{N}[\boldsymbol{\sigma}_{\alpha j} - \phi_j\rho_j C_{\alpha j}\boldsymbol{u}_{\alpha j}\otimes\boldsymbol{u}_{\alpha j}], &\quad (2.14)\\
\phi_j\rho_j\boldsymbol{T}_j &= \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}(\boldsymbol{t}_{\alpha j} + r_{\alpha j}\boldsymbol{u}_{\alpha j}), &\quad (2.15)
\end{aligned}
$$

where $\boldsymbol{u}_{\alpha j} := \boldsymbol{v}_{\alpha j} - \boldsymbol{v}_j$ is the relative velocity of constituent $\mathscr{C}_{\alpha j}$ with respect to phase velocity $\boldsymbol{v}_j$.

The balance of momentum for the mixture as a whole is found by summing Equation (2.13) over all phases $\mathscr{F}_j$ ($j = S, F$), i.e.

$$
\frac{\partial(\rho\boldsymbol{v})}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}\otimes\boldsymbol{v}) - \nabla\cdot\boldsymbol{\sigma} - \rho\boldsymbol{g} = \rho(R\boldsymbol{v} + \boldsymbol{T}), \qquad (2.16)
$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{T}$ are mixture overall Cauchy stress tensor, and momentum production, respectively, i.e.

$$
\begin{aligned}
\boldsymbol{\sigma} &:= \sum_{j=F,S}[\boldsymbol{\sigma}_j - \phi_j\rho_j(\boldsymbol{v_j} - \boldsymbol{v})\otimes(\boldsymbol{v_j} - \boldsymbol{v})], &\quad (2.17)\\
\rho\boldsymbol{T} &:= \sum_{j=S,F}\phi_j\rho_j[\boldsymbol{T}_j + R_j(\boldsymbol{v}_j - \boldsymbol{v})]. &\quad (2.18)
\end{aligned}
$$

2.2.3 Energy Balance Law – First Principle of Thermodynamics

The balance of energy of constituent $\mathscr{C}_{\alpha j}$ ($\alpha \in \{0, ..., N\}$, $j = S, F$) reads

$$
\begin{aligned}
&\frac{\partial}{\partial t}\Big[\phi_j\rho_j C_{\alpha j}\Big(E_{\alpha j} + \frac{1}{2}v_{\alpha j}^2\Big)\Big] + \nabla\cdot\Big[\phi_j\rho_j C_{\alpha j}\Big(E_{\alpha j} + \frac{1}{2}v_{\alpha j}^2\Big)\boldsymbol{v}_{\alpha j}\Big]\\
&\quad = \nabla\cdot(\boldsymbol{\sigma}_{\alpha j}.\boldsymbol{v}_{\alpha j}) + \nabla\cdot\boldsymbol{q}_{\alpha j} + \phi_j\rho_j C_{\alpha j}\boldsymbol{g}\cdot\boldsymbol{v}_{\alpha j} + \phi_j\rho_j C_{\alpha j}h_{\alpha j}\\
&\qquad + \phi_j\rho_j C_{\alpha j}\Big[r_{\alpha j}\Big(E_{\alpha j} + \frac{1}{2}v_{\alpha j}^2\Big) + \boldsymbol{t}_{\alpha j}\cdot\boldsymbol{v}_{\alpha j} + e_{\alpha j}\Big], \qquad (2.19)
\end{aligned}
$$

where $E_{\alpha j}$ is internal energy density, $\boldsymbol{q}_{\alpha j}$ is heat flux vector, $h_{\alpha j}$ is an energy source related to both radiative effects and pore-scale mechanical interactions among constituents (cf. (19) for details), and terms $r_{\alpha j}(E_{\alpha j} + \frac{1}{2}v_{\alpha j}^2)$, $\boldsymbol{t}_{\alpha j}\cdot\boldsymbol{v}_{\alpha j}$, and $e_{\alpha j}$ are energy sources accounting for mass production, and interactions of constituent $\mathscr{C}_{\alpha j}$ with all other constituents.

Summing Equation (2.19) over all $N+1$ constituents $\mathscr{C}_{\alpha j}$ ($\alpha \in \{0, \dots, N\}$) in phase $\mathscr{F}_j$ yields the balance of energy for phase $\mathscr{F}_j$, i.e.

$$\begin{aligned}
&\frac{\partial}{\partial t}\Big[\phi_j\rho_j\Big(E_j + \frac{1}{2}v_j^2\Big)\Big] + \nabla\cdot\Big[\phi_j\rho_j\Big(E_j + \frac{1}{2}v_j^2\Big)\boldsymbol{v}_j\Big] \\
&\quad = \nabla\cdot(\boldsymbol{\sigma}_j.\boldsymbol{v}_j) + \nabla\cdot\boldsymbol{q}_j + \phi_j\rho_j\boldsymbol{g}\cdot\boldsymbol{v}_j + \phi_j\rho_j h_j \\
&\qquad + \phi_j\rho_j\Big[R_j\Big(E_j + \frac{1}{2}v_j^2\Big) + \boldsymbol{T}_j\cdot\boldsymbol{v}_j + Q_j\Big]. \qquad (2.20)
\end{aligned}$$

Here, E_j and $\boldsymbol{q}_j$ are overall internal energy density and heat flux vector of phase $\mathscr{F}_j$, respectively, h_j accounts for energy sources due to both radiation and relative motion of constituents with respect to phase velocity, and Q_j is the source of energy due to mass production, mechanical interactions among constituents, and thermal effects. Quantities E_j, $\boldsymbol{q}_j$, h_j, and Q_j are defined by [1]

$$\begin{aligned}
\phi_j\rho_j E_j &:= \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\Big(E_{\alpha j} + \frac{1}{2}u_{\alpha j}^2\Big), && (2.21)\\
\boldsymbol{q}_j &:= \sum_{\alpha=0}^{N}\Big[\boldsymbol{q}_{\alpha j} - \phi_j\rho_j C_{\alpha j}\Big(E_{\alpha j} + \frac{1}{2}u_{\alpha j}^2\Big)\boldsymbol{u}_{\alpha j} + \boldsymbol{\sigma}_{\alpha j}\cdot\boldsymbol{u}_{\alpha j}\Big], && (2.22)\\
\phi_j\rho_j h_j &:= \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}(h_{\alpha j} + \boldsymbol{g}\cdot\boldsymbol{u}_{\alpha j}), && (2.23)\\
\phi_j\rho_j Q_j &:= \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\Big[e_{\alpha j} + \boldsymbol{t}_{\alpha j}\cdot\boldsymbol{u}_{\alpha j} + r_{\alpha j}\Big(E_{\alpha j} - E_j + \frac{1}{2}u_{\alpha j}^2\Big)\Big]. && (2.24)
\end{aligned}$$

In order to obtain the balance of energy for the mixture as a whole, we sum Equation (2.20) over the fluid- and solid-phase, i.e.

$$\begin{aligned}
\frac{\partial}{\partial t}\Big[\rho\Big(E + \frac{1}{2}v^2\Big)\Big] + \nabla\cdot\Big[\rho\Big(E + \frac{1}{2}v^2\Big)\boldsymbol{v}\Big] &= \nabla\cdot(\boldsymbol{\sigma}.\boldsymbol{v} + \boldsymbol{q}) + \rho\boldsymbol{g}\cdot\boldsymbol{v} + \rho h \\
&\quad + \rho\Big[R\Big(E + \frac{1}{2}v^2\Big) + \boldsymbol{T}\cdot\boldsymbol{v} + Q\Big]. \qquad (2.25)
\end{aligned}$$

where E and $\boldsymbol{q}$ are mixture internal energy and heat flux vector, respectively, h is the mixture energy source due to radiation and phase mechanical interactions, and Q is an energy source due mass production, mechanical interactions, and thermal effects. These quantities are defined

---

[1] All these quantities are composed of an *inner* (or averaged) part, given by the first terms on the RHS of Equations (2.21)-(2.24), and diffusive contributions identified with the second to fourth terms on the RHS of Equations (2.21)-(2.24).

by

$$\rho E \;:=\; \sum_{j=F,S} \phi_j\rho_j\Big(E_j + \frac{1}{2}(\boldsymbol{v}_j - \boldsymbol{v})^2\Big), \tag{2.26}$$

$$\boldsymbol{q} \;:=\; \sum_{j=F,S} \Big[\boldsymbol{q}_j - \phi_j\rho_j\Big(E_j + \frac{1}{2}(\boldsymbol{v}_j - \boldsymbol{v})^2\Big)(\boldsymbol{v}_j - \boldsymbol{v}) + \boldsymbol{\sigma}_j \cdot (\boldsymbol{v}_j - \boldsymbol{v})\Big], \tag{2.27}$$

$$\rho h \;:=\; \sum_{j=S,F} \phi_j\rho_j[h_j + \boldsymbol{g} \cdot (\boldsymbol{v}_j - \boldsymbol{v})], \tag{2.28}$$

$$\rho Q \;:=\; \sum_{j=S,F} \phi_j\rho_j\Big[R_j\Big(E_j - E + \frac{1}{2}(\boldsymbol{v}_j - \boldsymbol{v})^2\Big) + \boldsymbol{T}_j \cdot (\boldsymbol{v}_j - \boldsymbol{v}) + Q_j\Big]. \tag{2.29}$$

2.3 Clausius-Duhem Inequality

Clausius-Duhem Inequality is usually taken as the basis of a phenomenological treatment of Thermodynamics of Continua (Maugin, 1999). This is essentially the picture given by B. D. Coleman, W. Noll, C. A. Truesdell and their co-workers in the 1960s (cfr. Maugin (1999) and references therein) while establishing the foundations of Rational Thermodynamics. Such a theory postulates that those notions which precisely could be defined only at *equilibrium* in *Thermostatics* (Giles, 1964; Callen, 1985), exist *a priori* for any thermo-mechanical state, even largely outside from equilibrium (Maugin, 1999). Consequently, the notions of *temperature*, Θ, and *entropy*, η, are granted to any state, and their existence is assumed, so that the formal bases of this thermodynamics are the *a priori* statement of the first and second of Thermodynamics.

The importance of the Clausius-Duhem inequality lies in the fact that it is able to provide a simultaneous description of the mechanics and thermodynamics of the body by evidencing the *independent thermo-mechanical variables* which are the “most naturally suitable” for the body phenomenological characterization.

Since it is possible to apply the Clausius-Duhem inequality to any kind of body behaviour, it acquires the meaning of a *constraint* which has to be respected for the processes undergone by the body itself to be *thermo-mechanically admissible*. This is the basis of the Theory of the Constitutive Law.

2.4 Entropy Principle – Second Principle of Thermodynamics

In order to obtain Clausius-Duhem form of the entropy balance for constituent $\mathscr{C}_{\alpha j}$, we introduce the Helmholtz free energy density of constituent $\mathscr{C}_{\alpha j}$,

$$A_{\alpha j} := E_{\alpha j} - \Theta S_{\alpha j}, \tag{2.30}$$

substitute Equation (2.30) into energy balance law (2.19), and combine the result with Equation (2.20) so to obtain [1]

$$\begin{aligned}\Theta\phi_j\rho_j C_{\alpha j}\Gamma_{\alpha j} \quad = \quad & -\phi_j\rho_j C_{\alpha j}\frac{D_{\alpha j}A_{\alpha j}}{Dt} - \phi_j\rho_j C_{\alpha j}S_{\alpha j}\frac{D_{\alpha j}\Theta}{Dt} + \boldsymbol{\sigma}_{\alpha j} : \nabla\boldsymbol{v}_{\alpha j} \\ & + \boldsymbol{q}_{\alpha j}\cdot\frac{\nabla\Theta}{\Theta} + \phi_j\rho_j C_{\alpha j}r_{\alpha j}\Theta S_{\alpha j} + \phi_j\rho_j C_{\alpha j}e_{\alpha j} \\ & - \phi_j\rho_j C_{\alpha j}\Theta(r_{\alpha j}S_{\alpha j} + \eta_{\alpha j}). \end{aligned} \tag{2.31}$$

Summing over all $N+1$ constituents in phase $\mathscr{F}_j$, and accounting for Leibniz rule of differentiation and mass balance, lead to the following identity [2] :

$$\begin{aligned}\sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\frac{D_{\alpha j}A_{\alpha j}}{Dt} \;=\; & \phi_j\rho_j\frac{D_j A_j}{Dt} + \sum_{\alpha=0}^{N}\nabla\cdot[\phi_j\rho_j C_{\alpha j}A_{\alpha j}\boldsymbol{u}_{\alpha j}] \\ & - \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}r_{\alpha j}(A_{\alpha j} - A_j), \end{aligned} \tag{2.32}$$

where A_j is the Helmholtz free energy density of phase $\mathscr{F}_j$. In order for Equation (2.32) to hold, quantity A_j has to be defined as the sum of the $N+1$ single-constituent Helmholtz free energy densities, i.e.

$$\phi_j\rho_j A_j := \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}A_{\alpha j}. \tag{2.33}$$

---

[1] The symbol

$$\frac{D_{\alpha j}}{Dt} := \frac{\partial}{\partial t} + \boldsymbol{v}_{\alpha j}\cdot\nabla$$

represents the *convective* derivative operator with respect to the motion of constituent $\mathscr{C}_{\alpha j}$.

[2] The symbol

$$\frac{D_j}{Dt} := \frac{\partial}{\partial t} + \boldsymbol{v}_j\cdot\nabla$$

is said to be the *convective* derivative operator with respect to the motion of phase $\mathscr{F}_j$.

By summing Equation (2.31) over all $N+1$ constituents α (with $\alpha \in \{0,\dots,N\}$), using Equation (2.33), and performing some algebraic manipulations, the expression of entropy production for phase $\mathscr{F}_j$ reads

$$\begin{aligned}
\Theta\phi_j\rho_j\Gamma_j = & -\phi_j\rho_j\frac{D_jA_j}{Dt} - \phi_j\rho_j S_j\frac{D_j\Theta}{Dt} - \sum_{\alpha=0}^{N}\nabla\cdot(\phi_j\rho_j C_{\alpha j}A_{\alpha j}\boldsymbol{u}_{\alpha j}) \\
& + \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j} r_{\alpha j}(A_{\alpha j} - A_j) + \sum_{\alpha=0}^{N}\boldsymbol{\sigma}_{\alpha j} : \nabla\boldsymbol{u}_{\alpha j} \\
& + \left[\boldsymbol{\sigma}_j + \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\boldsymbol{u}_{\alpha j}\otimes\boldsymbol{u}_{\alpha j}\right] : \nabla\boldsymbol{v}_j \\
& + \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j} r_{\alpha j}\Theta S_{\alpha j} + \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j} e_{\alpha j} \\
& + \frac{\nabla\Theta}{\Theta}\cdot\left\{\boldsymbol{q}_j + \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\left(A_{\alpha j} + \frac{1}{2}u_{\alpha j}^2\right)\boldsymbol{u}_{\alpha j} - \boldsymbol{\sigma}_{\alpha j}\cdot\boldsymbol{u}_{\alpha j}\right]\right\} \\
& - \sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\Theta(r_{\alpha j}S_{\alpha j} + \eta_{\alpha j}).
\end{aligned} \tag{2.34}$$

After summing up Equation (2.34) over solid- and fluid-phase, we collect the terms of the above inequality as follows:

$$\sum_{j=S,F}\Theta\phi_j\rho_j\Gamma_j = \Theta\rho\Gamma_{\text{red}} - \sum_{j=S,F}\sum_{\alpha=0}^{N}\phi_j\rho_j C_{\alpha j}\Theta(r_{\alpha j}^{\text{tr}}S_{\alpha j} + \eta_{\alpha j}^{\text{tr}}). \tag{2.35}$$

In Equation (2.35), all sources of entropy directly ascribable to transfer processes between the solid- and fluid-phase (i.e. $r_{\alpha j}^{\text{tr}}S_{\alpha j} + \eta_{\alpha j}^{\text{tr}}$ where $\alpha \in \{0,\dots,N\}$ and $j = S, F$) are put together in the second term on the RHS. Since term $\Theta\rho\Gamma_{\text{red}}$ does not contain these sources of entropy explicitly, we call it *reduced expression of entropy production*. Following Hassanizadeh (19)(20), the second term on RHS of Equation (2.35) can be taken as non negative, for it represents the volume average of the entropy exchange occurring at the pore-scale (i.e. inside the RVE) through the fluid-solid interface. Indeed, by regarding the fluid-solid interface as the collection of discontinuity surfaces separating the fluid- from the solid-phase inside the RVE, the pore-scale expression of entropy transfer reads (31)

$$\sum_{j=S,F}\sum_{\alpha=0}^{N}[\rho_{\alpha j}^{p}S_{\alpha j}^{p}(\boldsymbol{w}_{\text{I}}^{p} - \boldsymbol{v}_{\alpha j}^{p}) + \Theta^{-1}\boldsymbol{q}_{\alpha j}^{p}]\cdot\boldsymbol{n}_{\text{I}} \geq 0, \tag{2.36}$$

where $\boldsymbol{q}^{p}_{\alpha j}$ is the pore-scale heat flux vector of constituent $\mathscr{C}_{\alpha j}$. Since the average of Equation (2.36) is still non negative, it is possible to conclude that

$$\sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} \Theta (r^{\text{tr}}_{\alpha j} S_{\alpha j} + \eta^{\text{tr}}_{\alpha j}) \geq 0. \tag{2.37}$$

The consequence of Equation (2.37) is that the reduced entropy production, Γ_{red}, satisfies the inequality $\Theta\rho\Gamma_{\text{red}} \geq 0$ on its own. For the whole mixture the reduced Clausius-Duhem inequality reads (58)

$$\begin{aligned}
\Theta\rho\Gamma_{\text{red}} \;=\; & - \sum_{j=S,F} \phi_j \rho_j \frac{D_j A_j}{Dt} - \sum_{j=S,F} \phi_j \rho_j S_j \frac{D_j \Theta}{Dt} - \sum_{j=S,F} \sum_{\alpha=0}^{N} \nabla \cdot (\phi_j \rho_j C_{\alpha j} A_{\alpha j} \boldsymbol{u}_{\alpha j}) \\
& + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} r^{\text{tr}}_{\alpha j} (A_{\alpha j} - A_j) + \sum_{j=S,F} \sum_{\alpha=0}^{N} \boldsymbol{\sigma}_{\alpha j} : \nabla \boldsymbol{u}_{\alpha j} \\
& + \sum_{j=S,F} \Big[\boldsymbol{\sigma}_j + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} \boldsymbol{u}_{\alpha j} \otimes \boldsymbol{u}_{\alpha j} \Big] : \nabla \boldsymbol{v}_j \\
& + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} r^{\text{tr}}_{\alpha j} \Theta S_{\alpha j} + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} e^{\text{tr}}_{\alpha j} \\
& + \frac{\nabla\Theta}{\Theta} \cdot \sum_{j=S,F} \Big\{ \boldsymbol{q}_j + \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} \Big(A_{\alpha j} + \frac{1}{2} u^2_{\alpha j} \Big) \boldsymbol{u}_{\alpha j} - \boldsymbol{\sigma}_{\alpha j} \cdot \boldsymbol{u}_{\alpha j} \Big] \Big\} \\
& + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} r^{\text{gr}}_{\alpha j} (A_{\alpha j} - A_j) \\
& + \sum_{j=S,F} \sum_{\alpha=0}^{N} \phi_j \rho_j C_{\alpha j} C_{\alpha j} (e^{\text{gr}}_{\alpha j} - \Theta \eta^{\text{gr}}_{\alpha j}) \geq 0.
\end{aligned} \tag{2.38}$$

For the sake of conciseness, we split the reduced expression of entropy production, $\rho\Gamma_{\text{red}}$, into the sum of four contributions, i.e.

$$\Theta\rho\Gamma_{\text{red}} = \Theta\rho\Gamma^{F}_{\text{red}} + \Theta\rho\Gamma^{S}_{\text{red}} + \Theta\rho\Gamma^{\text{tr}}_{\text{red}} + \Theta\rho\Gamma^{\text{gr}}_{\text{red}} \geq 0, \tag{2.39}$$

where $\rho\Gamma^{F}_{\text{red}}$ and $\rho\Gamma^{S}_{\text{red}}$ contain terms associated only to the fluid- and solid-phase, respectively, $\rho\Gamma^{\text{tr}}_{\text{red}}$ contains interaction terms due to mass transfer between the two phases, and $\Gamma^{\text{gr}}_{\text{red}}$ contains explicit growth contributions.

Essential information about the mixture thermo-mechanic behaviour can be gained by exploiting Clausius-Duhem inequality (2.39). To this end, if the mixture is subject to constraints, these constraints have to be used for a consistent analysis of the entropy inequality. According to the terminology of (18), this can be accomplished either in *strong* or*weak form*. In strong form, constraints are used for selecting independent thermomechanic variables, and expressing Clausius-Duhem inequality in terms of these variables only. In weak form, constraints are accounted for through the Lagrange multiplier technique, i.e. each constraint is premultiplied by an appropriate Lagrange multiplier, and the resulting expression is combined with Clausius-Duhem inequality in order to obtain a modified, or augmented, form of dissipation inequality. The equivalence between the strong and weak method was proven by Liu (25).

In the works by Liu (25), Liu and Müller (26), and Müller and Ruggeri (27), the modified expression of entropy inequality is obtained by adopting field equations as constraints. This approach was extended by Bennethum *et al.* (18), who included the kinematic restrictions

$$\sum_{\alpha=0}^{N} C_{\alpha F}\boldsymbol{u}_{\alpha F} = \mathbf{0}, \tag{2.40}$$

$$\sum_{\alpha=0}^{N} C_{\alpha S}\boldsymbol{u}_{\alpha S} = \mathbf{0}, \tag{2.41}$$

imposed on constituent relative velocities, $\boldsymbol{u}_{\alpha j}$, in the modified expression of Clausius-Duhem inequality.

In this section, following (18) and (58), we employ the Lagrange multiplier technique to kinematic relations (2.40) and (2.41), and mass balance of (i) fluid-phase as a whole, (ii) fluid constituents, (iii) solid-phase as a whole, and (iv) solid constituents.

By combining constraints (i)-(iv), and kinematic restrictions (2.40) and (2.41) with Clausius-Duhem inequality (2.39), the modified form of entropy inequality becomes (58)

$$\begin{aligned}
\widetilde{\Theta\rho\Gamma_{\mathrm{red}}} = {} & \Theta\rho\Gamma^{F}_{\mathrm{red}} + \Theta\rho\Gamma^{S}_{\mathrm{red}} + \Theta\rho\Gamma^{\mathrm{tr}}_{\mathrm{red}} + \Theta\rho\Gamma^{\mathrm{gr}}_{\mathrm{red}} \\
& + \sum_{j=S,F} \lambda_j \Big\{ \rho_j \frac{D_j\phi_j}{Dt} + \phi_j \frac{D_j\rho_j}{Dt} + \phi_j\rho_j \nabla\cdot\boldsymbol{v}_j - \phi_j\rho_j R_j \Big\} \\
& + \sum_{j=S,F}\sum_{\alpha=0}^{N} \lambda_{\alpha j} \Big\{ \phi_j\rho_j \frac{D_j C_{\alpha j}}{Dt} + \nabla\cdot(\phi_j\rho_j C_{\alpha j}\boldsymbol{u}_{\alpha j}) - \phi_j\rho_j C_{\alpha j}(r_{\alpha j} - R_j) \Big\} \\
& + \sum_{j=S,F} \phi_j \boldsymbol{\Lambda}_j \cdot \sum_{\alpha=0}^{N} \nabla(\rho_j C_{\alpha j}\boldsymbol{u}_{\alpha j}) \geq 0.
\end{aligned} \tag{2.42}$$

2.5 Elements of the Theory of Constitutive Law

As stated at the beginning of Section 2.2, balance laws relate physical quantities in all cases (Truesdell and Toupin, 1960). They provide a set of necessary conditions which thermo-mechanic variables must respect. In this framework, Clausius-Duhem inequality represents a constraint which tells us whether a certain process is thermo-mechanically consistent. However, balance laws are *not* sufficient to formulate the thermo-mechanical problem in a self-consistent form for they involve a number of unknowns which is bigger than the number of equations. Therefore, a certain number of additional *non*-redundant conditions have to be imposed. These conditions must be consistent with phenomenological observations and experimental results, and must be able to predict the thermo-mechanic behaviour of the body. In order for the latter requirement to be satisfied, they must be consistent with the Clausius-Duhem inequality (Coleman and Noll, 1961). These conditions are called Constitutive Laws.

In order to set up a constitutive framework, a *set* of thermo-mechanic *degrees of freedom* has to be chosen. A physical quantity belonging to this set is said to be *independent constitutive variable* (ICV), and has the property of being observable and measurable “along” *any* thermo-mechanic process followed by the body.

Each ICV is associated with a *conjugated* or *dependent constitutive variable* (DCV). Usually, those physical quantities which are directly related to *intrinsic* source terms are not enlisted among constitutive variables. Rather, they are supposed to be known functions of independent coordinates (Liu, 2002).

The set of ICV has to be suitably chosen depending on the kind of problem one is concerned with. Within the set of ICV, we refer to *basic fields* (Liu, 2002) as to those fields from which the other ICV can be derived. In thermo-mechanic problems, basic fields are the configuration field, c, absolute temperature, Q, and mass density, r (sometimes, depending on the problem, absolute temperature is replaced by the entropy density, h). The gradients of basic fields, such as velocity, deformation gradient, and higher order gradients, make up the remaining DCV. Constitutive laws are usually written in the reference configuration and involve the material form (i.e., the Piola transforms) of fields (Marsden and Hughes, 1983; Eringen, 1980, 2002; Liu, 2002).

In general, a certain DCV, f, is expressed through a functional relation involving all ICVs, and space-time coordinates. This aspect of the constitutive relations describes the realm that the value of f at time t depends on all the values of f at instants of time $s \in [0; t[$, i.e. on the *past history* of *f*. If *j* is a generic function of time, we call *past history* of *j* the function φ^t such that $\varphi^t(s) = \varphi(t - s)$, for all $s \in [0; t[$ and $t \to \infty$ (Liu, 2002; Fabrizio and Morro, 1992). In the case $s = 0$, the past history of *j* reduces to $\varphi^t(0) = \varphi(t)$.

2.5.1 The Fundamental Axioms of the Theory of the Constitutive Law

A constitutive law descends on the phenomenological interpretation of the thermo-mechanic system which one wants to describe. Nevertheless, the production of experimental data is not sufficient to establish an exhaustive and consistent Constitutive Theory. For this reason it is necessary to determine a set of *universal* requirements which permit one to extrapolate a methodological writing of the constitutive laws.

The main requirements a constitutive framework should be based can be summarized in the following axioms.

2.5.1.1 Axiom of Causality

The axiom of causality states that configuration field, *c*, temperature, Q (or entropy density, *h*), and mass density, *r*, are the basic fields for any thermo-mechanic behaviour of the body. In this framework, all physical quantities, except the gradients of *c* and Q (or *h*), are the DCV.

2.5.1.2 Axiom of Determinism

The axiom of determinism states that the value of a certain DCV at time *t* and material point, *X*, is determined by the histories $\chi^t(s, Y) = \chi(t - s, Y)$, and $\hat{\Theta}^t(s, Y) = \hat{\Theta}(t - s, Y)$ for every $s \in [0; t[$, and $Y \in \mathrm{B}_R$. This axiom is actually a principle of *exclusion*, because it excludes the dependence of the constitutive behaviour of the body on any instant of time external to the interval $[0; t]$, and any point external to the region of space instantaneously occupied by the body. Therefore, by virtue of Axioms 1 and 2, a DCV, *f*, can be expressed through the definition of a functional, $\mathrm{F}^{(f)}$, such that (Day, 1972; Liu, 2002)

$$\hat{f}(t, X) = \underset{Y \in \mathrm{B}, s \in [0;t]}{\mathrm{F}^{(f)}} (t, X, \hat{\rho}^t(s, Y), \chi^t(s, Y), \hat{\Theta}^t(s, Y)). \tag{2.43}$$

The functional $\mathrm{F}^{(f)}$ is called *response functional* of *f*. It should be noted that Eq. (2.43) takes into account the occurrence of arbitrary *non-local* effects (Liu, 2002; Eringen, 2002) of any inhomogeneous body (i.e., a body the constitutive law of which explicitly depends on material coordinates) with *memory* of the past history.

2.5.1.3 Axiom of Equipresence

This axiom states that all DCVs must depend on the same list of ICVs. According to this statement, *no* variable is, at least in principle, *a priori* excluded from the determination of the response law (Day, 1972). There are, of course, exceptions which may occur depending on whether some particular classes of symmetry are found in the system under investigation. The search for material symmetries is of great interest both from the mathematical and the physical point of view, and, apart from leading to considerable computational simplifications, permits to reformulate typical Continuum Mechanics problems in terms of Field Theories. Within the rigorous mathematical framework established by Mathematics, this may lead to better appreciate the beauties of Physics.

2.5.1.4 Axiom of Material Objectivity

This axiom states that constitutive laws must be invariant under *rigid* coordinate transformations of the spatial reference frame, and time translations. This property is tightly related with the fact that physical quantities must be *observable*, and thus cannot depend on the observer. In order to prove this property, it is necessary to show that for two arbitrarily chosen reference frames, R and R', the functional $\mathrm{F}^{(f)}$ leads to the same description of the physical quantity f (Liu, 2002), i.e.

$$\mathrm{F}^{(f)}_{\mathrm{R}} = \mathrm{F}^{(f)}_{\mathrm{R}'}. \tag{2.44}$$

It should be noted that the concepts of *observability* and invariance under a certain class of coordinate transformations are tightly related to the concept of *gauge symmetry* (Felsager, 1998).

2.5.1.5 Axiom of Material Invariance

This axiom is an alternative version of the previous one. It states that constitutive laws must be invariant with respect to the *group* of orthogonal transformations, and time and material translations.

2.5.1.6 Axiom of Smooth Neighbourhood and Smooth Memory

This axiom states that the values of the ICVs at material points, Y, far enough from a material point, X, do not appreciably affect the values of the DCVs at X. Analogously, the values of the ICVs at times, s, far enough from the current instant of time, t, do not appreciably affect the values of DCVs at time t. This axiom implies that the effects of non-locality are supposed to die away in time and space. Thus, the correlation functions one may associate with a certain physical quantity are expected to be “damped” out of the space-time neighbourhood in which the constitutive variable is examined.

2.6 Classification of Materials

The axioms of Smooth Neighbourhood and Material Objectivity permit to re-define constitutive laws by introducing new response functionals which depend on time, t, material coordinates, X, and on basic fields and their derivatives (up to infinite order) evaluated at t and X, i.e.

$$\begin{aligned}\hat{f}(t,X) = \underset{s\in[0;t]}{\mathrm{G}^{(f)}}&(t, X, \hat{\rho}^t(s,X), \nabla_R \hat{\rho}^t(s,X), ..., \chi^t(s,X), \nabla_R \chi^t(s,X), ...\\ &..., \hat{\Theta}^t(s,X), \nabla_R \hat{\Theta}^t(s,X), ...).\end{aligned} \tag{2.45}$$

The expression (2.45) can be simplified by noticing that the term $\chi^t(s,X)$ can be eliminated by means of a suitable choice of the coordinate frame, i.e.

$$\begin{aligned}\hat{f}(t,X) = \underset{s\in[0;t]}{\mathrm{G}^{(f)}}&(t, X, \hat{\rho}^t(s,X), \nabla_R \hat{\rho}^t(s,X), ..., F^t(s,X), ...\\ &..., \hat{\Theta}^t(s,X), \nabla_R \hat{\Theta}^t(s,X), ...).\end{aligned} \tag{2.46}$$

Here, the history of the deformation gradient tensor, $F^t(s,X) = \nabla_R \chi^t(s,X)$, has been explicitly introduced.

The advantage of working with a constitutive relation of the kind reported in Eq. (2.46) is that it is easier to determine the best order of approximation for a certain behaviour of the modelled material. For instance, when a certain material shows a behaviour which can be safely approximated by truncating Eq. (2.46) up to the *p-th* gradient of the configuration field, and the *q-th* temperature gradient, the material is said to be of mechanic order p, and thermal order q. In the case in which $p = 1$, and $q = 1$, the material is said to be *simple*, and the constitutive law reduces to

$$\hat{f}(t,X) = \underset{s\in[0;t]}{\mathrm{G}^{(f)}}(t, X, F^t(s,X), \hat{\Theta}^t(s,X)). \tag{2.47}$$

In Eq. (2.47) mass density and its gradients have not been considered. In the literature, this approximation is used for all those problems in which mass variation processes are disregarded.

When the constitutive law does not show explicit dependence on time, only the present values of the ICVs, rather than their whole history, are considered. In this case, Eq. (2.47) becomes

$$\hat{f}(t,X) = \Upsilon^{(f)}(X, F(t,X), \hat{\Theta}(t,X)). \tag{2.48}$$

Equation (2.48) describes the thermo-mechanical behaviour of the so-called *thermo-elastic* materials. Moreover, if the thermal and mechanical responses are supposed to be independent one on the other, then we speak of *hyperelastic materials*, and mechanical constitutive variables are characterized by constitutive relations of the kind

$$\hat{f}(t, X) = \Psi^{(f)}(X, F(t, X)). \tag{2.49}$$

The explicit dependence of $\Psi^{(f)}$ on X accounts for the presence of material inhomogeneities. This issue and its Field Theory-related aspects will be treated in detail in the following.

2.6.1 Thermoelastic Materials

In this Section we would like to show how the Constitutive Laws are used to formulate the closure of a typical Continuum Physics problem. For the sake of simplicity, we shall assume that the body is made of a thermoelastic material, and neither sources or fluxes are taken into account.

First, we summarize the balance laws which are involved in a "classical" thermo-mechanical problem in the absence of any sources and fluxes. With respect to the reference configuration (where boundary conditions are known), these conditions are

Mass	$\partial_t \rho_R = 0$
Linear Momentum	$\rho_R \partial_t^2 \chi = \nabla_R \cdot T$
Angular Momentum	$\sigma = \sigma^T \Rightarrow FT = (FT)^T$
First Principle of Thermodynamics	$\rho_R(\partial_t \hat{\mathrm{U}}) = \langle T \mid \partial_t F \rangle - \nabla_R \cdot Q$
Second Principle of Thermodynamics	$\rho_R(\partial_t \hat{\eta}) \geq -\nabla_R \cdot \left(\frac{Q}{\hat{\Theta}}\right)$

The relations above consist of fifteen scalar conditions involving the nineteen unknowns $\{\rho_R, \chi, T, \hat{\mathrm{U}}, \hat{\Theta}, Q, \hat{\eta}\}$. In order to formulate this problem in closed form, it is necessary to invoke the symmetry of the Cauchy stress tensor, and to enforce the constitutive relations.
Since mass sources are not considered, the mass density in the reference configuration, ρ_R, does not depend on time, i.e. $\rho_R(t, X) = \rho_R^{(0)}(X)$, and the map $\rho_R^{(0)}$ can be regarded as an initial condition. Moreover, since the material is assumed to be thermoelastic, we may rewrite the Clausius-Duhem inequality in the form

$$\begin{aligned} &-\rho_R\{\partial_t[\mathrm{F}^{(\psi)} \circ (I, F, \hat{\Theta}) + [\mathrm{F}^{(\eta)} \circ (I, F, \hat{\Theta})]\partial_t \hat{\Theta}\} + \\ &+\left\langle \mathrm{F}^{(T)} \circ (I, F, \hat{\Theta}) \,\middle|\, \partial_t F \right\rangle - \hat{\Theta}^{-1} \nabla_R \hat{\Theta} \cdot [\mathrm{F}^{(q)} \circ (I, F, \hat{\Theta})] \geq 0. \end{aligned} \tag{2.50}$$

By writing the time derivative of $\mathrm{F}^{(\psi)}$ in explicit form, we obtain

$$\begin{aligned}
&\left\langle -\rho_R \left[\tfrac{\partial \mathrm{F}^{(\psi)}}{\partial F} \circ (I, F, \hat{\Theta})\right] \,\middle|\, \partial_t F \right\rangle - \rho_R \left[\tfrac{\partial \mathrm{F}^{(\psi)}}{\partial \hat{\Theta}} \circ (I, F, \hat{\Theta})\right] \partial_t \hat{\Theta} + \\
&-\rho_R [\mathrm{F}^{(\eta)} \circ (I, F, \hat{\Theta})] \partial_t \hat{\Theta} + \left\langle \mathrm{F}^{(T)} \circ (I, F, \hat{\Theta}) \,\middle|\, \partial_t F \right\rangle + \\
&-\hat{\Theta}^{-1} \nabla_R \hat{\Theta} \cdot [\mathrm{F}^{(q)} \circ (I, F, \hat{\Theta})] \geq 0.
\end{aligned} \tag{2.51}$$

We note that the Clausius-Duhem inequality is satisfied as an equality if, and only if, the following conditions are respected

$$\begin{aligned}
T &= \mathrm{F}^{(T)} \circ (I, F, \hat{\Theta}) = \rho_R \left[\tfrac{\partial \mathrm{F}^{(\psi)}}{\partial F} \circ (I, F, \hat{\Theta})\right], \\
\hat{\eta} &= \mathrm{F}^{(\eta)} \circ (I, F, \hat{\Theta}) = -\left[\tfrac{\partial \mathrm{F}^{(\psi)}}{\partial \hat{\Theta}} \circ (I, F, \hat{\Theta})\right], \\
Q &= \mathrm{F}^{(q)} \circ (I, F, \hat{\Theta}) = 0.
\end{aligned} \tag{2.52}$$

Equations (2.52) enable us to state that, in a thermoelastic material, the heat flux vector vanishes identically, and, consequently the entropy time variation is solely due to intrinsic heat sources. Therefore, in the absence of sources of any kind, the Second Principle of Thermodynamics can be reformulated as an equality stating that entropy does not vary in time, i.e.

$$\rho_R(\partial_t \hat{\eta}) = 0 \Rightarrow \hat{\eta}(t, X) = \hat{\eta}^{(0)}(X). \tag{2.53}$$

A consequence to this statement is that thermoelastic materials are in *thermal equilibrium*. This can be proven by noting that, since internal energy density and Cauchy stress tensor are given by

$$\begin{aligned}
&\hat{\mathrm{U}} = \hat{\psi} + \hat{\Theta}\hat{\eta} = \mathrm{F}^{(\psi)} \circ (I, F, \hat{\Theta}) - \hat{\Theta} \left[\tfrac{\partial \mathrm{F}^{(\psi)}}{\partial \hat{\Theta}} \circ (I, F, \hat{\Theta})\right] \\
&\hat{\sigma} = \tfrac{1}{J} F T \Rightarrow \begin{cases} \hat{\sigma}^{ab} = \tfrac{1}{J} F^b{}_A T^{aA} \\ \hat{\sigma}^a{}_b = \tfrac{1}{J} T^a{}_A (F^T)^A{}_b \, , \end{cases}
\end{aligned} \tag{2.54}$$

the First Principle of Thermodynamics writes

$$\rho_R(\partial_t \hat{\mathrm{U}}) = \langle T \mid \partial_t F \rangle \Rightarrow \rho_R \left[\frac{\partial \mathrm{F}^{(\psi)}}{\partial \hat{\Theta}} \circ (I, F, \hat{\Theta})\right] \partial_t \hat{\Theta} = 0, \tag{2.55}$$

i.e. temperature does not depend on time.

In conclusion, we say that a thermoelastic material is *thermodynamically admissible* if, and only if, stress, internal energy and entropy are derivable from a potential, $\mathrm{F}^{(\psi)}$, and the heat flux vector is zero.

It is worthwhile to remind that Eqs. (2.53) and (2.55) state that, in the absence of sources and fluxes, only *isoentropic and isothermal* processes are allowed. Moreover, since these conditions are equivalent to say that the substantial derivatives of entropy and temperature are zero (i.e. $D_t \eta = 0$, and $D_t \Theta = 0$), we conclude that entropy and temperature are *constant* throughout the time evolution of each material point, X.

In the Engineers' jargon, this can represented by attaching a $(\hat{\Theta}^{(0)}(X); \hat{\eta}^{(0)}(X))$-Gibbs plane to each material point, X. In this plane, a thermodynamic state is represented by a *point*.

2.7 Linear Theory of Elasticity

In case of hyperelastic materials, the Helmholtz free energy density is expressed through the functional relation

$$\hat{\psi} = \Phi \circ (I, F). \tag{2.56}$$

Equation (2.56) can be rewritten in terms of the Lagrange strain tensor (cfr. Chapter 1), e, i.e.

$$\hat{\psi} = \Psi \circ (I, \varepsilon). \tag{2.57}$$

By deriving Eq. (2.57) with respect to e, we obtain the *second Piola-Kirchhoff stress tensor*, S, i.e.

$$S = \frac{\partial \Psi}{\partial \varepsilon} \circ (I, \varepsilon). \tag{2.58}$$

This fully material stress tensor is related to the first Piola-Kirchhoff stress tensor, T, through the definition

$$S = F^{-1} T \Rightarrow S^{AB} = (F^{-1})^{A}{}_{a} T^{aB}. \tag{2.59}$$

Consequently, the Lagrangian form of the Cauchy stress tensor is given by

$$\hat{\sigma} = \frac{1}{J} T F^T = \frac{1}{J} F S F^T \Rightarrow \hat{\sigma}^{a}{}_{b} = \frac{1}{J} F^{a}{}_{A} S^{A}{}_{B} (F^T)^{B}{}_{b}. \tag{2.60}$$

In the limit of small strains, the potential Y is well approximated by its CityplaceTaylor expansion up to the second order, i.e.

$$\begin{aligned} \Psi \circ (I, \varepsilon) \cong \; & \Psi \circ (I, O) + \left[\tfrac{\partial \Psi}{\partial \varepsilon^{AB}} \circ (I, O)\right] \varepsilon^{AB} + \\ & + \tfrac{1}{2} \left[\tfrac{\partial^2 \Psi}{\partial \varepsilon^{AB} \partial \varepsilon^{CD}} \circ (I, O)\right] \varepsilon^{AB} \varepsilon^{CD}. \end{aligned} \tag{2.61}$$

Since the zero-order term can be set to be equal to zero, and the first-order term is identically zero because *no* stress can exist at *zero* strain, we conclude that

$$\Psi \circ (I, \varepsilon) \cong \frac{1}{2} \left[\frac{\partial^2 \Psi}{\partial \varepsilon^{AB} \partial \varepsilon^{CD}} \circ (I, O)\right] \varepsilon^{AB} \varepsilon^{CD}. \tag{2.62}$$

The four-order tensor featuring in Eq. (2.62) is called *elasticity tensor* and is denoted by

$$\frac{\partial^2 \Psi}{\partial \varepsilon^{AB} \partial \varepsilon^{CD}} \circ (I, O) = \mathrm{L}_{ABCD} \circ (I, O). \tag{2.63}$$

In general, the dependence on the identity second-order tensor, I, means that the elasticity tensor may depend explicitly on material coordinates, X; therefore, we write $\mathrm{L}(I(X), O) = L(X)$.

Equation (2.62) allows us to determine the second Piola-Kirchhoff stress tensor, S. Using lower indexes only, we obtain

$$S = \frac{\partial \Psi}{\partial \varepsilon} \circ (I, \varepsilon) \cong L\varepsilon \Rightarrow S_{AB}(t, X) = L_{ABCD}(X)\varepsilon_{CD}(t, X). \tag{2.64}$$

By virtue of the definition of Eq. (2.60), we note that, in the small strain regime, the second Piola-Kirchhoff stress tensor can be approximated with the Lagrangian form of the Cauchy stress, i.e.

$$S_{AB}(t, X) \cong \hat{\sigma}_{ab}(t, X). \tag{2.65}$$

Consequently, Eq. (2.64) can be written as

$$\hat{\sigma}_{ab}(t, X) = L_{abcd}(X)\varepsilon_{cd}(t, X). \tag{2.66}$$

Within the Linear Theory of Elasticity, the elasticity tensor, L, is the representative of all of the material symmetries of the material. In particular, while the dependence of L on X deals with the invariance of material elastic properties under the group of translations (*homogeneity*), the symmetry of the tensor L with respect to its pairs of indexes takes into account of the invariance of material elastic properties under the group of rotations (*isotropy*). These concepts will be discussed in detail in the next Chapter.

Chapter 3

Evolution of a fibre-reinforced growing mixture

3.1 Introduction

In this Chapter it will be studied a biological mixture consisting of a fluid- and a solid-phase. The latter will be assumed to comprise two sub-phases, i.e. matrix and fibre-like inclusion, moving with the common phase velocity,$\mathbf{v}_S$. Each phase will be modelled as a mixture on its own with several constituents. Because of mass exchanges between phases, the solid-phase experiences growth (or resorption). Growth, and the material inhomogeneities related to it, will be described through the multiplicative decomposition of the solid-phase deformation gradient tensor, and the introduction of the growth velocity gradient.

Through Onsager's principle, it will be proven that inhomogeneity velocity "gradient" is related to the Mandel stress tensor of the solid-phase, and chemical potentials of fluid constituents. This relation will be used in order to show that, in response to growth (or adsorption), development of material inhomogeneities may trigger fibre reorientation in the solid-phase by inducing the evolution in time of its texture tensor (112)

The macroscopic mechanical behaviour of biological tissues is influenced by the presence of inclusions. For example, in the case of articular cartilage, the mechanical properties and geometric distribution of collagen fibres enhance the tissue resistance to external loads, and determine the tissue material symmetry.

If inclusions evolve in time, the response of the tissue to external stimuli adapts to the current organisation of the inclusions. This rearrangement of the internal structure, known as *remodelling* (3), implies that tissue material symmetries evolve in time. For this reason, an accurate characterisation of the tissue mechanical behaviour should be able to predict how inclusions evolve, and how their evolution is related to the quantities that determine the mechanical state of the tissue.

Tools of investigation are different depending on the phenomenon that has to be described. In linear elasticity, models are usually based on the theory of composite materials with spheroidal inclusions (cf., for example, (43)–(45)). According to this approach, the effective strain in the inclusions, $\tilde{\boldsymbol{\varepsilon}}$, is expressed through the relation $\tilde{\boldsymbol{\varepsilon}} = \mathbb{A} : \boldsymbol{\varepsilon}$, where $\boldsymbol{\varepsilon}$ is the strain field "felt" by the composite as a whole, and $\mathbb{A}$ is a fourth-order tensor called *strain intensification tensor*.

Inclusions may also exhibit statistical orientation. In this case, it is possible to introduce a probability density distribution, which describes the probability of finding a fibre-like inclusion aligned along a given direction in space (this approach was used, for example, in (62)(64) for modelling articular cartilage).

The texture tensor, Ξ, is defined by $\Xi = \boldsymbol{\xi} \otimes \boldsymbol{\xi}$, where $\boldsymbol{\xi}$ is a unit vector describing the local alignment of a fibre-like inclusion along a prescribed direction of space.

When growth is considered, the change of internal structure of the tissue is also driven by the adaptive re-distribution of its mass density as new material is added (or subtracted) to the pre-existing one. In the case of a materially uniform continuum body (i.e. a body whose points, made of the same material, can be brought to attain the same state simultaneously) described by a first-order constitutive theory, Epstein and Maugin (52) pointed out that the process of growth is essentially governed by temporal changes of mass density, and distortions of material-point neighbourhoods in the reference configuration of the body. Distortions, and related residual stresses, arise because of the possible loss of geometric compatibility of material-point neighbourhoods as growth takes place. Growth is thus viewed as a process capable of developing body material inhomogeneities.

We would like to approach the problem of growth and remodelling in the context of Mixture Theory. For our purposes, we consider a mixture consisting of a fluid- and a solid-phase, and we assume that the solid-phase is composed by a matrix and fibre-like inclusions. In the following, we refer to matrix and fibre-like inclusions as to solid sub-phases. We remark that, since fibre-like inclusions are regarded as a phase, their dimension is not seen in the model, while their orientation is accounted for by the solid-phase texture tensor, Ξ_S. According to this description, the solid-phase of the mixture studied in this paper describes a homogenised system consisting of matrix and fibres.

3.2 Model Description

We consider a class of biological tissues that can be macroscopically modelled as mixtures composed of a fluid- and a solid-phase. The former is a multi-constituent fluid experiencing single-phase flow, and the latter is a deformable medium consisting of a porous matrix and fibre-like inclusions. We refer to matrix and fibre-like inclusions as to solid sub-phases. In the following, we denote the fluid-phase by $\mathscr{F}_F$, and the solid-phase by $\mathscr{F}_S = \mathscr{F}_M \cup \mathscr{F}_I$, where $\mathscr{F}_M$ and $\mathscr{F}_I$ represent the matrix, and inclusion sub-phase, respectively.

Following the picture proposed by Bennethum *et al.* (18), we assume that the fluid-phase, $\mathscr{F}_F$, and the sub-phases $\mathscr{F}_M$ and $\mathscr{F}_I$ are mixtures on their own, which comprise the same number of constituents. Constituents 0-th and 1-st confer the sub-phases $\mathscr{F}_M$ and $\mathscr{F}_I$ the mechanical properties of a solid, respectively. The N-th constituent is identified with water, and all other constituents ($\gamma = 2, \dots, N-1$) represent, for example, nutrients, byproducts of cellular metabolic reactions, chemical agents, and molecular species. The α-th constituent in phase $\mathscr{F}_j$ (with $\alpha \in \{0, \dots, N\}$ and $j \in \{F\} \cup \{M, I\}$) is denoted by $\mathscr{C}_{\alpha j}$. If a given constituent is present in one phase but absent in the other two phases, its mass exchange term is set identically equal to zero, and it is *formally* regarded as present with zero concentration.

We require that the mixture satisfies the *saturation condition*. According to this condition, the sum of solid- and fluid-phase volume fractions, denoted by ϕ_F and ϕ_S, respectively, is constrained to equal unity at all times and all points of the mixture, i.e. $\phi_F + \phi_S = 1$. We remark that, due to the presence of matrix and inclusions, the volume fraction of the solid-phase as a whole, ϕ_S, is actually defined by the sum of the volume fractions of the solid sub-phases $\mathscr{F}_M$ and $\mathscr{F}_I$, i.e. $\phi_S := \phi_M + \phi_I$. Following (19), we define the mass density of fluid-phase, $\mathscr{F}_j$ (with $j \in \{F\} \cup \{M, I\}$), by the sum

$$\rho_j := \sum_{\alpha=0}^{N} \rho_{\alpha j}, \tag{3.1}$$

where $\rho_{\alpha j}$ (with $\alpha \in \{0, \dots, N\}$) is the mass density of constituent $\mathscr{C}_{\alpha j}$ in the phase $\mathscr{F}_j$. The mass fractions of constituents $\mathscr{C}_{\alpha j}$ are defined by the ratios $C_{\alpha j} := \rho_{\alpha j}/\rho_j$, and are thus linearly dependent through the constraint $\sum_{\alpha=0}^{N} C_{\alpha j} = 1$. The mass density of the solid-phase is given by $\phi_S \rho_S = \phi_M \rho_M + \phi_I \rho_I$, whereas densities ρ_M and ρ_I are defined as in eq. (3.1)

3.2.1 Balance laws and Source terms

As saw in Chapter 2 , considering eq.(2.3) and Tables 2.1 and 2.2 we can find the the following overall source terms:

Mass

$$R_j := \sum_{\alpha=0}^{N} C_{\alpha j} R_{\alpha j}, \tag{3.2}$$

Momentum

$$\mathbf{T}_j := \sum_{\alpha=0}^{N} C_{\alpha j}(R_{\alpha j}\mathbf{u}_{\alpha j} + \mathbf{T}_{\alpha j}), \tag{3.3}$$

Energy

$$Q_j := \sum_{\alpha=0}^{N} C_{\alpha j}\Big[Q_{\alpha j} + \mathbf{T}_{\alpha j}\cdot\mathbf{u}_{\alpha j} + R_{\alpha j}\Big(E_{\alpha j} - E_j + \frac{1}{2}\mathrm{u}_{\alpha j}^2\Big)\Big], \tag{3.4}$$

Entropy

$$\eta_j := \sum_{\alpha=0}^{N} C_{\alpha j}[\eta_{\alpha j} + R_{\alpha j}(S_{\alpha j} - S_j)], \tag{3.5}$$

Moreover by virtue of eqs. (3.2)–(3.4), the fact that the mixture is closed is expressed by requiring

$$\begin{aligned}
0 &= \sum_{j\in\{F,M,I\}} \phi_j\rho_j R_j, && (3.6)\\
\mathbf{0} &= \sum_{j\in\{F,M,I\}} \phi_j\rho_j(\mathbf{T}_j + R_j\mathbf{v}_j), && (3.7)\\
0 &= \sum_{j\in\{F,M,I\}} \phi_j\rho_j\Big[Q_j + \mathbf{T}_j\cdot\mathbf{v}_j + R_j\Big(E_j + \frac{1}{2}\mathrm{v}_j^2\Big)\Big], && (3.8)\\
0 &\le \sum_{j\in\{F,M,I\}} \phi_j\rho_j(\eta_j + R_j S_j). && (3.9)
\end{aligned}$$

that represent averaged thermodynamic exchange interactions occurring at the interface between the fluid- and the solid-phase.

Finally, substituting the Helmholtz free energy densities, $A_{\alpha j}$, into the balance of entropy and under the hypothesis that the mixture undergoes only isothermal processes, the expression of entropy production for constituent $\mathscr{C}_{\alpha j}$ become :

$$\begin{aligned}
\Theta\phi_j\rho_j C_{\alpha j}\Gamma_{\alpha j} &= -\phi_j\rho_j C_{\alpha j}\frac{\mathrm{D}_{\alpha j}A_{\alpha j}}{\mathrm{D}t} - \phi_j\rho_j C_{\alpha j}S_{\alpha j}\frac{\mathrm{D}_{\alpha j}\Theta}{\mathrm{D}t} + \boldsymbol{\sigma}_{\alpha j} : \nabla\mathbf{v}_{\alpha j} && (3.10)\\
&\quad +\phi_j\rho_j C_{\alpha j}R_{\alpha j}\Theta S_{\alpha j} + \phi_j\rho_j C_{\alpha j}Q_{\alpha j} - \phi_j\rho_j C_{\alpha j}\Theta(R_{\alpha j}S_{\alpha j} + \eta_{\alpha j})\\
&\quad +\phi_j\rho_j C_{\alpha j}(Q_{\alpha j}^{*} - \Theta\eta_{\alpha j}^{*}),
\end{aligned}$$

that summed over all constituents $\mathscr{C}_{\alpha j}$ (with $\alpha \in \{0, \dots, N\}$) leads to the expression of *entropy production of phase* $\mathscr{F}_j$, $\Gamma_j := \sum_{\alpha=0}^{N} C_{\alpha j}\Gamma_{\alpha j}$ ($j \in \{F\} \cup \{M, I\}$), i.e. as shown by Grillo *et al.* (112) :

$$\begin{aligned} \Theta\phi_j\rho_j\Gamma_j \;=\; & -\phi_j\rho_j\frac{\mathrm{D}_jA_j}{\mathrm{D}t} - \phi_j\rho_jS_j\frac{\mathrm{D}_j\Theta}{\mathrm{D}t} - \sum_{\alpha=0}^{N}\nabla\cdot(\phi_j\rho_jC_{\alpha j}A_{\alpha j}\mathbf{u}_{\alpha j}) \\ & + \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}R_{\alpha j}(A_{\alpha j} - A_j) + \sum_{\alpha=0}^{N}\boldsymbol{\sigma}_{\alpha j} : \nabla\mathbf{u}_{\alpha j} \\ & + \Big[\boldsymbol{\sigma}_j + \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}\mathbf{u}_{\alpha j}\otimes\mathbf{u}_{\alpha j}\Big] : \nabla\mathbf{v}_j + \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}R_{\alpha j}\Theta S_{\alpha j} \\ & + \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}Q_{\alpha j} - \sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}\Theta(R_{\alpha j}S_{\alpha j} + \eta_{\alpha j}) \\ & + \phi_j\rho_j(Q_j^{*} - \Theta\eta_j^{*}). \end{aligned} \tag{3.11}$$

3.2.2 Reduced Entropy Inequality

The expression of entropy production for the mixture as a whole is obtained by summing eq. (3.11) over all phases $\mathscr{F}_j$ (with $j \in \{F\} \cup \{I, M\}$). In order to do that, we first need to compute the sum $\sum_{j\in\{F,I,M\}}\sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}Q_{\alpha j}$. For the sake of simplicity, we hypothesise here that: (i) in the solid sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$, constituents $\mathscr{C}_{\alpha I}$ and $\mathscr{C}_{\alpha M}$ (with $\alpha \in \{0, \dots, N\}$) have *no* diffusive velocity (i.e. $\mathbf{u}_{\alpha I} \equiv \mathbf{0}$, and $\mathbf{u}_{\alpha M} \equiv \mathbf{0}$, $\forall\alpha \in \{0, \dots, N\}$), and (ii) that sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$ move with the same velocity, i.e. $\mathbf{v}_I \equiv \mathbf{v}_M \equiv \mathbf{v}_S$, where $\mathbf{v}_S$ is thus the velocity of the solid-phase as a whole. By using these assumptions, definitions (3.2)–(3.4), and restrictions (3.6)–(3.8), the sum $\sum_{j\in\{F,I,M\}}\sum_{\alpha=0}^{N}\phi_j\rho_jC_{\alpha j}Q_{\alpha j}$ reads:

$$\begin{aligned} & \sum_{\alpha=0}^{N}\phi_I\rho_IC_{\alpha I}Q_{\alpha I} + \sum_{\alpha=0}^{N}\phi_M\rho_MC_{\alpha M}Q_{\alpha M} + \sum_{\alpha=0}^{N}\phi_F\rho_FC_{\alpha F}Q_{\alpha F} \\ & = -\phi_F\rho_F\mathbf{T}_F\cdot\mathbf{w}_{FS} - \phi_F\rho_FR_F\frac{1}{2}\mathrm{w}_{FS}^2 - \sum_{\alpha=0}^{N}\phi_F\rho_FC_{\alpha F}\mathbf{T}_{\alpha F}\cdot\mathbf{u}_{\alpha F} \\ & - \sum_{\alpha=0}^{N}\phi_I\rho_IC_{\alpha I}R_{\alpha I}E_{\alpha I} - \sum_{\alpha=0}^{N}\phi_M\rho_MC_{\alpha M}R_{\alpha M}E_{\alpha M} - \sum_{\alpha=0}^{N}\phi_F\rho_FC_{\alpha F}R_{\alpha F}\Big[E_{\alpha F} + \frac{1}{2}\mathrm{u}_{\alpha F}^2\Big]. \end{aligned} \tag{3.12}$$

We notice that the sum over all phases $\mathscr{F}_j$ (with $j \in \{F\} \cup \{I, M\}$) of the second last term on the RHS of eq. (3.11) gives the averaged form of the overall entropy production due to exchange processes occurring at the fluid-solid interface. This entropy production is zero if eq. (3.9) is satisfied as an equality (18). We assume that this is the case, and, by making use of eq. (3.12), hypotheses (i) and (ii), and eqs. (3.2)–(3.4) and (3.6)–(3.8), we define a *reduced* form of overall entropy production, Γ_{red}, such that

$$\begin{aligned}
\Theta\rho\Gamma_{\mathrm{red}} \quad = \quad & -\phi_S\rho_S\frac{\mathrm{D}_S A_S}{\mathrm{D}t} - \phi_F\rho_F\frac{\mathrm{D}_F A_F}{\mathrm{D}t} - \phi_S\rho_S S_S\frac{\mathrm{D}_S\Theta}{\mathrm{D}t} - \phi_F\rho_F S_F\frac{\mathrm{D}_F\Theta}{\mathrm{D}t} \\
& + \sum_{\alpha=0}^{N}\Big[\boldsymbol{\sigma}_{\alpha F} - \phi_F\rho_F C_{\alpha F} A_{\alpha F}\boldsymbol{I}\Big] : \nabla\mathbf{u}_{\alpha F} \\
& - \sum_{\alpha=0}^{N}\Big[\nabla(\phi_F\rho_F C_{\alpha F} A_{\alpha F}) + \phi_F\rho_F C_{\alpha F}\mathbf{T}_{\alpha F}\Big]\cdot\mathbf{u}_{\alpha F} \\
& + \Big[\boldsymbol{\sigma}_F + \sum_{\alpha=0}^{N}\phi_F\rho_F C_{\alpha F}\mathbf{u}_{\alpha F}\otimes\mathbf{u}_{\alpha F}\Big] : \nabla\mathbf{v}_F + \boldsymbol{\sigma}_S : \nabla\mathbf{v}_S - \phi_F\rho_F\mathbf{T}_F\cdot\mathbf{w}_{FS} \\
& - \phi_S\rho_S R_S\Big[A_S - A_F - \frac{1}{2}\mathrm{w}_{FS}^2\Big] + \phi_S\rho_S A_S^* - \sum_{\alpha=0}^{N}\phi_F\rho_F C_{\alpha F} R_{\alpha F}\frac{1}{2}\mathrm{u}_{\alpha F}^2 \geq 0,
\end{aligned} \tag{3.13}$$

where $\rho := \sum_{j\in\{F,I,M\}}\phi_j\rho_j$ is the mass density of the mixture, $\phi_S\rho_S A_S := \sum_{j\in\{I,M\}}\phi_j\rho_j A_j$ and $\phi_S\rho_S S_S := \sum_{j\in\{I,M\}}\phi_j\rho_j S_j$ are the Helmholtz free energy density and entropy density of the solid-phase $\mathscr{F}_S$ (i.e. $\mathscr{F}_S = \mathscr{F}_I \cup \mathscr{F}_M$), respectively, $\mathbf{w}_{FS} := \mathbf{v}_F - \mathbf{v}_S$ is the fluid-phase *filtration velocity*, and $\phi_S\rho_S A_S^* := \sum_{k=I,M}\phi_k\rho_k(Q_k^* - \Theta\eta_k^*)$ is the rate of dissipation due to remodelling and growth.

3.2.3 Lagrange Multiplier Method

If the mixture is subject to constraints, these constraints should be accounted for when the expression of entropy production (in our case, eq. (3.13)) is exploited. A possible way of doing that consists in the application of the *Lagrange multiplier technique*: each constraint is multiplied by an appropriate Lagrange multiplier, and the resulting expression is combined with the expression of entropy production, in order to obtain a modified form of the entropy inequality. The reader is referred to the works by Liu (25), Liu and Müller (61), and Müller and Ruggeri (27) for details. The procedure used in our paper is based on the papers (18) and (58). For our purposes, we adopt as constraints the balance of mass of constituents $\mathscr{C}_{\beta j}$ (with $\beta \in \{0, \dots, N-1\}$ and $j \in \{F\} \cup \{I, M\}$), the balance of mass of all phases $\mathscr{F}_j$ (with $j \in \{F\} \cup \{I, M\}$) (cf., for example, (17)), and the requirement that the weighted sum of all diffusive velocities of fluid constituents $\mathscr{C}_{\alpha F}$ ($\alpha \in \{0, \dots, N\}$) is null, i.e. $\sum_{\alpha=0}^{N} C_{\alpha F}\mathbf{u}_{\alpha F} = \mathbf{0}$.

The modified expression of entropy production reads

$$\begin{aligned}
\Theta\rho\widetilde{\Gamma_{\mathrm{red}}} = {} & \Theta\rho\Gamma_{\mathrm{red}} \\
& +\pi\Big\{\frac{\phi_I}{\rho_I}\frac{\mathrm{D}_S\rho_I}{\mathrm{D}t}+\frac{\phi_M}{\rho_M}\frac{\mathrm{D}_S\rho_M}{\mathrm{D}t}+\frac{\phi_F}{\rho_F}\frac{\mathrm{D}_S\rho_F}{\mathrm{D}t}+\mathbf{w}_{FS}\cdot\nabla\phi_F+\frac{\phi_F}{\rho_F}\mathbf{w}_{FS}\cdot\nabla\rho_F \\
& \quad +\phi_S\nabla\cdot\mathbf{v}_S+\phi_F\nabla\cdot\mathbf{v}_F-\phi_I R_I-\phi_M R_M-\phi_F R_F\Big\} \\
& +\sum_{k\in\{I,M\}}\sum_{\beta=0}^{N-1}\lambda_{\beta k}\Big\{\phi_k\rho_k\frac{\mathrm{D}_S C_{\beta k}}{\mathrm{D}t}-\phi_k\rho_k C_{\beta k}(R_{\beta k}-R_k)\Big\} \\
& +\sum_{\beta=0}^{N-1}\lambda_{\beta F}\Big\{\phi_F\rho_F\frac{\mathrm{D}_F C_{\beta F}}{\mathrm{D}t}+\nabla\cdot(\phi_F\rho_F C_{\beta F}\mathbf{u}_{\beta F})-\phi_F\rho_F C_{\beta F}(R_{\beta F}-R_F)\Big\} \\
& +\phi_F\mathbf{\Lambda}_F:\sum_{\alpha=0}^{N}\nabla(\rho_F C_{\alpha F}\mathbf{u}_{\alpha F})\geq 0.
\end{aligned} \tag{3.14}$$

The quantities π, $\lambda_{\beta k}$ (where $\beta\in\{0,\dots,N-1\}$ and $k\in\{I,M\}$), and $\mathbf{\Lambda}_F$ are Lagrange multipliers. Their determination follows from the study of eq. (3.14) according to Coleman-Noll method.

We remark that, because of the definition of the solid-phase volume fraction, $\phi_S := \phi_I+\phi_M$, and the saturation condition, $\phi_F+\phi_S = 1$, the summation of the mass balance laws of all phases implies that no convective derivative of volume fraction, ϕ_S (or ϕ_F), can feature in eq. (3.14). Another consequence of the approach followed in the present paper is that, since the summation of the mass balance laws of all phases leads to a single balance of mass for the mixture as a whole, the enforcement of the resulting balance law as a constraint for $\Theta\rho\Gamma$ requires the introduction of a single Lagrange multiplier, i.e. π. Although this approach differs from the approach followed in (58), it is probably more appropriate for the development of the following theory.

3.3 Constitutive Framework

In order to close the field equations to be solved, a constitutive framework has to be introduced. This is done by selecting a set of *independent constitutive variables* (ICV), and treating the remaining unknowns as *dependent constitutive variables* (DCV). In the context of mixtures, however, this procedure alone does not usually provide conditions for volume fractions. Bennethum *et al.* (18) pointed out that this problem of closure is due to the loss of information in the averaging process that leads from the pore-scale analysis of the mixture to the macroscopic field equations. The solution to this problem can be obtained by following different approaches.

In the work by Wilmański (55), a thermodynamic model of compressible porous materials is presented with a balance law for porosity, whereas in the work by Sciarra *et al.* (56), volume fraction is regarded as a microstructural parameter that is introduced so to enlarge the space of admissible deformations with respect to the classical theory of mixtures. More frequently, additional conditions on the mass density of phases are imposed. For example, in the case of biphasic mixtures, it is rather customary to assume that the solid-phase (or the fluid-phase) is *intrinsically incompressible* [1]. This assumption can be relaxed if the solid-phase is modelled as a mixture of solid sub-phases (17). Indeed, even though the mass density of each sub-phase is assumed to be constant, the mass density of the solid-phase as a whole does not need to be constant because volume fractions of solid sub-phases are allowed to change in space and time. In our paper, however, we do not assume the incompressibility of the fluid- and the solid sub-phase. Rather, we assume that the mass densities of the fluid-phase, $\mathscr{F}_F$, and the solid sub-phases, $\mathscr{F}_I$ and $\mathscr{F}_M$, are functions of the mass fractions, $C_{\beta j}$ (with $\beta \in \{0, \dots, N-1\}$, and $j \in \{F, I, M\}$).

3.3.1 Growth

Following the picture proposed by Epstein and Maugin (52), growth is here viewed as a process causing the development of material inhomogeneities in the reference configuration of a body due to the presence of mass sources, or sinks, acting inside the body itself. Since, in the case of surface (or appositional) growth, a reference configuration for the body is not defined (cf., for example, (17) for explanation), we consider here volumetric (or interstitial) growth only. Growth is thus assumed to be responsible for inducing the time variation of the mass density of the body in its reference configuration. Material inhomogeneities [2] are related to the incompatibility of deformation arising as growth occurs (the reader is referred, for example, to the work by Rodriguez *et al.* (5) for explanation, and the connection of incompatible deformation with residual stresses). The anelastic deformation induced by growth is described through Kröner's *incompatibility method*, which consists of decomposing the deformation gradient tensor into the product of an elastic and an anelastic contribution.

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[1] The j-th phase of a mixture is said to be incompressible, if the convective derivative of its mass density is zero, i.e.

$$\frac{\mathrm{D}_j \rho_j}{\mathrm{D}t} = 0.$$

In the case of mixtures whose phases exchange mass, the assumption that the solid-phase is incompressible does not necessarily imply that $J_S = \det(\mathbf{F}_S) = 1$, where $\mathbf{F}_S$ is the deformation gradient tensor of the solid phase.

[2] According to Noll's terminology, by inhomogeneities we mean here distortions.

In order to define a reference configuration for the mixture, we adhere to Biot's approach (65), and the framework proposed by Quiligotti (40), and Quiligotti *et al.* (66). Accordingly, the solid-phase is taken as the "control" phase to which a reference configuration is associated. In the study presented in our paper, growth (or adsorption) is described as a process concerning the solid sub-phases of the tissue, $\mathscr{F}_I$ and $\mathscr{F}_M$, as a result of the mass exchange between the fluid-phase, $\mathscr{F}_F$, and sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$. Although we have assumed that solid sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$ move with the common velocity $\mathbf{v}_S$ (which is said to be the solid-phase velocity), growth may occur independently. Following (60), this is accounted for by assuming that, according to Kröner's method, the solid-phase deformation gradient tensor, $\mathbf{F}_S$, admits the multiplicative decomposition

$$\mathbf{F}_S = \mathbf{F}_I^{\mathrm{e}}\mathbf{F}_I^{\mathrm{an}} = \mathbf{F}_M^{\mathrm{e}}\mathbf{F}_M^{\mathrm{an}}, \tag{3.15}$$

where $\mathbf{F}_I^{\mathrm{e}}$ and $\mathbf{F}_M^{\mathrm{e}}$ measure the true elastic deformation of the inclusions and matrix, respectively, while $\mathbf{F}_I^{\mathrm{an}}$ and $\mathbf{F}_M^{\mathrm{an}}$ describe the *anelastic* part of deformation related to the production of material inhomogeneities due to growth in sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$, respectively. Each tensor $\mathbf{F}_k^{\mathrm{an}}$ (with $k \in \{I, M\}$) maps the tangent space of the reference configuration of the mixture into the tangent space of an intermediate, elastically released configuration, which is referred to as to the *natural configuration* of sub-phase $\mathscr{F}_k$ (with $k \in \{I, M\}$). The quantities $\mathbf{F}_S$, $\mathbf{F}_I^{\mathrm{an}}$, and $\mathbf{F}_M^{\mathrm{an}}$ should be treated as free unknowns.

3.3.2 Remodelling

In order to account for the presence of inclusions, and the possibility of remodelling, we introduce a *unit* vector λ_I^N, which represents the alignment of fibre-like inclusions in the natural configuration of phase $\mathscr{F}_I$. An alternative description of anisotropy can be given by the texture tensor $\Xi_I^N := \lambda_I^N \otimes \lambda_I^N$. Unit vectors λ_I^N and $\boldsymbol{\xi}_S$, and texture tensors Ξ_I^N and Ξ_S are related to the each other through

$$\boldsymbol{\xi}_S = \frac{1}{\sqrt{\mathrm{Tr}[\mathbf{F}_I^{\mathrm{e}}(\lambda_I^N \otimes \lambda_I^N)(\mathbf{F}_I^{\mathrm{e}})^T]}}\mathbf{F}_I^{\mathrm{e}}\lambda_I^N, \tag{3.16}$$

$$\Xi_S = \frac{1}{\mathrm{Tr}[\mathbf{F}_I^{\mathrm{e}}\Xi_I^N(\mathbf{F}_I^{\mathrm{e}})^T]}\mathbf{F}_I^{\mathrm{e}}\Xi_I^N(\mathbf{F}_I^{\mathrm{e}})^T. \tag{3.17}$$

According to eqs. (3.16) and (3.17), the alignment of fibre-like inclusions in the current configuration, described by $\boldsymbol{\xi}_S$ (or Ξ_S), can be obtained if the fibre arrangement in the natural configuration of phase $\mathscr{F}_I$, described by λ_I^N (or Ξ_I^N), is known.

When remodelling occurs, the change of tissue anisotropy is described by an evolution law for either the unit vector λ_I^N, or the texture tensor Ξ_I^N. Therefore, vector λ_I^N (or tensor Ξ_I^N) has to be treated as a free unknown for the tissue. However, since the unit vector λ_I^N is constrained by the relation $\|\lambda_I^N\| = 1$, it may be convenient to select as independent free unknowns only the angles ϑ and φ such that $\lambda_I^N = \sin(\varphi)\cos(\vartheta)\mathbf{e}_1 + \sin(\varphi)\cos(\vartheta)\mathbf{e}_2 + \cos(\varphi)\mathbf{e}_3$, where $\{\mathbf{e}_J\}_{J=1}^3$ are the basis unit vectors of the three-dimensional Euclidean space.

3.3.3 Unknowns

We count the unknowns featuring in the modified expression of entropy production (cf. eq. (3.14)). In particular, we split these unknowns in three sets, i.e. *free unknowns*, $\mathscr{U}_{\text{free}}$, *dependent unknowns*, $\mathscr{U}_{\text{dep}}$, and Lagrange multipliers, $\mathscr{M}$. Therefore, we conclude that the set of free and dependent unknowns, and Lagrange multipliers are given by

$$\mathscr{U}_{\text{free}} = \{\phi_I, \phi_M, C_{\beta I}, C_{\beta M}, C_{\beta F}, \mathbf{u}_{\beta F}, \mathbf{w}_{FS}, \Theta, \varphi, \vartheta, \mathbf{F}_I^{\text{e}}, \mathbf{F}_M^{\text{e}}, \mathbf{F}_I^{\text{an}}, \mathbf{F}_M^{\text{an}}\}, \tag{3.18}$$

$$\mathscr{U}_{\text{dep}} = \{A_S, A_F, S_S, S_F, \boldsymbol{\sigma}_{\beta F}, A_{\beta F}, \mathbf{T}_{\beta F}, \boldsymbol{\sigma}_F, \boldsymbol{\sigma}_S, \mathbf{T}_F, R_S, R_{\beta F}, \rho_I, \rho_M, \rho_F\}, \tag{3.19}$$

$$\mathscr{M} = \{\pi, \lambda_{\beta I}, \lambda_{\beta M}, \lambda_{\beta F}, \mathbf{\Lambda}_F\}. \tag{3.20}$$

For the exploitation of the expression of entropy production (3.14), quantities $\mathbf{F}_I^{\text{e}}$ and $\mathbf{F}_M^{\text{e}}$ are replaced by the Green-Lagrange strain tensors $\mathbf{E}_I^{\text{e}} := \frac{1}{2}[(\mathbf{F}_I^{\text{e}})^T\mathbf{F}_I^{\text{e}} - \boldsymbol{I}_I^N]$ and $\mathbf{E}_M^{\text{e}} := \frac{1}{2}[(\mathbf{F}_M^{\text{e}})^T\mathbf{F}_M^{\text{e}} - \boldsymbol{I}_M^N]$ (where $\boldsymbol{I}_I^N$ and $\boldsymbol{I}_M^N$ are the identity tensors in the natural configuration of $\mathscr{F}_I$ and $\mathscr{F}_M$, respectively), while quantities $\mathbf{F}_I^{\text{an}}$ and $\mathbf{F}_M^{\text{an}}$ are replaced by the *inhomogeneities velocity gradients* $\mathbf{L}_I^{\text{an}}$ and $\mathbf{L}_M^{\text{an}}$, defined by

$$\mathbf{L}_I^{\text{an}} := \frac{\mathrm{D}_S\mathbf{F}_I^{\text{an}}}{\mathrm{D}t}(\mathbf{F}_I^{\text{an}})^{-1}, \qquad \text{and} \qquad \mathbf{L}_M^{\text{an}} := \frac{\mathrm{D}_S\mathbf{F}_M^{\text{an}}}{\mathrm{D}t}(\mathbf{F}_M^{\text{an}})^{-1}. \tag{3.21}$$

Quantities featuring in balance laws, but not present in the lists above, are related to the above listed variables through either kinematic restrictions or their own definition. We remark that fluid-phase mass density is taken as dependent unknown (cf. eq. (3.19)) because we assume that it is prescribed as a constitutive function of mass fractions of fluid constituents. Furthermore, solid-phase velocity, $\mathbf{v}_S$, does not feature in eq. (3.18) because it has been replaced by deformation gradient tensor, $\mathbf{F}_S$, and then by tensors $\mathbf{F}_I^{\text{e}}$, $\mathbf{F}_M^{\text{e}}$, $\mathbf{F}_I^{\text{an}}$, and $\mathbf{F}_M^{\text{an}}$ through eq. (3.15).

3.3.4 Helmholtz free energy densities

In our constitutive framework, the set of independent constitutive variables (ICV) is obtained through the union of the set of free unknowns, $\mathscr{U}_{\text{free}}$, and a set of variables containing the gradients of volume and mass fractions, and the *inhomogeneity velocity gradients*, $\mathbf{L}^{\text{an}}_I$ and $\mathbf{L}^{\text{an}}_M$, while the set of dependent constitutive variables (DCV) is identified with the set of dependent unknowns, $\mathscr{U}_{\text{dep}}$, i.e.

$$\begin{aligned} \text{ICV} &= \mathscr{U}_{\text{free}} \cup \left\{ \nabla C_{\beta F}, \nabla C_{\beta I}, \nabla C_{\beta M}, \frac{\mathrm{D}_S \varphi}{\mathrm{D}t}, \frac{\mathrm{D}_S \vartheta}{\mathrm{D}t} \right\}, && (3.22) \\ \text{DCV} &= \{ A_S, A_F, S_S, S_F, \boldsymbol{\sigma}_{\beta F}, A_{\beta F}, \mathbf{T}_{\beta F}, \boldsymbol{\sigma}_F, \boldsymbol{\sigma}_S, \mathbf{T}_F, R_S, R_{\beta F}, \rho_I, \rho_M, \rho_F \}, && (3.23) \end{aligned}$$

where $\beta \in \{0, \dots, N-1\}$.

If the Axiom of equipresence were rigorously applied, the Helmholtz free energy densities, A_F and A_S should be given as constitutive functions of all ICV's. However, it is possible to show that letting A_F and A_S depend only on a subset of ICV minimizes the algebraic calculations necessary for our purposes without leading to thermodynamic inconsistencies. For this reason, we assume here that

$$A_F := \widehat{A}_F(\rho_F, \mathrm{C}_F, \Theta), \qquad \text{and} \qquad A_S := \widehat{A}_S(\rho_I, \rho_M, \mathrm{C}_I, \mathrm{C}_M, \Theta, \mathbf{F}, \mathbf{F}^{\text{an}}_I, \mathbf{F}^{\text{an}}_M, \varphi, \vartheta), \quad (3.24)$$

where $\mathrm{C}_j \equiv \{C_{0j}, \dots, C_{(N-1)j}\}$ (with $j \in \{F\} \cup \{I, M\}$). Moreover, by prescribing that the mass densities of both the solid sub-phases, $\mathscr{F}_I$ and $\mathscr{F}_M$, and the fluid-phase, $\mathscr{F}_F$, are given by constitutive (or state) functions of the mass fractions of constituents, i.e.

$$\rho_F := \widehat{\rho}_F(\mathrm{C}_F), \quad \rho_k := \widehat{\rho}_k(\mathrm{C}_k), \quad k \in \{I, M\}, \quad (3.25)$$

we write the constitutive expressions of $\widehat{A}_F$ and $\widehat{A}_S$ as

$$\begin{aligned} \widehat{A}_F(\rho_F, \mathrm{C}_F, \Theta) &= \widehat{\Psi}_F(\mathrm{C}_F, \Theta), && (3.26) \\ \widehat{A}_S(\rho_I, \rho_M, \mathrm{C}_I, \mathrm{C}_M, \Theta, \mathbf{F}, \mathbf{F}^{\text{an}}_I, \mathbf{F}^{\text{an}}_M, \varphi, \vartheta) &= \widehat{\Psi}_S(\mathrm{C}_I, \mathrm{C}_M, \Theta, \mathbf{F}, \mathbf{F}^{\text{an}}_I, \mathbf{F}^{\text{an}}_M, \varphi, \vartheta). && (3.27) \end{aligned}$$

3.4 Exploitation of the entropy production inequality

Substitution of eqs. (3.26) and (3.27) into (3.13), the result into (3.14), and application of Coleman–Noll procedure to the resulting expression of entropy production leads to the constitutive laws reported below.

3.4.1 Lagrange Multipliers

Lagrange multipliers are found to be:

$$\lambda_{\beta I} = \frac{\partial \widehat{\Psi}_I}{\partial C_{\beta I}} - \frac{\pi}{\widehat{\rho}_I^2}\frac{\partial \widehat{\rho}_I}{\partial C_{\beta I}}, \qquad \lambda_{\beta M} = \frac{\partial \widehat{\Psi}_M}{\partial C_{\beta M}} - \frac{\pi}{\widehat{\rho}_M^2}\frac{\partial \widehat{\rho}_M}{\partial C_{\beta M}}, \qquad \lambda_{\beta F} = \frac{\partial \widehat{\Psi}_F}{\partial C_{\beta F}} - \frac{\pi}{\widehat{\rho}_F^2}\frac{\partial \widehat{\rho}_F}{\partial C_{\beta F}}. \tag{3.28}$$

Quantities $\lambda_{\beta j}$ (with $\beta \in \{0, \ldots, N-1\}$ and $j \in \{F\} \cup \{I, M\}$) are identified with the *relative chemical potential* of constituent $\mathscr{C}_{\beta j}$, i.e. $\lambda_{\beta j} \equiv m_{\beta j} := \mu_{\beta j} - \mu_{Nj}$, where $\mu_{\beta j}$ and μ_{Nj} are the *absolute* chemical potentials of constituents $\mathscr{C}_{\beta j}$ and $\mathscr{C}_{Nj}$ in phase $\mathscr{F}_j$, respectively (cf., for example, (18)). We remark that, by definition, $\lambda_{Nj} \equiv m_{Nj} \equiv 0$ for all $\mathscr{F}_j$, $j \in \{F, I, M\}$. Finally, Lagrange multiplier $\mathbf{\Lambda}_F$ is found to be (18) (20)

$$\mathbf{\Lambda}_F = A_{NF}\boldsymbol{I} - \frac{1}{\phi_F \rho_F C_{NF}}\boldsymbol{\sigma}_{NF}, \tag{3.29}$$

where A_{NF}, C_{NF}, and $\boldsymbol{\sigma}_{NF}$ are Helmholtz free energy density, mass fraction, and Cauchy stress tensor of constituent $\mathscr{C}_{NF}$ in the fluid-phase.

3.4.2 Entropies and Cauchy stress tensors

Entropy densities of the solid- and fluid-phase are related to the derivatives of the corresponding Helmholtz free energy density with respect to temperature, i.e.

$$S_S = -\frac{\partial \widehat{\Psi}_S}{\partial \Theta}, \qquad \text{and} \qquad S_F = -\frac{\partial \widehat{\Psi}_F}{\partial \Theta}. \tag{3.30}$$

Furthermore, the Cauchy stress tensors of fluid-phase constituents, fluid-phase as a whole, and solid-phase are given by

$$\boldsymbol{\sigma}_{\alpha F} = \phi_F \rho_F C_{\alpha F}(A_{\alpha F} - \lambda_{\alpha F})\boldsymbol{I} - \phi_F \rho_F C_{\alpha F}\mathbf{\Lambda}_F, \tag{3.31}$$

$$\boldsymbol{\sigma}_F = -\phi_F \rho_F \lambda_F \boldsymbol{I} - \sum_{\alpha=0}^{N} \phi_F \rho_F C_{\alpha F}\mathbf{u}_F \otimes \mathbf{u}_F = -\phi_F \pi \boldsymbol{I} - \sum_{\alpha=0}^{N} \phi_F \rho_F C_{\alpha F}\mathbf{u}_F \otimes \mathbf{u}_F, \tag{3.32}$$

$$\boldsymbol{\sigma}_S = -\phi_S \pi \mathbf{I} + \boldsymbol{\sigma}_I^{\mathrm{e}} + \boldsymbol{\sigma}_M^{\mathrm{e}}. \tag{3.33}$$

We remark that, in order for eq. (3.31) to be consistent with eq. (3.32), the sum over all constituents in the fluid-phase, $\mathscr{C}_{\alpha F}$ ($\alpha \in \{0, \ldots, N\}$), of the Cauchy stress tensors $\boldsymbol{\sigma}_{\alpha F}$ must be equal to the inner part of the fluid-phase Cauchy stress tensor, $\boldsymbol{\sigma}_F$, i.e.

$$\sum_{\alpha=0}^{N} \boldsymbol{\sigma}_{\alpha F} = -\phi_F \pi. \tag{3.34}$$

By using Equation (3.29), this condition can be used in order to show that

$$\mu_{\alpha F} = A_{\alpha F} + \frac{\pi_{\alpha F}}{\rho_F C_{\alpha F}}, \tag{3.35}$$

where $\pi_{\alpha F}$ is the partial pressure of the fluid-phase constituent $\mathscr{C}_{\alpha F}$ ($\alpha \in \{0, \dots, N\}$). Moreover, the Cauchy stress tensor of constituent $\mathscr{C}_{\alpha F}$ is given by $\boldsymbol{\sigma}_{\alpha F} = -\phi_F \pi_{\alpha F} \boldsymbol{I}$, and partial pressures $\pi_{\alpha F}$ satisfy

$$\sum_{\alpha=0}^{N} \pi_{\alpha F} = \pi. \tag{3.36}$$

Finally, the sum of the quantities $\boldsymbol{\sigma}_I^{\mathrm{e}}$ and $\boldsymbol{\sigma}_M^{\mathrm{e}}$ represents the elastic part of solid-phase overall Cauchy stress tensor. These two tensors are defined by

$$\begin{aligned} \boldsymbol{\sigma}_I^{\mathrm{e}} &:= \frac{1}{J_S} \mathbf{F}_I^{\mathrm{e}} \frac{\partial \overline{W}_I}{\partial \mathbf{E}_I^{\mathrm{e}}} (\mathbf{F}_I^{\mathrm{e}})^T + \phi_I \rho_I (A_S - A_I) \boldsymbol{I} \\ &= \phi_I \rho_I \mathbf{F}_I^{\mathrm{e}} \frac{\partial A_I}{\partial \mathbf{E}_I^{\mathrm{e}}} (\mathbf{F}_I^{\mathrm{e}})^T + \phi_I \rho_I (A_S - A_I) \boldsymbol{I}, \end{aligned} \tag{3.37}$$

$$\begin{aligned} \boldsymbol{\sigma}_M^{\mathrm{e}} &:= \frac{1}{J_S} \mathbf{F}_M^{\mathrm{e}} \frac{\partial \overline{W}_M}{\partial \mathbf{E}_M^{\mathrm{e}}} (\mathbf{F}_M^{\mathrm{e}})^T + \phi_M \rho_M (A_S - A_M) \boldsymbol{I} \\ &= \phi_M \rho_M \mathbf{F}_M^{\mathrm{e}} \frac{\partial A_M}{\partial \mathbf{E}_M^{\mathrm{e}}} (\mathbf{F}_M^{\mathrm{e}})^T + \phi_M \rho_M (A_S - A_M) \boldsymbol{I}, \end{aligned} \tag{3.38}$$

where $\overline{W}_I := J_S W_I$, $\overline{W}_M := J_S W_M$, and $W_I := \phi_I \rho_I A_I$ (with $j \in \{I, M\}$), and their sum is such that the elastic part of the Cauchy stress tensor of the solid-phase as a whole is given by

$$\boldsymbol{\sigma}_S^{\mathrm{e}} = \frac{1}{J_S} \mathbf{F}_I^{\mathrm{e}} \frac{\partial \overline{W}_I}{\partial \mathbf{E}_I^{\mathrm{e}}} (\mathbf{F}_I^{\mathrm{e}})^T + \frac{1}{J_S} \mathbf{F}_M^{\mathrm{e}} \frac{\partial \overline{W}_M}{\partial \mathbf{E}_M^{\mathrm{e}}} (\mathbf{F}_M^{\mathrm{e}})^T. \tag{3.39}$$

Equations (3.37)-(3.38) are obtained by computing the total differential of Ψ_S and using the fact that, because of the multiplicative decomposition of $\mathbf{F}_S$, the hypothesis of *density preserving growth* (which implies that $\mathrm{Tr}(\mathbf{L}_k^{\mathrm{an}}) = R_k$), and the constraint $\rho_k \equiv \widehat{\rho_k}(\mathrm{C}_k)$, each volume fraction ϕ_k can be written as a function of the elastic part of deformation, $\mathbf{E}_k^{\mathrm{e}}$, and mass fraction of constituents in subphase $\mathscr{F}_k$, i.e. $\phi_k \equiv \widehat{\phi_k}(\mathbf{E}_k^{\mathrm{e}}, \mathrm{C}_k)$, where

$$\frac{\partial \phi_k}{\partial \mathbf{E}_k^{\mathrm{e}}} = -\phi_k \mathbf{C}_k^{\mathrm{e}\,-T}, \qquad \frac{\partial \phi_k}{\partial C_{\beta k}} = -\frac{\phi_k}{\rho_k} \frac{\partial \widehat{\rho_k}}{\partial C_{\beta k}}, \tag{3.40}$$

and $\mathbf{C}_k^{\mathrm{e}} := \mathbf{F}_k^{\mathrm{e}\,T} \mathbf{F}_k^{\mathrm{e}}$. Moreover, as done in (11), the Helmholtz free energy density of sub-phase $\mathscr{F}_k$, A_k ($k \in \{I, M\}$), is assumed to depend on the overall deformation only through the elastic part of deformation associated with $\mathscr{F}_k$, i.e. $\mathbf{E}_k^{\mathrm{e}}$.

3.4.3 Residual entropy production inequality

By virtue of eqs. (3.28)–(3.39), under the assumptions of small diffusive velocities of fluid-phase constituents, small fluid-phase filtration velocity (i.e. $\|\mathbf{u}_{\alpha F}\|^2 \ll 1$, and $\|\mathbf{w}_{FS}\|^2 \ll 1$), negligible inertial terms in momentum balance laws, and accounting for the kinematic constraints on the growth velocity gradients $\mathbf{L}_I^{\text{an}}$ and $\mathbf{L}_M^{\text{an}}$ (60), i.e.

$$\mathrm{Tr}(\mathbf{L}_I^{\text{an}}) = \mathbf{L}_I^{\text{an}} : \boldsymbol{I}_I^N = R_I, \qquad \text{and} \qquad \mathrm{Tr}(\mathbf{L}_M^{\text{an}}) = \mathbf{L}_M^{\text{an}} : \boldsymbol{I}_M^N = R_M, \tag{3.41}$$

the expression of *residual* of entropy production can be written as

$$\begin{aligned}
\Theta\rho\widetilde{\Gamma}_{\text{red}} = {} & \sum_{\alpha=0}^{N} \mathbf{u}_{\alpha F}\cdot\Big\{-\phi_F\rho_F C_{\alpha F}\Big(\nabla\mu_{\alpha F}-\mathbf{g}\Big)\Big\} + \mathbf{w}_{FS}\cdot\Big\{-\phi_F\rho_F\mathbf{T}_F+\pi\nabla\phi_F\Big\} \\
& -\sum_{\beta=0}^{N-1}\phi_I\rho_I C_{\beta I}R_{\beta I}\Big\{\lambda_{\beta I}-\lambda_{\beta F}\Big\} - \sum_{\beta=0}^{N-1}\phi_M\rho_M C_{\beta M}R_{\beta M}\Big\{\lambda_{\beta M}-\lambda_{\beta F}\Big\} \\
& +\phi_I\rho_I\mathbf{L}_I^{\text{an}} : \Big\{\frac{1}{J_S\phi_I\rho_I}\mathbf{B}_I^{\text{e}} - \Big(A_I+\frac{\pi}{\rho_I}-\sum_{\beta=0}^{N-1}C_{\beta I}\lambda_{\beta I}\Big)\boldsymbol{I}_I^N \\
& \qquad + \Big(A_F+\frac{\pi}{\rho_F}-\sum_{\beta=0}^{N-1}C_{\beta F}\lambda_{\beta F}\Big)\boldsymbol{I}_I^N\Big\} \\
& +\phi_M\rho_M\mathbf{L}_M^{\text{an}} : \Big\{\frac{1}{J_S\phi_M\rho_M}\mathbf{B}_M^{\text{e}} - \Big(A_M+\frac{\pi}{\rho_M}-\sum_{\beta=0}^{N-1}C_{\beta M}\lambda_{\beta M}\Big)\boldsymbol{I}_M^N \\
& \qquad + \Big(A_F+\frac{\pi}{\rho_F}-\sum_{\beta=0}^{N-1}C_{\beta F}\lambda_{\beta F}\Big)\boldsymbol{I}_M^N\Big\} \\
& +\phi_S\rho_S A_S^* - \phi_S\rho_S\frac{\mathrm{D}_S\varphi}{\mathrm{D}t} : \frac{\partial\widehat{\Psi}_S}{\partial\varphi} - \phi_S\rho_S\frac{\mathrm{D}_S\vartheta}{\mathrm{D}t} : \frac{\partial\widehat{\Psi}_S}{\partial\vartheta} \geq 0,
\end{aligned} \tag{3.42}$$

where we introduced the notation

$$\mathbf{B}_I^{\text{e}} := \mathbf{C}_I^{\text{e}}\frac{\partial\overline{W}_I}{\partial\mathbf{E}_I^{\text{e}}}, \qquad \text{and} \qquad \mathbf{B}_M^{\text{e}} := \mathbf{C}_M^{\text{e}}\frac{\partial\overline{W}_M}{\partial\mathbf{E}_M^{\text{e}}}, \tag{3.43}$$

with $\mathbf{C}_I^{\text{e}} = (\mathbf{F}_I^{\text{e}})^T\mathbf{F}_I^{\text{e}}$, $\mathbf{C}_M^{\text{e}} = (\mathbf{F}_M^{\text{e}})^T\mathbf{F}_M^{\text{e}}$, and $J_S = \det(\mathbf{F}_S)$.

Further conditions on the unknowns can be obtained by studying inequality (3.42) in the case of thermodynamic equilibrium, i.e. at the state at which all non-equilibrium variables

$$\text{Non-equilibrium variables} = \Big\{\frac{\mathrm{D}_S\varphi}{\mathrm{D}t}, \frac{\mathrm{D}_S\vartheta}{\mathrm{D}t}, \mathbf{u}_{\alpha F}, \mathbf{w}_{FS}, \mathbf{L}_I^{\text{an}}, \mathbf{L}_M^{\text{an}}, R_{\beta I}, R_{\beta M}\Big\} \tag{3.44}$$

($\beta \in \{0, \ldots, N-1\}$) vanish identically. At equilibrium, entropy production is zero, i.e. it attains its minimum value. Therefore, it is possible to characterise equilibrium by requiring the "gradient", and the "Hessian"of the residual entropy production with respect to non-equilibrium variables to be zero, and be positive–definite, respectively. For this purpose, inspired by (71), we assume that the quantity $\phi_S \rho_S A_S^*$ can be written as

$$\phi_S \rho_S A_S^* = \phi_S \rho_S A_S^{**} + \phi_I \rho_I \mathbf{L}_I^{\mathrm{an}} : \mathbf{H}_I + \phi_M \rho_M \mathbf{L}_M^{\mathrm{an}} : \mathbf{H}_M, \tag{3.45}$$

where $\mathbf{H}_I$ and $\mathbf{H}_M$ are two second-order tensors related growth. Under this assumption, the equilibrium conditions are fulfilled by the following set of Onsager's relations:

$$\mathbf{u}_{\beta F} = -\mathbf{M}_{\beta F} \nabla m_{\beta F}, \tag{3.46}$$

$$\mathbf{w}_{FS} = -\mathbf{M}_F (\phi_F \rho_F \mathbf{T}_F - \pi \nabla \phi_F), \tag{3.47}$$

$$R_{\beta I} = -\mathrm{Z}_{\beta I} (m_{\beta I} - m_{\beta F}), \tag{3.48}$$

$$R_{\beta M} = -\mathrm{Z}_{\beta M} (m_{\beta M} - m_{\beta F}), \tag{3.49}$$

$$\begin{aligned} \mathbf{L}_I^{\mathrm{an}} \;=\; \mathbb{M}_I : \Big\{ & \frac{1}{J_S \phi_I \rho_I} \mathbf{B}_I^{\mathrm{e}} + \mathbf{H}_I - \Big(A_I + \frac{\pi}{\rho_I} - \sum_{\beta=0}^{N-1} C_{\beta I} m_{\beta I} \Big) \boldsymbol{I}_I^N \\ & + \Big(A_F + \frac{\pi}{\rho_F} - \sum_{\beta=0}^{N-1} C_{\beta F} m_{\beta F} \Big) \boldsymbol{I}_I^N \Big\}, \end{aligned} \tag{3.50}$$

$$\begin{aligned} \mathbf{L}_M^{\mathrm{an}} \;=\; \mathbb{M}_M : \Big\{ & \frac{1}{J_S \phi_M \rho_M} \mathbf{B}_M^{\mathrm{e}} + \mathbf{H}_M - \Big(A_M + \frac{\pi}{\rho_M} - \sum_{\beta=0}^{N-1} C_{\beta M} m_{\beta M} \Big) \boldsymbol{I}_M^N \\ & + \Big(A_F + \frac{\pi}{\rho_F} - \sum_{\beta=0}^{N-1} C_{\beta F} m_{\beta F} \Big) \boldsymbol{I}_M^N \Big\}, \end{aligned} \tag{3.51}$$

$$A_S^{**} - \frac{\mathrm{D}_S \varphi}{\mathrm{D}t} : \frac{\partial \widehat{\Psi}_S}{\partial \varphi} - \frac{\mathrm{D}_S \vartheta}{\mathrm{D}t} : \frac{\partial \widehat{\Psi}_S}{\partial \vartheta} \geq 0, \tag{3.52}$$

where we used the definitions of relative chemical potentials, $\lambda_{\beta I} = m_{\beta I}$, $\lambda_{\beta M} = m_{\beta M}$, and $\lambda_{\beta F} = m_{\beta F}$ (with $\beta \in \{0, \ldots, N-1\}$), given in eqs. (3.28). If some constituents are not exchanged, then the index β in eqs. (3.48)-(3.49) ranges in the subset of constituents that are actually exchanged, i.e. those for which $R_{\beta j} \neq 0$. Coefficients $\mathrm{Z}_{\beta I}$, $\mathrm{Z}_{\beta M}$ are positive scalars, $\mathbf{M}_{\beta F}$, $\mathbf{M}_F$ are positive-definite second-order tensors, and $\mathbb{M}_I$, $\mathbb{M}_M$ are positive-definite fourth-order tensors endowed with the major symmetry (cf. Loret and Simões (60)). In general, each of these coefficients may be a function of all independent constitutive variables. We remark that eqs. (3.46)–(3.51) are obtained by inverting the near-equilibrium expansions of the coefficients of non-equilibrium variables (3.44), i.e. the terms between braces in eq. (3.42).

Onsager's relation (3.46) provides diffusion–dispersion Fick's law for the fluid-phase constituent $\mathscr{C}_{\beta F}$. Indeed, by multiplying both side of eq. (3.46) by $\phi_F \rho_F C_{\beta F}$, and defining the diffusive–dispersive mass flux constituent $\mathscr{C}_{\beta F}$ as $\mathbf{J}_{\beta F} = \phi_F \rho_F C_{\beta F} \mathbf{u}_{\beta F}$, we obtain

$$\mathbf{J}_{\beta F} = -\phi_F \rho_F C_{\beta F} \mathbf{M}_{\beta F} \nabla m_{\beta F}, \tag{3.53}$$

where tensor $\mathbf{M}_{\beta F}$ is proportional to the diffusive–dispersive tensor associated with constituent $\mathscr{C}_{\beta F}$.

Equation (3.47) gives Darcy's law of flow for the filtration velocity of the fluid-phase. This law is obtained by expressing the momentum exchange $\phi_F \rho_F \mathbf{T}_F$ through the balance of momentum for the fluid-phase, approximating the fluid-phase Cauchy stress tensor by $\boldsymbol{\sigma}_F \approx -\phi_F \pi \boldsymbol{I}$ (cf. eq. (3.32)), and invoking the hypothesis of negligible inertial terms, i.e.

$$\phi_F \rho_F \mathbf{T}_F = \nabla(\phi_F \pi) - \phi_F \rho_F \mathbf{g}. \tag{3.54}$$

Substitution of eq. (3.54) into Onsager's relation (3.47) leads to

$$\mathbf{w}_{FS} = -\mathbf{K}_F (\nabla \pi - \rho_F \mathbf{g}). \tag{3.55}$$

where $\mathbf{K}_F = \phi_F \mathbf{M}_F$ is said to be the fluid-phase permeability tensor.

Onsager's relations (3.48) and (3.49) imply that the source (or sink) of mass of constituent $\mathscr{C}_{\beta k}$ (with $k \in \{I, M\}$) depends on the difference between the relative chemical potential of that constituent, $m_{\beta k}$, and the relative chemical potential of constituent $\mathscr{C}_{\beta F}$ in the fluid-phase, $m_{\beta F}$. Since, at equilibrium, the relative chemical potential of a given constituent has to be the same for any phase, the conditions $m_{\beta I} \equiv m_{\beta F}$ and $m_{\beta M} = m_{\beta F}$ imply that sources (or sinks) $R_{\beta I}$ and $R_{\beta M}$ have to vanish at equilibrium. Furthermore, since $\phi_F \rho_F C_{\beta F} R_{\beta F} = -(\phi_I \rho_I C_{\beta I} R_{\beta I} + \phi_M \rho_M C_{\beta M} R_{\beta M})$, also the source (or sink) of mass for constituent $\mathscr{C}_{\beta F}$ in the fluid-phase has to be zero at equilibrium. Results (3.46)–(3.49) were obtained by Bennethum *et al.* in (18), and have been here slightly generalized to the case of a solid-phase consisting of two sub-phases (i.e. matrix and fibre-like inclusion sub-phases).

Equations (3.50) and (3.51) represent the growth laws for the solid sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$, respectively. These relations can be rewritten by defining, for solid sub-phases $\mathscr{F}_I$ and $\mathscr{F}_M$, and for the fluid-phase $\mathscr{F}_F$, the following Mandel-type stress tensors

$$\mathbf{B}_I = \mathbf{B}_I^{\mathrm{e}} + J_S \phi_I \rho_I \sum_{\beta=0}^{N-1} C_{\beta I} m_{\beta I} \boldsymbol{I}_I^N, \tag{3.56}$$

$$\mathbf{B}_M = \mathbf{B}_M^{\mathrm{e}} + J_S \phi_M \rho_M \sum_{\beta=0}^{N-1} C_{\beta M} m_{\beta M} \boldsymbol{I}_M^N, \tag{3.57}$$

$$\mathbf{B}_{FI} = J_S \phi_I \rho_I \sum_{\beta=0}^{N-1} C_{\beta F} m_{\beta F} \boldsymbol{I}_I^N, \quad \text{and} \quad \mathbf{B}_{FM} = J_S \phi_M \rho_M \sum_{\beta=0}^{N-1} C_{\beta F} m_{\beta F} \boldsymbol{I}_M^N. \tag{3.58}$$

Substitution of definitions (3.56)–(3.58) into eqs. (3.50) and (3.51) yields

$$\mathbf{L}_I^{\mathrm{an}} = \mathbb{M}_I : \left\{ \frac{1}{J_S \phi_I \rho_I} \Big(\mathbf{B}_I - \mathbf{B}_{FI} \Big) + \mathbf{H}_I - \left[\left(A_I + \frac{\pi}{\rho_I} \right) - \left(A_F + \frac{\pi}{\rho_F} \right) \right] \boldsymbol{I}_I^N \right\}, \tag{3.59}$$

$$\mathbf{L}_M^{\mathrm{an}} = \mathbb{M}_M : \left\{ \frac{1}{J_S \phi_M \rho_M} \Big(\mathbf{B}_M - \mathbf{B}_{FM} \Big) + \mathbf{H}_M - \left[\left(A_M + \frac{\pi}{\rho_M} \right) - \left(A_F + \frac{\pi}{\rho_F} \right) \right] \boldsymbol{I}_M^N \right\}. \tag{3.60}$$

Equations (3.59) and (3.60) are a generalisation of the results reported in (58). Similar growth laws have been previously proposed by Loret and Simões (60), Fusi *et al.* (13) for a fluid-solid mixture with mass exchange between constituents, Ambrosi and Guana (67) in the monophasic continuum, and by Ambrosi *et al.* (15) for a non-homogeneous monophasic body. Following (71)(126), tensors $\mathbf{H}_I$ and $\mathbf{H}_M$ may be taken as

$$\mathbf{H}_I = -\frac{1}{J_S \phi_I \rho_I} \mathbf{B}_I^0, \quad \text{and} \quad \mathbf{H}_M = -\frac{1}{J_S \phi_M \rho_M} \mathbf{B}_M^0, \tag{3.61}$$

where $\mathbf{B}_I^0$ and $\mathbf{B}_M^0$ are external "forces" that, at equilibrium, balance $\mathbf{B}_I$ and $\mathbf{B}_M$, respectively.

By accounting for Onsager's relations (3.46)–(3.49), and (3.59)–(3.60), we conclude that inequality (3.52) has to be verified in order for the entropy principle to be respected. In the next section, we investigate the consequences of this requirement.

3.5 Evolution of fibre-like inclusions

Since the solid-phase Helmholtz free energy density, $\widehat{\Psi}_S$, is assumed to be a dependent constitutive variable, the derivative of $\widehat{\Psi}_S$ with respect to texture tensor Ξ_I^N can be regarded as known. Therefore, it can be concluded that, in inequality (3.52), unknown quantities are $\mathrm{D}_S \boldsymbol{\Xi}_I^N / \mathrm{D}t$ and A_S^{**}.

Following Chadwick (46), Imatani and Maugin (53), and Maugin and Imatani (54), a formulation of remodelling can be obtained on the basis of the evolution of the texture tensor $\boldsymbol{\Xi}_I^N$, i.e.

$$\frac{\mathrm{D}_S \boldsymbol{\Xi}_I^N}{\mathrm{D}t} = \boldsymbol{\Xi}_I^N (\mathbf{L}_I^{\mathrm{an}})^T + \mathbf{L}_I^{\mathrm{an}} \boldsymbol{\Xi}_I^N - 2(\mathbf{L}_I^{\mathrm{an}} : \boldsymbol{\Xi}_I^N) \boldsymbol{\Xi}_I^N. \tag{3.62}$$

We remark that, by virtue of eq. (3.17), texture tensor $\boldsymbol{\Xi}_S$ is determined if tensors $\boldsymbol{\Xi}_I^N$ and $\mathbf{F}_I^{\mathrm{e}}$ are known. Therefore, if $\boldsymbol{\Xi}_I^N$ is the solution of the evolution law (3.62), texture tensor $\boldsymbol{\Xi}_S$ can be computed directly through eq. (3.17)

In the case in which vector λ_I^N is embedded in the continuum, we propose to use Onsager's relation (3.59) in order to express the growth velocity gradient, $\mathbf{L}_I^{\mathrm{an}}$, for the fibre-like inclusion sub-phase $\mathscr{F}_I$. By doing that, tensor $\mathbf{L}_I^{\mathrm{an}}$ is a function of Mandel-type stress tensors $\mathbf{B}_I$ and $\mathbf{B}_{FI}$, as well as other thermodynamic quantities. This confirms that Mandel stress is the driving force for remodelling.

As an example, following Olsson and Klarbring (126), we assume that the growth law (3.59) takes on the simplified form

$$\mathbf{L}_I^{\mathrm{an}} = M_I \left\{ \frac{1}{J_S \phi_I \rho_I} \left(\mathbf{B}_I - \mathbf{B}_{FI} - \mathbf{B}_I^0 \right) - \left[\left(A_I + \frac{\pi}{\rho_I} \right) - \left(A_F + \frac{\pi}{\rho_F} \right) \right] \boldsymbol{I}_I^N \right\}, \tag{3.63}$$

where M_I is a positive scalar coefficient. We notice that the growth velocity gradient $\mathbf{L}_I^{\mathrm{an}}$ contains hydrostatic contributions. Since hydrostatic terms cannot play any role in the evolution equation of $\boldsymbol{\Xi}_I^N$, by introducing the notation

$$M_I^* = \frac{M_I}{J_S \phi_I \rho_I}, \tag{3.64}$$

eq. (3.62) becomes

$$\frac{\mathrm{D}_S \boldsymbol{\Xi}_I^N}{\mathrm{D}t} = \boldsymbol{\Xi}_I^N M_I^* (\mathbf{B}_I^{\mathrm{e}} - \mathbf{B}_I^0)^T + M_I^* (\mathbf{B}_I^{\mathrm{e}} - \mathbf{B}_I^0) \boldsymbol{\Xi}_I^N - 2[M_I^* (\mathbf{B}_I^{\mathrm{e}} - \mathbf{B}_I^0) : \boldsymbol{\Xi}_I^N] \boldsymbol{\Xi}_I^N, \tag{3.65}$$

where only the *elastic* part of the Mandel-type stress tensor $\mathbf{B}_I$ is the driving force for remodelling. We remark that, in the example described above, the fluid-phase Mandel-type stress tensor plays no role in remodelling due to the fact that it is a hydrostatic tensor.

This result shows that, in the simple case studied in this section, only the elastic Mandel-type stress tensor, $\mathbf{B}_I^{\mathrm{e}}$, acts as a driving force for the reorientation of fibre-like inclusions.

Chapter 4

Growth and Mass Transfer in Multi-Constituent Biological Materials

4.1 Introduction

A biphasic and multiconstituent material describes macroscopically the growth and mass transfer in a biological tissue. One phase is fluid, and the other one is solid. Our goals in this chapter are (i) to discuss possible evolution laws for both mass transfer and growth, and (ii) to characterize the equilibrium of the system. In order to do that we distinguish between the phases and growth exchange interactions in the solid-phase. Kröner's decomposition allows us to find an elastic, $\mathbf{F}_e$, and inelastic, $\mathbf{F}_a$, part of the deformation gradient tensor, $\mathbf{F} = \mathbf{F}_e\mathbf{F}_a$. This approch has origin in the Theory of Plasticity and it is one of the milestones of the mathematical modelling of volumetric growth.

In monophasic continua, if growth is the only inelastic process, $\mathbf{F}_a$ defines the generally incompatible and inelastic deformation due to growth (100). Within a first-order constitutive framework, the material derivative of $\mathbf{F}_a$ is constrained by $R = \mathrm{Tr}\{\mathbf{L}_a\}$, where $\mathbf{L}_a := (\mathrm{D}_t\mathbf{F}_a)(\mathbf{F}_a)^{-1}$, and R is the rate at which the medium grows. If a constitutive law for $\mathbf{L}_a$ is found, then the identity $(\mathrm{D}_t\mathbf{F}_a) = \mathbf{L}_a\mathbf{F}_a$ is the evolution law of $\mathbf{F}_a$. In multiphasic continua, which aim at a more realistic modelling of biological tissues, there are usually other processes that concur, together with growth, to the variation of mass of the phases. Sometimes, the growth of one phase (typically the solid one) is identified with the mass that this phase acquires because of the exchange processes with all other phases. Also in this context, the variation of mass, assumed to trigger inelastic deformation, is related to $\mathbf{F}_a$.The search for evolution laws of

$\mathbf{F}_a$ has become the subject of several papers dealing with the Thermomechanics of volumetric growth.

Inspired by the Thermodynamics of Irreversible Processes, we will determine $\mathbf{L}_a$ directly from the Dissipation Inequality (cf., for example, (13)-(112)).

To meet the purposes of this Chapter it will be presented the results obtained by Grillo and Wittum (2), showing possible evolution laws for both mass transfer and growth in multi-constituent biological materials, and studing the equilibrium of the system.

4.2 Definitions

The studied biphasic material comprises a fluid-phase, $\mathscr{F}_F$, and a solid-phase, $\mathscr{F}_S$. The volume fraction of $\mathscr{F}_j$, with $j \in \{F, S\}$, is denoted by ϕ_j. The saturation condition applies, i.e. $\sum_{j=F,S} \phi_{1j} = 1$. Each phase contains $(N+1)$ constituents. The α-th constituent of $\mathscr{F}_j$ is denoted by $C_{\alpha j}$, with $\alpha \in \{0, \dots, N\}$. The "true" mass density of $\mathscr{F}_j$ is defined by $\rho_j := \sum_{\alpha=0}^{N} \rho_{\alpha j}$, where $\rho_{\alpha j}$ is the mass density of $C_{\alpha j}$. The composition of $\mathscr{F}_j$ is described by the mass fractions $\omega_{\alpha j} := \rho_{\alpha j}/\rho_j$, which are constrained by $\sum_{\alpha=0}^{N} \omega_{\alpha j} = 1$.

The velocity of $\mathscr{F}_F$ is defined by $\mathbf{v}_F := \sum_{\alpha=0}^{N} \omega_{\alpha F} \mathbf{v}_{\alpha F}$, $\mathbf{v}_{\alpha F}$ being the velocity of $C_{\alpha F}$. The diffusion of $C_{\alpha F}$ in the fluid-phase is described by the mass flux $\mathbf{j}_{\alpha F} := \phi_F \rho_F \omega_{\alpha F} \mathbf{u}_{\alpha F}$, with $\mathbf{u}_{\alpha F} := \mathbf{v}_{\alpha F} - \mathbf{v}_F$. By definition, $\sum_{\alpha=0}^{N} \mathbf{j}_{\alpha F} = \mathbf{0}$. The velocity at which the fluid-phase moves as a whole through the solid-phase is the *filtration velocity* $\mathbf{w}_{FS} := \mathbf{v}_F - \mathbf{v}_S$, where $\mathbf{v}_S$ is the velocity of $\mathscr{F}_S$.

In our model, the constituents of $\mathscr{F}_S$ are assumed to move at the same velocity $\mathbf{v}_S$. The deformation gradient tensor of $\mathscr{F}_S$ is $\mathbf{F} := \mathrm{Grad}(\chi_S)$, and χ_S is the solid-phase motion (74).

The Helmholtz free energies per unit mass of $C_{\alpha j}$ and $\mathscr{F}_j$ are $\Psi_{\alpha j}$ and Ψ_j, respectively, with $\Psi_j := \sum_{\alpha=0}^{N} \omega_{\alpha j} \Psi_{\alpha j}$. We also introduce the Gibbs free energy density of $\mathscr{F}_j$, $G_j := \sum_{\alpha=0}^{N} \omega_{\alpha j} \mu_{\alpha j}$, where $\mu_{\alpha j}$ is the chemical potential of $C_{\alpha j}$. The difference $\widetilde{\mu}_{\beta j} := \mu_{\beta j} - \mu_{Nk}$ is the *relative* chemical potential of $C_{\beta j}$.

The overall mass source R_j of $\mathscr{F}_j$ may represent the superposition of different processes. The term R_j^t accounts for the interphase mass transfer. If $\mathscr{F}_j$ grows, the term R_j^g is introduced, so that $R_j = R_j^t + R_j^g$. We assume that $\mathscr{F}_F$ and $\mathscr{F}_S$ exchange mass with each other, and that $\mathscr{F}_S$ undergoes also growth. Therefore, we define $R_F = R_F^t$ and $R_S = R_S^t + R_S^g$. Since the biphasic medium as a whole is closed with respect to the exchange interactions, the restriction $\sum_{j=F,S} \phi_j \rho_j R_j^t = 0$ applies. Because of growth, however, the biphasic medium is *open*.

If both mass transfer and growth lead to inelastic deformation, we decompose the tensor $\mathbf{F}_a$ as $\mathbf{F}_a = \mathbf{F}_g\mathbf{F}_t$. Here, we have exploited the analogy with the Theory of Plasticity a little further. Indeed, decompositions of $\mathbf{F}_a$ of this form are encountered in Plasticity when damage is present (72). The inelastic velocity "gradient" reads

$$\mathbf{L}_a = \mathbf{L}_g + \mathbf{F}_g\mathbf{L}_t(\mathbf{F}_g)^{-1}, \tag{4.1}$$

with $\mathbf{L}_g := (\mathrm{D}_t\mathbf{F}_g)(\mathbf{F}_g)^{-1}$ and $\mathbf{L}_t := (\mathrm{D}_t\mathbf{F}_t)(\mathbf{F}_t)^{-1}$ such that $\mathrm{Tr}\{\mathbf{L}_g\} = R^g_S$, $\mathrm{Tr}\{\mathbf{L}_t\} = R^t_S$, and $\mathrm{Tr}\{\mathbf{L}_a\} = R_S = R^t_S + R^g_S$.

4.3 Constitutive Results

Since the phases vary their mass by exchanging constituents, the composition of $\mathscr{F}_F$ and $\mathscr{F}_S$ is variable. Thus, the phases are in principle not intrinsically incompressible, and ρ_F and ρ_S are functions of composition. Assuming constant temperature, the Helmholtz free energy densities Ψ_F and Ψ_S are prescribed constitutive functions as specified below

$$\Psi_F := \Psi_F(\omega_{0F}, \ldots, \omega_{(N-1)F}), \quad \text{and} \quad \Psi_S := \Psi_S(\mathbf{F}_e, \omega_{0S}, \ldots, \omega_{(N-1)S}). \tag{4.2}$$

The fact that ρ_F and ρ_S are independent on pressure requires to consider pressure as a Lagrange multiplier. In this case, the study of the Dissipation Inequality for a multi-constituent biphasic medium comprising a macroscopically inviscid fluid-phase and an elastic solid-phase leads to the constitutive results (cf., for example, (58)(112)):

$$\begin{aligned} \mathbf{T}_S \quad &= \quad -\phi_S p\mathbf{I} + \mathbf{T}^e_S = -\phi_S p\mathbf{I} + \phi_S\rho_S \tfrac{\partial\Psi_S}{\partial\mathbf{F}_e}(\mathbf{F}_a)^{-T}\mathbf{F}^T, \quad \text{and} \\ &\mathbf{T}_F = -\phi_F p\mathbf{I} - \textstyle\sum_{\alpha=0}^{N}\mathbf{u}_\alpha \otimes \mathbf{j}_{\alpha F} \end{aligned} \tag{4.3}$$

$$\widetilde{\mu}_{\beta j} \quad = \quad \frac{\partial G_j}{\partial\omega_{\beta j}} = \frac{\partial\Psi_j}{\partial\omega_{\beta j}} - \frac{p}{\rho_j^2}\frac{\partial\rho_j}{\partial\omega_{\beta j}}, \quad \text{with } \beta \in \{0, \ldots, N-1\}, \quad \text{and} \quad G_j = \Psi_j + \frac{p}{\rho_j}. \tag{4.4}$$

4.4 Study of the Residual Dissipation Inequality

We assume that the biphasic medium is in chemical and thermal equilibrium. For such a system, the residual Dissipation inequality can be written as (cf. (58)(112))

$$\mathrm{D}^{res} = -\textstyle\sum_{\beta=0}^{N-1}\mathbf{j}_{\beta F}\cdot\mathbf{b}_{\beta F} - \mathbf{w}_{FS}\cdot\mathbf{b}_F + \sum_{\beta=0}^{N-1}\omega_{\beta S}R^t_{\beta S}\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\} + \mathbf{L}_t : \mathbf{Q}_t + \mathbf{L}_g : \mathbf{H}_g \geq 0. \tag{4.5}$$

The quantity $\mathbf{b}_{\beta F}$ is the dissipative part of the rate at which the constituent $C_{\beta F}$ exchanges momentum with all other constituents, while $\mathbf{b}_F := \mathbf{F}_F - p \ \mathrm{grad}(\phi_F)$ is the dissipative part of $\mathbf{F}_F$, the latter being the rate of exchange of momentum between $\mathscr{F}_F$ and $\mathscr{F}_S$. The third summand represents the dissipation due to the exchange of constituents between $\mathscr{F}_F$ and $\mathscr{F}_S$, where $R^t_{\beta S}$ is the rate of transfer of the β-th constituent from $\mathscr{F}_F$ into $\mathscr{F}_S$, and vice versa. The fourth term, instead, accounts for the dissipation due to the overall interphase mass transfer. The second-order tensor $\mathbf{Q}_t$ is defined by

$$\mathbf{Q}_t = \{\phi_S \rho_S [(G_F - \textstyle\sum_{\beta=0}^{N-1} \omega_{\beta F} \widetilde{\mu}_{\beta F}) - (G_S - \textstyle\sum_{\beta=0}^{N-1} \omega_{\beta S} \widetilde{\mu}_{\beta S})]\mathbf{I}_e + (J_e)^{-1} (\mathbf{F}_g)^T \mathbf{B}_e (\mathbf{F}_g)^{-T} + \mathbf{M}_t\}, \tag{4.6}$$

where $\mathbf{I}_e$ is the identity tensor in the relaxed configuration, $J_e = \det(\mathbf{F}_e)$, and $\mathbf{B}_e$ is the elastic Mandel stress tensor of the solid-phase, i.e.

$$\mathbf{B}_e = J_e \phi_S \rho_S (\mathbf{F}_e)^T \tfrac{\partial \Psi_S}{\partial \mathbf{F}_e}. \tag{4.7}$$

These results are obtained by enforcing the condition $\phi_S \rho_S \omega_{\beta S} R^t_{\beta S} = -\phi_F \rho_F \omega_{\beta F} R^t_{\beta F}$, which states that the constituent leaving $\mathscr{F}_F$ enters $\mathscr{F}_S$, and vice versa.

Following (73)(71), we define the second-order tensor $\mathbf{H}_g$ by

$$\mathbf{H}_g = (J_e)^{-1} \mathbf{B}_e + \mathbf{M}_g. \tag{4.8}$$

The tensors $\mathbf{M}_t$ and $\mathbf{M}_g$ originate from the *non-standard* dynamics put forward in (71) for monophasic media. These tensors are generelized forces conjugated to the generalized velocities $\mathbf{L}_t$ and $\mathbf{L}_g$, respectively. The adjective “non-standard” refers to the fact that, in the present theory, the space of test velocities of the biphasic medium is augmented by $\mathbf{L}_t$ and $\mathbf{L}_g$. Following the terminology of (71), we call $\mathbf{M}_g$ and $\mathbf{M}_t$ *outer remodelling couples*, for they drive the rearrangement of the internal structure of the medium in response to inelastic processes described by $\mathbf{L}_t$ and $\mathbf{L}_g$.

We consider the set $\mathrm{T} = \{\mathbf{L}_t, \mathbf{L}_g, \mathbf{Q}_t, \mathbf{H}_g\} \subset \mathrm{Lin}$, where Lin is the set of all linear maps from a finite-dimensional vector space V into itself. Any tensor $\mathbf{T} \in \mathrm{T}$ admits the unique decomposition

$$\mathbf{T} = [\mathbf{T}]_S + [\mathbf{T}]_A, \tag{4.9}$$

where $[\ \cdot\ ]_S$ and $[\ \cdot\ ]_A$ are operators that extract the symmetric and antisymmetric part of $\mathbf{T}$, respectively. Let us also introduce the space of symmetric tensors, $\mathrm{Sym} \subset \mathrm{Lin}$, and the spaces of spherical and deviatoric tensors, denoted by Sph and Dev, respectively. Since $[\mathbf{T}]_S \in \mathrm{Sym}$, and $\mathrm{Sym} = \mathrm{Sph} \oplus \mathrm{Dev}$, we perform the further decomposition

$$\mathbf{T} = \tfrac{1}{3}\mathrm{Tr}\{\mathbf{T}\}\mathbf{I} + \mathrm{Dev}\{[\mathbf{T}]_S\} + [\mathbf{T}]_A. \tag{4.10}$$

By applying (5.34) in (4.5), and performing the scalar products, we obtain:

$$\begin{aligned} \mathrm{D}^{res} \;=\; & -\textstyle\sum_{\beta=0}^{N-1}\mathbf{j}_{\beta F}\cdot\mathbf{b}_{\beta F} - \mathbf{w}_{FS}\cdot\mathbf{b}_F + \sum_{\beta=0}^{N-1}\omega_{\beta S}R^t_{\beta S}\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\} \\ & +\mathrm{Tr}\{\mathbf{L}_t\}\tfrac{1}{3}\mathrm{Tr}\{\mathbf{Q}_t\} + \mathrm{Dev}\{[\mathbf{L}_t]_S\} : \mathrm{Dev}\{[\mathbf{Q}_t]_S\} + [\mathbf{L}_t]_A : [\mathbf{Q}_t]_A \\ & +\mathrm{Tr}\{\mathbf{L}_g\}\tfrac{1}{3}\mathrm{Tr}\{\mathbf{H}_g\} + \mathrm{Dev}\{[\mathbf{L}_g]_S\} : \mathrm{Dev}\{[\mathbf{H}_g]_S\} + [\mathbf{L}_g]_A : [\mathbf{H}_g]_A \geq 0. \end{aligned} \tag{4.11}$$

In (4.5), we choose the following quantities as the independent thermodynamic variables that vanish at equilbrium

$$\Phi = \Upsilon \cup \Sigma = \{(\mathbf{j}_{\beta F})_{\beta=0}^{N-1}, \mathbf{w}_{FS}\} \cup \{(\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\})_{\beta=0}^{N-1}, \mathbf{Q}_t, \mathbf{H}_g\}, \tag{4.12}$$

and we postulate that, for an isotropic medium, D^{res} admits the simple form

$$\begin{aligned} \mathrm{D}^{res}(\Phi) \;:=\; & \textstyle\sum_{\beta=0}^{N-1}\mathbf{j}_\beta\cdot(\mathbf{A}_{\beta F}\mathbf{j}_{\beta F}) + \mathbf{w}_{FS}\cdot(\mathbf{A}_F\mathbf{w}_{FS}) + \sum_{\beta=0}^{N-1}K_{\beta S}(\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\})^2 \\ & +2\textstyle\sum_{\beta=0}^{N-1}K_{\beta S}(\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\})\frac{\mathrm{Tr}\{\mathbf{Q}_t\}}{3} + \mathbf{Q}_t : \gimel^\star_t[\mathbf{Q}_t] + \mathbf{H}_g : \gimel_g[\mathbf{H}_g] \geq 0. \end{aligned} \tag{4.13}$$

The symmetric and positive definite tensors $\mathbf{A}_F$ and $\mathbf{A}_{\beta F}$ are the inverse of the permeability and mobility of constituent $C_{\alpha F}$, respectively. The positive scalars $K_{\beta S}$ are related to the rates at which constituents are exchanged between the phases, while $\gimel^\star_t$ and $\gimel_g$ are the positive definite fourth-order tensors defined below (75)(76)

$$\begin{aligned} \gimel^\star_t[\mathbf{Q}_t] &= l_t\mathrm{Tr}\{\mathbf{Q}_t\}\mathbf{I}_e + 2m_t[\mathbf{Q}_t]_S + 2n_t[\mathbf{Q}_t]_A = \\ &\ (3l_t + 2m_t)\tfrac{1}{3}\mathrm{Tr}\{\mathbf{Q}_t\}\mathbf{I}_e + 2m_t\mathrm{Dev}\{[\mathbf{Q}_t]_S\} + 2n_t[\mathbf{Q}_t]_A, \end{aligned} \tag{4.14}$$

$$\begin{aligned} \gimel_g[\mathbf{H}_g] &= l_g\mathrm{Tr}\{\mathbf{H}_g\}\mathbf{I}_e + 2m_g[\mathbf{H}_g]_S + 2n_g[\mathbf{H}_g]_A = \\ &\ (3l_g + 2m_g)\tfrac{1}{3}\mathrm{Tr}\{\mathbf{H}_g\}\mathbf{I}_e + 2m_g\mathrm{Dev}\{[\mathbf{H}_g]_S\} + 2n_g[\mathbf{H}_g]_A. \end{aligned} \tag{4.15}$$

The hypothesis of isotropic medium allows for deducing that the dissipation defined in (5.16) is fully decoupled into a volumetric and deviatoric part (51)(77)[1].

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[1] A potential is said to be *fully decoupled* when the associated fourth-order tensor $\gimel$ satisfies $\mathbb{V} : \gimel : \mathbb{D} = 0$ and $\mathbb{D} : \gimel : \mathbb{V} = 0$, where $\mathbb{V}$ and $\mathbb{D}$ are the operators extracting the volumetric and deviatoric part of given tensor $\mathbf{T} \in \mathrm{Lin}$, i.e. $V_{ijkl} = \frac{1}{3}\delta_{ij}\delta_{kl}$, and $D_{ijkl} = \delta_{ik}\delta_{jl} - V_{ijkl}$. If $\mathbf{T} \in \mathrm{Sym}$, then $D_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - V_{ijkl}$.

4.4.1 Evolution Laws

We determine the evolution laws for the quantities Φ by applying the Principle of Maximum Dissipation (78). By defining the list of thermodynamic quantities dual of Φ as

$$\Pi = \Omega \cup \Lambda = \{(\mathbf{b}_{\beta F})_{\beta=0}^{N-1}, \mathbf{b}_F\} \cup \{(\omega_{\beta S} R_{\beta S}^t)_{\beta=0}^{N-1}, \mathbf{L}_t, \mathbf{L}_g\}, \tag{4.16}$$

the evolution laws for Π are given by $\Pi = \frac{1}{2}\partial_\Phi \mathrm{D}^{res}$.

After some calculations, we obtain:

$$\begin{aligned}
\mathbf{b}_{\beta F} &= -\mathbf{A}_{\beta F}\mathbf{j}_{\beta F}, && (4.17)\\
\mathbf{b}_F &= -\mathbf{A}_F\mathbf{w}_F, && (4.18)\\
\omega_{\beta S} R_{\beta S}^t &= K_{\beta S}(\phi_S\rho_S\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\} + \tfrac{\mathrm{Tr}\{\mathbf{Q}_t\}}{3}) = \\
&\quad \phi_S\rho_S K_{\beta S}(\mu_{\beta F} - \mu_{\beta S} + \tfrac{\mathrm{Tr}\{(J_e)^{-1}\mathbf{B}_e\}+\mathrm{Tr}\{\mathbf{M}_t\}}{3\phi_S\rho_S}), && (4.19)\\
\mathbf{L}_t &= \textstyle\sum_{\beta=0}^{N-1} \tfrac{\phi_S\rho_S K_{\beta S}}{3}\{\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\}\mathbf{I}_e + \gimel_t^{\star}[\mathbf{Q}_t], && (4.20)\\
\mathbf{L}_g &= \gimel_g[\mathbf{H}_g] = (3l_g + 2m_g)\tfrac{1}{3}\mathrm{Tr}\{\mathbf{H}_g\}\mathbf{I}_e + 2m_g\mathrm{Dev}\{[\mathbf{H}_g]_S\} + 2n_g[\mathbf{H}_g]_A. && (4.21)
\end{aligned}$$

Since $\sum_{\alpha=0}^N \omega_{\alpha S} R_{\alpha S}^t = R_S^t = \mathrm{Tr}\{\mathbf{L}_t\}$, we enforce the condition $\sum_{\alpha=0}^N \frac{K_{\alpha S}}{3} = (3l_t + 2m_t)$, so that $\mathbf{L}_t$ can be rewritten as

$$\mathbf{L}_t = \textstyle\sum_{\alpha=0}^N \frac{\phi_S\rho_S K_{\alpha S}}{3}\{(\mu_{\alpha F} - \mu_{\alpha S}) + \frac{\mathrm{Tr}\{\mathbf{H}_t\}}{3\phi_S\rho_S}\}\mathbf{I}_e + 2m_t\mathrm{Dev}\{[\mathbf{H}_t]_S\} + 2n_t[\mathbf{H}_t]_A, \tag{4.22}$$

where $\mathbf{H}_t := (J_e)^{-1}(\mathbf{F}_g)^T\mathbf{B}_e(\mathbf{F}_g)^{-T}+\mathbf{M}_t$, and $K_{\alpha S} \equiv K_{\alpha S}(\omega_{0S}, \ldots, \omega_{(N-1)S})$ for all $\alpha \in \{0, \ldots, N\}$.

Equations ([Ons3]–[LLt]) generalize the results of [Bennethum2000], and are perhaps more physical than the evolution laws determined in [GrilloIJES]. The improvement is in the fact that ([Ons3]–[Ons4]) are now coupled (see also the fourth term in ([Delta])). This coupling is, in our opinion, necessary in order to have a diagonal representation of the constituent mass exchange terms, i.e.

$\omega_{\alpha S} R_{\alpha S}^t = \phi_S\rho_S K_\alpha\{\mu_{\alpha F} - \mu_{\alpha S} + \frac{\mathrm{Tr}\{\mathbf{H}_t\}}{3\phi_S\rho_S}\}$.

4.4.2 Characterization of Equilibrium

In Mixture Theory, the state of thermodynamic equilibrium is characterized by the vanishing of the quantities Υ and Λ. From (4.17–4.18) it follows that setting $\Upsilon = 0$ is equivalent to have zero diffusion fluxes, i.e. $\mathbf{j}_{\beta F} = \mathbf{0}$ with $\beta \in \{0, \ldots, N-1\}$, and zero filtration velocity, i.e. $\mathbf{w}_{FS} = \mathbf{0}$. Furthermore, in a neighbourhood of equilibrium, (4.17–4.18) allow for the determination of the Fick and Darcy's laws, respectively. On the other hand, the evolution laws (4.19–4.22) rephrase the equilibrium conditions for Λ in terms of their conjugated thermodynamic quantities Σ. Therefore, setting $\Sigma = 0$ provides the circumstances under which the multi-constituent biphasic material experiences neither interphase mass transfer nor growth.

Let us start with growth. From the condition $\mathbf{L}_g = \mathbf{0}$, we deduce that a sufficient condition for impeding growth is that $\mathbf{H}_g = \mathbf{0}$. If this is the case, then the non-standard generalized force $\mathbf{M}_g$ must satisfy the equality $\mathbf{M}_g = -(J_e)^{-1}\mathbf{B}_e$. Thus, by regarding $\mathbf{H}_g$ as the dissipative part of $\mathbf{M}_g$, we draw two conclusions: (i) the negative of the Mandel stress tensor, devided by J_e, is the equilibrium part of $\mathbf{M}_g$, and (ii) out of equilibrium, $\mathbf{M}_g$ reads

$$\mathbf{M}_g = -(J_e)^{-1}\mathbf{B}_e + \mathbf{H}_g = -(J_e)^{-1}\mathbf{B}_e + \gimel_g^{-1}[\mathbf{L}_g]. \tag{4.23}$$

Thus, the growing medium behaves as a "visco-elastic" material in which $(J_e)^{-1}\mathbf{B}_e$, which is entirely defined by the body elastic behaviour, plays the role of a generalized equilibrium stress, whereas the inverse tensor $\gimel_g^{-1}$ provides the "viscosities". The characterization of the types of growth that may occur in a tissue can be instead discussed by looking at the tensor decomposition in (4.21). For example, if $\mathrm{Dev}\{[\mathbf{H}_g]_S\} = \mathbf{0}$ and $[\mathbf{H}_g]_A = \mathbf{0}$, then we have spherical growth.

Let us now look at mass transfer. From (4.22) we notice that the condition $\mathbf{L}_t = \mathbf{0}$ is fulfilled when $\mathrm{Dev}\{[\mathbf{H}_t]_S\} = \mathbf{0}$, $[\mathbf{H}_t]_A = \mathbf{0}$, and

$$\mu_{\alpha F} - \mu_{\alpha S} + \tfrac{\mathrm{Tr}\{\mathbf{H}_t\}}{3\phi_S \rho_S} = 0, \quad \forall\, \alpha \in \{0, \ldots, N\}. \tag{4.24}$$

The latter set of equations implies that, at equilibrium, the spherical part of $\mathbf{H}_t$ modulates the difference of chemical potential of the α-th constituent simultaneously present in the fluid- and in the solid-phase. This might be understood as a chemo-mechanical coupling. Moreover, if we prescribe $\mathrm{Tr}\{\mathbf{H}_t\} = 0$, then we re-obtain the Gibbsean characterization of equilibrium, i.e. $\mu_{\alpha F} - \mu_{\alpha S} = 0$ for all $\alpha \in \{0, \ldots, N\}$. This result cannot be obtained if the tensor $\mathbf{M}_t$, which is instrinsic in the non-standard dynamics of (71), is not introduced in the model. Indeed, if one sets $\mathbf{M}_t = \mathbf{0}$, then the imbalance of chemical potentials in (4.24) would be always compensated for by $\mathrm{Tr}\{(J_e)^{-1}\mathbf{B}_e\}/(3\phi_S\rho_S)$, which does not vanish at equilibrium for it is already an equilibrium quantity. From the discussion above we draw two conclusions: (i) for mass transfer, there are two non-equilrium stresses (cf. (4.20)), one of which is proportional to $\{E\widetilde{\mu}_{\beta F} - \widetilde{\mu}_{\beta S}\}\mathbf{I}_e$, and the other one is given by $\mathbf{Q}_t$ in (4.6), and (ii) out of equilibrium, $\mathbf{L}_t$ is driven by $\mathbf{M}_t$ and the generalized imbalance of Eshelby-like stress tensors determined by rewriting (4.6) as follows

$$\begin{aligned}\mathbf{Q}_t \;=\;& \phi_S \rho_S (\mathbf{F}_g)^T \{[G_F \mathbf{I}_e - \textstyle\sum_{\beta=0}^{N-1} \omega_{\beta F} \frac{\partial G_F}{\partial \omega_{\beta F}} \mathbf{I}_e] \\ & -[G_S \mathbf{I}_e - (\textstyle\sum_{\beta=0}^{N} \omega_{\beta S} \frac{\partial G_S}{\partial \omega_{\beta S}} \mathbf{I}_e + (\mathbf{F}_e)^T \frac{\partial G_S}{\partial \mathbf{F}_e})]\}(\mathbf{F}_g)^{-T} + \mathbf{M}_t. \qquad (4.25)\end{aligned}$$

To the best of our understanding, mass transfer and growth are different processes. In our model, the difference is given by the explicit presence of chemical potentials in the evolution law of $\mathbf{L}_t$.

Chapter 5

Remodeling in Fiber-Reinforced, Multi-Constituent Materials

5.1 Introduction

After the introduction, in the previous chapters, of many important concepts such as the Mixture Theory, the mass balances and the kinematics of anelastic processes, we will obtain the expression of residual dissipation as shown by Grillo *et al.* (136) and we will study the residual dissipation inequality improving some of the results presented in (2, 58, 112).
We adapt the model of fiber reorientation put forward by Olsson and Klarbring (126) to the case of a multi-constituent solid with statistical distribution of fibers. Morever the latter model in the presence of chemical agents will also prepresent the starting point for the next and last chapter. We conceive the solid phase of the mixture as a composite material whose fibers are distributed according to some probability density distribution. The procedure for determining the evolution laws of the variables describing the reorientation of fibers is similar to that used for mass transfer and growth. The novelty, however, is conceptual since we view these variables either as the parameters specifying the probability density distribution or as the probability density distribution itself.

5.2 Dissipation

We require that every constituent $\mathscr{C}_{aj}$ of the mixture is characterized by its Helmholtz free energy density $\rho_{aj}\psi_{aj}$. Adding these quantities over all constituents of the j-th phase yields

$\rho_j\psi_j = \sum_a \rho_{aj}\psi_{aj}$, while the addition over all phases leads to the Helmholtz free energy density of the mixture, i.e. $\rho\psi := \sum_j \sum_a \rho_{aj}\psi_{aj}$.

In the case of constant and uniform temperature, the energy imbalance is postulated, for any part $\mathscr{V}_t$ of $\mathscr{B}_t$, in the form

$$\int_{\mathscr{V}_t} \mathrm{D} = -\mathrm{d}_t \int_{\mathscr{V}_t} (\mathrm{K} + \rho\psi) + \mathrm{P}^{\mathrm{ext}}_{\mathrm{st}} + \mathrm{P}^{\mathrm{ext}}_{\text{n-st}} + \int_{\partial\mathscr{V}_t} \boldsymbol{q}_\psi \cdot \boldsymbol{n} + \int_{\mathscr{V}_t} \overset{g}{\Psi} \geq 0, \tag{5.1}$$

where the time derivative on the right-hand side is taken with respect to the motion of the mixture as a whole, $\mathrm{P}^{\mathrm{ext}}_{\mathrm{st}}$ and $\mathrm{P}^{\mathrm{ext}}_{\text{n-st}}$ are the standard and non-standard external powers, respectively,

$$\mathrm{P}^{\mathrm{ext}}_{\mathrm{st}} = \int_{\mathscr{V}_t} \{\textstyle\sum_j \sum_a \rho_{aj} \boldsymbol{b}_{aj} \cdot \boldsymbol{v}_{aj}\} + \int_{\partial\mathscr{V}_t} \textstyle\sum_j \sum_a \boldsymbol{\tau}_{aj} \cdot \boldsymbol{v}_{aj}, \tag{5.2}$$

$$\mathrm{P}^{\mathrm{ext}}_{\text{n-st}} = \int_{\mathscr{V}_t} \{\mathbf{Y}^{\mathrm{ext}} : \mathrm{D}_S \mathbf{K} + \mathbf{Z}^{\mathrm{ext}} : \mathrm{D}_S \mathbf{G} + \textstyle\sum_n \mathrm{R}^{\mathrm{ext}}_n \mathrm{D}_S \zeta_n\}, \tag{5.3}$$

$\boldsymbol{q}_\psi$ is a (pseudo-)flux of energy ($\boldsymbol{n}$ is the unit vector normal to $\partial\mathscr{V}_t$), which arises in response to the relative velocities $\boldsymbol{u}_{aj}$, $\boldsymbol{u}_S$ and $\boldsymbol{u}_F$, i.e.

$$\boldsymbol{q}_\psi = -\{\textstyle\sum_j \sum_a \rho_{aj}\psi_{aj}\boldsymbol{u}_{aj} + \rho_S\psi_S\boldsymbol{u}_S + \rho_F\psi_F\boldsymbol{u}_F\}, \tag{5.4}$$

and $\overset{g}{\Psi}$ collects all the energy production terms induced by growth (6), i.e.,

$$\overset{g}{\Psi} = \textstyle\sum_a \rho_{aS} [\underset{aS}{\overset{g}{\Psi}} + \boldsymbol{p}_{aS} \cdot \boldsymbol{v}_{aS} + \gamma_{aS} (\frac{|\boldsymbol{v}_{aS}|^2}{2} + \psi_{aS})], \tag{5.5}$$

where $\underset{aS}{\overset{g}{\Psi}}$ represents a supply of energy which is, in general, not expressed in terms of mechanic power.

5.2.1 Saturation Constraint

Following (2, 13, 17, 112), we account for saturation in the balance of mass of the mixture as a whole, which is now regarded as a constraint and written as follows

$$\begin{aligned} p\,\mathrm{C} \;=\; & \textstyle\sum_j \rho_j \frac{p}{\hat{\rho}_j^2} \mathrm{D}_S \hat{\rho}_j + \frac{p}{\hat{\rho}_F} \mathrm{grad}(\rho_F) \cdot \boldsymbol{w}_{FS} + \phi_F\, p\, \mathrm{div}(\boldsymbol{w}_{FS}) \\ & + p\, \mathrm{div}(\boldsymbol{v}_S) - \Big(\frac{p}{\hat{\rho}_S} - \frac{p}{\hat{\rho}_F}\Big) \rho_S r_S - \frac{p}{\hat{\rho}_S} \rho_S \gamma_S = 0, \end{aligned} \tag{5.6}$$

where p is an unknown Lagrange multiplier having the physical meaning of pressure. We append now (5.6) to (5.1), and evaluate the integral $\int_{\mathscr{V}_t} \{\mathrm{D} + p\,\mathrm{C}\}$ which, after localization, yields the inequality $\tilde{\mathrm{D}} = \mathrm{D} + p\,\mathrm{C} \geq 0$. In order to study this result, we introduce the Gibbs free energy density of the phase $\mathscr{F}_j$,

$$G_j = \psi_j + \frac{p}{\hat{\rho}_j} \tag{5.7}$$

and, after several algebraic manipulations, rewrite the local form of (5.1) as

$$\tilde{\mathrm{D}} = -\textstyle\sum_j \rho_j \Big(\mathrm{D}_S \psi_j - \dfrac{p}{\hat{\rho}_j^2} \mathrm{D}_S \hat{\rho}_j\Big) + \tilde{\mathrm{D}}_{\mathrm{I}} + \tilde{\mathrm{D}}_{\mathrm{II}} + \tilde{\mathrm{D}}_{\mathrm{III}} \geq 0. \tag{5.8}$$

In monophasic theories, the Gibbs free energy density is usually defined as the Legendre transformation of the Helmholtz free energy density ψ, i.e. $G = \psi - \frac{1}{\rho_R}\mathbf{S} : \mathbf{E}$, where ρ_R is the mass density measured with respect to the reference configuration, $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor, and $\mathbf{E}$ is the Green-Lagrange strain tensor. In this respect, our definition of G_j reflects the (partial) Legendre transformation of ψ_j with respect to the mass density $\hat{\rho}_j$. We use this definition because of the assumption on $\{\hat{\rho}_j\}_{j=S,F}$, which are independent on pressure in our formulation.

The term $\tilde{\mathrm{D}}_{\mathrm{I}}$ provides information about the standard stresses, and is defined by

$$\begin{aligned} \tilde{\mathrm{D}}_{\mathrm{I}} &= (\mathbf{T}_S + \mathbf{T}_F + p\mathbf{I}) : \mathrm{grad}(\boldsymbol{v}_S) + (\mathbf{T}_F + \phi_F p\mathbf{I}) : \mathrm{grad}(\boldsymbol{w}_{FS}) \\ &\quad + \textstyle\sum_j \sum_b \{\tilde{\mathbf{T}}_{bj} - \rho_{bj}\tilde{\psi}_{bj}\mathbf{I}\} : \mathrm{grad}(\boldsymbol{u}_{bj}), \end{aligned} \tag{5.9}$$

where $\mathbf{T}_F = \sum_a \mathbf{T}_{aF}$ and $\mathbf{T}_S = \sum_a \mathbf{T}_{aS}$ are the peculiar Cauchy stress tensors of the fluid phase and solid phase as a whole, respectively, while $\tilde{\mathbf{T}}_{bj} = \mathbf{T}_{bj} - \frac{\omega_{bj}}{\omega_{Nk}}\mathbf{T}_{Nk}$ and $\tilde{\psi}_{bj} = \psi_{bj} - \psi_{Nk}$ represent the relative stress and energy in constituent $\mathscr{C}_{bj}$ (cf. (18, 20)). The term $\tilde{\mathrm{D}}_{\mathrm{II}}$ describes the exchange of momentum among phases and constituents, and can be written as follows

$$\begin{aligned} \tilde{\mathrm{D}}_{\mathrm{II}} &= -\Big[\rho_F \mathrm{grad}(\psi_F) + \rho_F \boldsymbol{m}_F - \frac{p}{\hat{\rho}_F}\mathrm{grad}(\rho_F)\Big] \cdot \boldsymbol{w}_{FS} \\ &\quad - \textstyle\sum_j \sum_b \{\mathbf{T}_{Nk}\mathrm{grad}(\frac{\omega_{bj}}{\omega_{Nk}}) + \mathrm{grad}(\rho_{bj}\tilde{\psi}_{bj}) + \rho_{bj}\tilde{\boldsymbol{m}}_{bj}\} \cdot \boldsymbol{u}_{bj}, \end{aligned} \tag{5.10}$$

where $\tilde{\boldsymbol{m}}_{bj} = \boldsymbol{m}_{bj} - \boldsymbol{m}_{Nk}$ denotes the relative production of momentum of constituent $\mathscr{C}_{bj}$ due to exchange interactions. Finally, the summand $\tilde{\mathrm{D}}_{\mathrm{III}}$ contains all terms related to mass transfer, growth as well as the non-standard external power, i.e.

$$\begin{aligned} \tilde{\mathrm{D}}_{\mathrm{III}} &= \textstyle\sum_a \rho_{aS}\, r_{aS} \{\frac{|\boldsymbol{u}_{aF}|^2}{2} - \frac{|\boldsymbol{u}_{aS}|^2}{2} + \frac{|\boldsymbol{w}_{FS}|^2}{2} + (G_F - G_S)\} \\ &\quad + \textstyle\sum_a [\rho_{aS} \underset{aS}{\overset{g}{\Psi}} + \rho_{aS}\gamma_{aS}(\psi_{aS} - G_S)] \\ &\quad + \mathbf{Y}^{\mathrm{ext}} : \mathrm{D}_S \mathbf{K} + \mathbf{Z}^{\mathrm{ext}} : \mathrm{D}_S \mathbf{G} + \textstyle\sum_n \mathrm{R}_n^{\mathrm{ext}} \mathrm{D}_S \zeta_n. \end{aligned} \tag{5.11}$$

5.2.2 Constitutive Framework

We consider a simplified constitutive framework in which ψ_F is a given function of the composition of $\mathscr{F}_F$, and ψ_S depends on the composition of $\mathscr{F}_S$, the elastic part of deformation, $\mathbf{F}_E$, and the remodeling parameters $\{\zeta_n\}_{n=1}^{\mathrm{I}}$, i.e.

$$\psi_F = \psi_F(\{\omega_{bF}\}_{b=0}^{N-1}), \quad \psi_S = \psi_S(\mathbf{F}\mathbf{K}^{-1}\mathbf{G}^{-1}, X, \{\omega_{bj}\}_{b=0}^{N-1}, \{\zeta_n\}_{n=1}^{\mathrm{I}}). \tag{5.12}$$

The quantities enlisted among the arguments of the Helmholtz free energy densities defined in (5.12) belong to the set of the independent constitutive variables. This set contains also the relative velocities $\boldsymbol{u}_{bj}$ and $\boldsymbol{w}_{FS}$ (which describe mass diffusion phenomena and filtration of the fluid through the solid phase) and the time derivatives of $\mathbf{G}$, $\mathbf{K}$ and ζ_n in order to account for mass transfer, growth and reorientation of fibers. On the contrary, the gradients of $\boldsymbol{v}_S$, $\boldsymbol{w}_{FS}$ and $\boldsymbol{u}_{bj}$ are assumed to be neither independent nor dependent constitutive variables.

With this constitutive framework, we substitute (5.12) into (5.8) in order to obtain a modified form of dissipation, which will be studied by means of the Coleman-Noll method, i.e.

$$\tilde{\mathrm{D}} = \tilde{\mathrm{D}}_{\mathrm{I}}^{(1)} + \tilde{\mathrm{D}}_{\mathrm{II}}^{(1)} + \tilde{\mathrm{D}}_{\mathrm{III}}^{(1)} \geq 0. \tag{5.13}$$

The indices "(1)" have been introduced to highlight that the summands of (5.13) are obtained by combining $\tilde{\mathrm{D}}_{\mathrm{I}}$, $\tilde{\mathrm{D}}_{\mathrm{II}}$ and $\tilde{\mathrm{D}}_{\mathrm{III}}$ with the first term on the right-hand-side of (5.8). By defining the auxiliary quantities

$$\begin{aligned} g_{bj} &= \frac{\partial G_j}{\partial \omega_{bj}}, && (5.14)\\ \mathbf{\Pi} &= {\mathbf{F}_E}^T\Big(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\Big) + \mathbf{Z}^{\mathrm{int}}\mathbf{G}^T, && (5.15)\\ \mathbf{\Delta} &= {\mathbf{F}_E}^T\Big(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\Big) + \mathbf{G}^{-T}\mathbf{Y}^{\mathrm{int}}\mathbf{K}^T\mathbf{G}^T, && (5.16)\\ \mathrm{N}_n &= -\Big(\rho_S \frac{\partial \psi_S}{\partial \zeta_n}\Big) + \mathrm{R}_n^{\mathrm{int}}, && (5.17) \end{aligned}$$

the contributions $\tilde{\mathrm{D}}_{\mathrm{I}}^{(1)}$, $\tilde{\mathrm{D}}_{\mathrm{II}}^{(1)}$, and $\tilde{\mathrm{D}}_{\mathrm{III}}^{(1)}$ can be written as

$$\begin{aligned} \tilde{\mathrm{D}}_{\mathrm{I}}^{(1)} = & \Big\{-\Big(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\Big)\mathbf{F}_A^{-T}\mathbf{F}^T + \mathbf{T}_S + \mathbf{T}_F + p\mathbf{I}\Big\} : \mathrm{grad}(\boldsymbol{v}_S) && (5.18)\\ & +\Big\{\mathbf{T}_F + \phi_F p\mathbf{I}\Big\} : \mathrm{grad}(\boldsymbol{w}_{FS})\\ & +\textstyle\sum_j \sum_b \Big\{\tilde{\mathbf{T}}_{bj} + \rho_{bj}(g_{bj} - \tilde{\psi}_{bj})\mathbf{I}\Big\} : \mathrm{grad}(\boldsymbol{u}_{bj}), \end{aligned}$$

$$\begin{aligned}\tilde{\mathrm{D}}^{(1)}_{\mathrm{II}} &= -\Big\{\rho_F \boldsymbol{m}_F - p\ \mathrm{grad}(\phi_F)\Big\}\cdot \boldsymbol{w}_{FS} \\ &\quad -\textstyle\sum_j \sum_b \Big\{\mathbf{T}_{Nk}\mathrm{grad}(\frac{\omega_{bj}}{\omega_{Nk}}) - \mathrm{grad}[\rho_{bj}(g_{bj} - \tilde{\psi}_{bj})] \\ &\quad +\rho_{bj}\tilde{\boldsymbol{m}}_{bj} + \rho_{bj}\mathrm{grad}(g_{bj})\Big\}\cdot \boldsymbol{u}_{bj},\end{aligned} \tag{5.19}$$

$$\begin{aligned}\tilde{\mathrm{D}}^{(1)}_{\mathrm{III}} &= \mathbf{\Pi} : \mathbf{\Lambda} + \mathbf{\Delta} : \mathbf{V} + \textstyle\sum_n \mathrm{N}_n \mathrm{D}_S \zeta_n \\ &\quad +\textstyle\sum_a \rho_{aS}\, r_{aS}\Big\{\frac{|\boldsymbol{u}_{aF}|^2}{2} - \frac{|\boldsymbol{u}_{aS}|^2}{2}\Big\} + \sum_b \rho_{bS}\, r_{bS}\,(g_{bF} - g_{bS}) \\ &\quad +\rho_S\, r_S\Big\{(G_F - \textstyle\sum_b \omega_{bF} g_{bF}) - (G_S - \sum_b \omega_{bS}\, g_{bS}) + \frac{|\boldsymbol{w}_{FS}|^2}{2}\Big\} \\ &\quad -\textstyle\sum_b \rho_{bS}\,\gamma_{bS}\, g_{bS} - \rho_S\,\gamma_S\,(G_S - \sum_b \omega_{bS}\, g_{bS}) \\ &\quad +\textstyle\sum_a \{\rho_{aS} \overset{g}{\underset{aS}{\Psi}} + \rho_{aS}\,\gamma_{aS}\,\psi_{aS}\} \geq 0.\end{aligned} \tag{5.20}$$

5.2.3 Bowen's chemical potential and standard results

Bowen (18, 20, 92) introduced the tensor field $\boldsymbol{\nu}_{aj} = \psi_{aj}\mathbf{I} - \frac{1}{\rho_{aj}}\mathbf{T}_{aj}$ and called it *tensorial chemical potential*. This tensor has the property

$$\tilde{\boldsymbol{\nu}}_{bj} := \boldsymbol{\nu}_{bj} - \boldsymbol{\nu}_{Nk} = \tilde{\psi}_{bj}\mathbf{I} - \frac{1}{\rho_{bj}}\tilde{\mathbf{T}}_{bj}, \tag{5.21}$$

which allows for writing

$$\begin{aligned}&\textstyle\sum_j \sum_b \Big\{\tilde{\mathbf{T}}_{bj} + \rho_{bj}(g_{bj} - \tilde{\psi}_{bj})\mathbf{I}\Big\} : \mathrm{grad}(\boldsymbol{u}_{bj}) \\ &= \textstyle\sum_j \sum_b \Big\{\rho_{bj}(g_{bj}\mathbf{I} - \tilde{\boldsymbol{\nu}}_{bj})\Big\} : \mathrm{grad}(\boldsymbol{u}_{bj}).\end{aligned} \tag{5.22}$$

If $\mathrm{grad}(\boldsymbol{u}_{bj})$ is no constitutive variable, equality (5.22) implies that $g_{bj}\mathbf{I} = \tilde{\boldsymbol{\nu}}_{bj}$ for all values of b and j. Analogously, if neither $\mathrm{grad}(\boldsymbol{v}_S)$ nor $\mathrm{grad}(\boldsymbol{w}_{FS})$ is a constitutive variable, we conclude that

$$\mathbf{T}_S + \mathbf{T}_F = -p\mathbf{I} + \left(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\right)\mathbf{F}_A^{-T}\mathbf{F}^T, \quad \mathbf{T}_F = -\phi_F p\mathbf{I}. \tag{5.23}$$

In order to look for further implications, let us start with the fluid phase. For this phase, the relation $\mathbf{T}_F = \sum_a \mathbf{T}_{aF}$ is valid. Thus, using Bowen's definition, we get

$$-\phi_F p\mathbf{I} = \rho_F \psi_F \mathbf{I} - \textstyle\sum_b \rho_{bF}\tilde{\boldsymbol{\nu}}_{bF} - \rho_F \boldsymbol{\nu}_{NF}. \tag{5.24}$$

Moreover, since $\tilde{\boldsymbol{\nu}}_{bF} = g_{bF}\mathbf{I}$, we conclude that $\boldsymbol{\nu}_{NF}$ is an isotropic tensor, indeed:

$$\boldsymbol{\nu}_{NF} = G_F\mathbf{I} - \textstyle\sum_b \omega_{bF}\tilde{\boldsymbol{\nu}}_{bF} = (G_F - \sum_b \omega_{bF} g_{bF})\mathbf{I}. \tag{5.25}$$

Finally, further use of Bowen's definition leads to conclude that $\boldsymbol{\nu}_{bF}$ is also isotropic, indeed

$$\boldsymbol{\nu}_{bF} = \tilde{\boldsymbol{\nu}}_{bF} + \boldsymbol{\nu}_{NF} = \boldsymbol{\nu}_{NF} + g_{bF}\mathbf{I} = (G_F - \textstyle\sum_{d=0}^{N-1}\omega_{dF}g_{dF})\mathbf{I} + g_{bF}\mathbf{I}. \tag{5.26}$$

It also follows that $\boldsymbol{\nu}_{aF} = \mu_{aF}\mathbf{I}$, where μ_{aF} is said to be the chemical potential of the constituent $\mathscr{C}_{aF}$. Consequently, all tensors $\mathbf{T}_{aF}$ are isotropic. Let us now look at the solid phase. Since

$$\mathbf{T}_S = \textstyle\sum_a \mathbf{T}_{aS} = -\phi_S p\mathbf{I} + \rho_S \dfrac{\partial\psi_S}{\partial\mathbf{F}_E}\mathbf{F}_A^{-T}\mathbf{F}^T, \tag{5.27}$$

use of Bowen's definition yields

$$\begin{aligned} \boldsymbol{\nu}_{NS} &= (G_S - \textstyle\sum_{b=0}^{N-1}\omega_{bS}g_{bS})\mathbf{I} - \dfrac{\partial\psi_S}{\partial\mathbf{F}_E}\mathbf{F}_A^{-T}\mathbf{F}^T, & (5.28)\\ \boldsymbol{\nu}_{bS} &= (G_S - \textstyle\sum_{d=0}^{N-1}\omega_{ds}g_{ds})\mathbf{I} + g_{bS}\mathbf{I} - \dfrac{\partial\psi_S}{\partial\mathbf{F}_E}\mathbf{F}_A^{-T}\mathbf{F}^T. & (5.29) \end{aligned}$$

Since all $\boldsymbol{\nu}_{aS}$ have the same non-spherical part, we rewrite them as

$$\boldsymbol{\nu}_{aS} = \mu_{aS}\mathbf{I} - \frac{\partial\psi_S}{\partial\mathbf{F}_E}\mathbf{F}_A^{-T}\mathbf{F}^T, \tag{5.30}$$

where μ_{aS} is the chemical potential of $\mathscr{C}_{aS}$. Moreover, we obtain $\tilde{\boldsymbol{\nu}}_{bj} = \tilde{\mu}_{bj}\mathbf{I} = g_{bj}\mathbf{I}$, with $\tilde{\mu}_{bj} := \mu_{bj} - \mu_{Nk}$. This means that g_{bj} equals the relative chemical potential of $\mathscr{C}_{bj}$. Chemical potentials are required to satisfy the relation $G_j = \sum_a \omega_{aj}\mu_{aj}$. Based on the results above, and assuming negligibility of the terms containing the square of relative velocities, we obtain the following form of the residual dissipation

$$\begin{aligned} \tilde{\mathrm{D}}_{\mathrm{res}} &= -\rho_F\boldsymbol{q}_F\cdot\boldsymbol{w}_{FS} - \textstyle\sum_j\sum_b \rho_{bj}\boldsymbol{q}_{bj}\cdot\boldsymbol{u}_{bj} & (5.31)\\ &\quad +\boldsymbol{\Pi}:\boldsymbol{\Lambda} + \boldsymbol{\Delta}:\mathbf{V} + \textstyle\sum_n \mathrm{N}_n\mathrm{D}_S\zeta_n \\ &\quad +\textstyle\sum_a \rho_{aS}r_{aS}(\mu_{aF} - \mu_{aS}) \\ &\quad +\textstyle\sum_a \rho_{aS}\gamma_{aS}(\mathrm{A}_{aS} + \psi_{aS} - \mu_{aS}) \geq 0, \end{aligned}$$

where we have set $\overset{g}{\underset{aS}{\Psi}} = \gamma_{aS}\mathrm{A}_{aS}$ (A_{aS} is an energy supply of constituent $\mathscr{C}_{aj}$, which vanishes if there is no growth), and introduced the dissipative forces $\rho_F\boldsymbol{q}_F$ and $\rho_{bj}\boldsymbol{q}_{bj}$, i.e.

$$\begin{aligned} \rho_F\boldsymbol{q}_F &:= \rho_F\boldsymbol{m}_F - p\,\mathrm{grad}(\phi_F), & (5.32)\\ \rho_{bj}\boldsymbol{q}_{bj} &:= \mathbf{T}_{Nk}\mathrm{grad}(\tfrac{\omega_{bj}}{\omega_{Nk}}) - \mathrm{grad}[\rho_{bj}(\tilde{\mu}_{bj} - \tilde{\psi}_{bj})] \\ &\quad +\rho_{bj}\tilde{\boldsymbol{m}}_{bj} + \rho_{bj}\mathrm{grad}(\tilde{\mu}_{bj}). \end{aligned}$$

5.3 Study of the residual dissipation inequality

Equation (5.31) collects all dissipative processes taken into account in the formulated problem. The first two terms on the right-hand side represent the dissipation due to fluid filtration through the porous medium and diffusion of species, respectively. Analogously to $\rho_F \boldsymbol{q}_F$ and $\rho_{bj}\boldsymbol{q}_{bj}$, the fields $\mathbf{\Pi}$, $\mathbf{\Delta}$ and N_n are generalized forces conjugate to the generalized velocities $\mathbf{\Lambda}$, $\mathbf{V}$ and $\mathrm{D}_S\zeta_n$, which describe growth, mass transfer and reorientation of fibers. The last two terms on the right-hand side of (5.31) have an analogous structure: the rates of mass production (or depletion) r_{aS} and γ_{aS} are associated with the force-like quantities $\rho_{aS}(\mu_{aF} - \mu_{aS})$ and $\rho_{aS}(\mathrm{A}_{aS} + \psi_{aS} - \mu_{aS})$.

If the external actions $\mathbf{Z}^{\mathrm{ext}}$ and $\mathbf{Y}^{\mathrm{ext}}$ were zero, their internal counterparts $\mathbf{Z}^{\mathrm{int}}$ and $\mathbf{Y}^{\mathrm{int}}$ would vanish too because of the field equations :

$$\mathbf{Y}^{\mathrm{int}} = \mathbf{Y}^{\mathrm{ext}}, \quad \mathbf{Z}^{\mathrm{int}} = \mathbf{Z}^{\mathrm{ext}}, \quad \mathrm{R}_n^{\mathrm{int}} = \mathrm{R}_n^{\mathrm{ext}} \tag{5.33}$$

moreover $\mathbf{\Pi}$ and $\mathbf{\Delta}$ would be equal to Mandel-like stress tensors, as prescribed by (5.15) and (5.16) (6, 95).

Recently, an attempt to study the dissipation inequality (5.31) by means of the Pericak-Spektor&Spector decomposition (76) was illustrated in (2). In this study, tensors $\mathbf{\Lambda}$ and $\mathbf{V}$ (denoted $\mathbf{L}_g$ and $\mathbf{L}_t$ with the formalism of (2)) were related with $\mathbf{\Pi}$ and $\mathbf{\Delta}$ (denoted by $\mathbf{H}_g$ and $\mathbf{H}_t$ in (2)). In the present paper, however, we follow a different path. We assume that $\mathbf{\Delta}$ and $\mathbf{\Pi}$ have the same symmetry as the Mandel stress, and look for thermodynamic restrictions only for the tensors $\mathrm{sym}(\mathbf{C\Lambda})$ and $\mathrm{sym}(\mathbf{CV})$. A motivation for following this path is outlined in (6).

Assuming $\mathbf{\Delta}$ and $\mathbf{\Pi}$ to have the same symmetry as the Mandel stress means requiring $\mathbf{C}^{-1}\mathbf{\Pi} = \mathbf{\Pi}^T\mathbf{C}^{-1}$ and $\mathbf{C}^{-1}\mathbf{\Delta} = \mathbf{\Delta}^T\mathbf{C}^{-1}$, where $\mathbf{C} = \mathbf{F}_E^T\mathbf{F}_E$. If this is the case, the product $\mathbf{\Pi} : \mathbf{\Lambda}$ can be rewritten as $\mathbf{C}^{-1}\mathbf{\Pi} : \mathrm{sym}(\mathbf{C\Lambda})$. Therefore, by using the abbreviations $\bar{\mathbf{\Pi}} = \mathbf{C}^{-1}\mathbf{\Pi}$, and $\bar{\mathbf{\Lambda}} = \mathrm{sym}(\mathbf{C\Lambda})$, we conclude that $\mathbf{\Pi} : \mathbf{\Lambda} = \bar{\mathbf{\Pi}} : \bar{\mathbf{\Lambda}}$. Furthermore, we can write the following relation

$$\mathbf{\Pi} : \mathbf{\Lambda} = \bar{\mathbf{\Pi}} : \bar{\mathbf{\Lambda}} = \tfrac{1}{3}\mathrm{tr}(\mathbf{\Pi})\mathrm{tr}(\mathbf{\Lambda}) + \overline{\mathbf{\Pi}'} : \overline{\mathbf{\Lambda}'}, \tag{5.34}$$

where we have set $\overline{\mathbf{\Pi}'} = \mathbf{C}^{-1}\mathbf{\Pi}'$ and $\overline{\mathbf{\Lambda}'} = \mathrm{sym}(\mathbf{C\Lambda}')$, with $\mathbf{\Pi}' = \mathrm{dev}(\mathbf{\Pi})$ and $\mathbf{\Lambda}' = \mathrm{dev}(\mathbf{\Lambda})$. Analogous considerations hold true also for the product $\mathbf{\Delta} : \mathbf{V}$.

5.3.1 Force-like quantities and their conjugate generalized velocities

The expression of residual dissipation can be written as the sum of terms, each of which is the scalar product of a force-like quantity multiplied by its conjugate generalized velocity. The purpose of this section is to identify the force-like quantities, their conjugate velocities, and discuss how dissipation is studied.

By using (5.34) and the constraints $\rho_S \mathrm{tr}(\mathbf{\Lambda}) = \rho_S \gamma_S = \sum_a \rho_{aS} \gamma_{aS}$ and $\rho_S \mathrm{tr}(\mathbf{V}) = \rho_S r_S = \sum_a \rho_{aS} r_{aS}$, we can rewrite the residual dissipation as

$$\begin{aligned}\mathrm{D}_{\mathrm{res}} \;=\;& -\rho_F \boldsymbol{q}_F \cdot \boldsymbol{w}_{FS} - \textstyle\sum_j \sum_b \rho_{bj} \boldsymbol{q}_{bj} \cdot \boldsymbol{u}_{bj} + \sum_n \mathrm{N}_n \mathrm{D}_S \zeta_n \\ & + \textstyle\sum_a \rho_{aS} \gamma_{aS} (\mathrm{A}_{aS} + \psi_{aS} - \mu_{aS} + \frac{\mathrm{tr}(\mathbf{\Pi})}{3\rho_S}) + \overline{\mathbf{\Pi}'} : \overline{\mathbf{\Lambda}'} \\ & + \textstyle\sum_a \rho_{aS} r_{aS} (\mu_{aF} - \mu_{aS} + \frac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}) + \overline{\mathbf{\Delta}'} : \overline{\mathbf{V}'} \geq 0.\end{aligned} \tag{5.35}$$

According to the study of dissipation provided by (78), we can define force-like quantities and their conjugate generalized velocities. The force-like quantities are given by

$$\Upsilon = \{-\rho_F \boldsymbol{q}_F, -\rho_{bj} \boldsymbol{q}_{bj}, \mathrm{N}_n, y_{aS}, \overline{\mathbf{\Pi}'}, s_{aS}, \overline{\mathbf{\Delta}'}\}, \tag{5.36}$$

where

$$y_{aS} = \rho_{aS} (\mathrm{A}_{aS} + \psi_{aS} - \mu_{aS} + \tfrac{\mathrm{tr}(\mathbf{\Pi})}{3\rho_S}), \tag{5.37}$$

$$s_{aS} = \rho_{aS} (\mu_{aF} - \mu_{aS} + \tfrac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}), \tag{5.38}$$

whereas the conjugate velocities are

$$\mathrm{X} = \{\boldsymbol{w}_{FS}, \boldsymbol{u}_{bj}, \mathrm{D}_S \zeta_n, \gamma_{aS}, \overline{\mathbf{\Lambda}'}, r_{aS}, \overline{\mathbf{V}'}\}. \tag{5.39}$$

The expression of residual dissipation can thus be put in the compact form $\mathrm{D}_{\mathrm{res}} = \Upsilon \cdot \mathrm{X} \geq 0$. Depending on the phenomena that have to be characterized, there are several possible methods to explore this inequality. A discussion on this subject can be found, for example, in (78). If coupled phenomena are excluded, the simplest approach to the dissipation inequality relies on the fact that requiring each summand of (5.35) to be non-negative is sufficient to ensure that $\mathrm{D}_{\mathrm{res}}$ is non-negative too.

We remark that, at this stage, excluding coupled phenomena from our treatment of the dissipation inequality is due to our ignorance about the physical meaning and modeling assumptions necessary for discussing couplings among completely different thermodynamic processes. Unlike thermodiffusion (a phenomenon leading to the Soret and Dufour effects (99, 113, 131), in which the diffusion of chemical species in dilute solutions couples with diffusion of heat), a field in which an extensive literature is available, there is –to our knowledge– no measurement of the coupling between, e.g., fluid motion and growth, or diffusion of species and reorientation of fibers. We cannot claim from the outset that such couplings do not exist, but we should be cautious in establishing relations just on the basis of formal analogies with different, though to a certain extent similarly modeled, physical phenomena. There are also some technical issues to be considered. Indeed, the study of coupling effects is based, in the case of thermodiffusion, on the assumption that Onsager's relations are valid. This is easy when the dissipation inequality has a "simple" form, which, in turn, might be too restrictive for the phenomena presented in our manuscript. For these reasons, we prefer to consider a simpler approach, in which no coupling is considered, and each summand of the dissipation inequality is viewed as an entity on its own, which should be non-negative.

5.3.2 Reorientation of fibers

The purpose of this section is to determine differential equations that define the evolution of the variables $\{\zeta\}_{n=1}^{\mathrm{I}}$ (cf. (5.41)). Our result is reported in (5.48), and consists in identifying the variables $\{\zeta\}_{n=1}^{\mathrm{I}}$ with the parameters that specify the probability density distribution with which the fibers are distribution in the solid phase.

Let us now consider the term describing the reorientation of fibers, i.e. $\sum_n \mathrm{N}_n \mathrm{D}_S \zeta_n$, and assume that, for each n, the product $\mathrm{N}_n \mathrm{D}_S \zeta_n$ is non-negative. Several possible hypotheses may be advocated in order to extract information from this requirement. In any case, the inequality $\mathrm{N}_n \mathrm{D}_S \zeta_n \geq 0$ should be studied jointly with the "non-standard" equation of motion $(5.33)_3$, which, by virtue of (5.17), can be now reformulated as $\mathrm{N}_n = -(\rho_S \frac{\partial \psi_S}{\partial \zeta_n}) + \mathrm{R}_n^{\mathrm{ext}}$. If we restrict our investigation to the case in which the extra-force N_n is obtainable from a constitutive relation involving $\mathrm{D}_S \zeta_n$, and in addition require this relation to be linear, we arrive at

$$\mathrm{N}_n = \overset{c}{\mathrm{N}}_n(\ldots, \mathrm{D}_S \zeta_n) = \overset{c}{\mathrm{N}}{}_n^0(\ldots) \mathrm{D}_S \zeta_n \tag{5.40}$$

where the superimposed "c" stands for "constitutive", and the dots mean that $\overset{c}{\mathrm{N}}_n$ and $\overset{c}{\mathrm{N}}{}_n^0$ may depend on all constitutive variables that need not vanish when dissipation is zero. Note that $\overset{c}{\mathrm{N}}{}_n^0(\ldots)$ has to be positive. By plugging (5.40) into the the non-standard equation of motion $(5.33)_3$, written with $\mathrm{N}_n = \overset{c}{\mathrm{N}}_n$, we find

$$\overset{c}{\mathrm{N}}{}_n^0(\ldots) \mathrm{D}_S \zeta_n = -\left(\rho_S \frac{\partial \psi_S}{\partial \zeta_n}\right) + \mathrm{R}_n^{\mathrm{ext}}. \tag{5.41}$$

This result slightly generalizes the presentation of the theory proposed by Olsson and Klarbring (126) for fiber reorientation in arteries. Their equation is retrieved in the monophasic case by letting $\overset{c}{\mathrm{N}}{}_n^0$ reduce to a positive constant, viewing the variables ζ_n as the angles that identify the direction of fibers in space, and taking the Helmholtz free energy function ψ_S as in the Holzapfel-Gasser-Ogden model (117), i.e. as the superposition of an isotropic contribution ψ_m due to the matrix, and an anisotropic contribution ψ_f due to the fibers, where

$$\psi_m = k_0(I_1 - 3), \quad \psi_f = \tfrac{k_1}{2k_2}[\mathrm{e}^{k_2(I_4-1)^2} + \mathrm{e}^{k_2(I_6-1)^2} - 2], \tag{5.42}$$

where k_0, k_1 and k_2 are material parameters, $I_1 = \mathrm{tr}(\mathbf{C})$, $I_4 = \mathrm{tr}(\mathbf{CA}_1)$ and $I_6 = \mathrm{tr}(\mathbf{CA}_2)$ are invariants, with $\mathbf{C} = \mathbf{F}_E^T\mathbf{F}_E$ being the Cauchy-Green stretch tensor in the intermediate configuration, and $\mathbf{A}_1$ and $\mathbf{A}_2$ the fabric tensors of two families of fibers. In (5.42), the free energy of the matrix and fibers, ψ_m and ψ_f, are assumed to provide, respectively, the isotropic and anisotropic contributions to the overall energy. As noticed for Darcy's and Fick's laws, the path followed here for modeling the reorientation of fibers is by no means the most general. Nevertheless, it is proposed only because it is believed to have some possible reliability in biological context (for example, in modeling arteries), where the external force $\mathrm{R}_n^{\mathrm{ext}}$ determines a target direction along which fibers align in response to mechanical stress (115, 126).

The model discussed above considers a deterministic distribution of fibers. More generally, however, fibers are oriented according to some normalized probability distribution

$$\wp : \mathbb{S}_X^2 \to \mathbb{R}_0^+, \qquad \int_{\mathbb{S}_X^2} \wp(\boldsymbol{M})\mathrm{d}S = 1, \tag{5.43}$$

which defines the probability to find, at a given material point X, a fiber aligned along the direction $\boldsymbol{M}$. Here, the unit vector $\boldsymbol{M}$ and the unit sphere $\mathbb{S}_X^2$ are thought to be associated with the intermediate configuration of the solid phase. By extending the superposition method (117) to a continuous infinity of families of fibers (102)(104)(107), it is possible to construct the Helmholtz free energy density of the solid phase on the basis of (5.43), i.e.

$$\rho_S\psi_S(\mathbf{C}, \{\zeta_n\}_{n=1}^{\mathrm{I}}) = \rho_m\psi_m(\mathbf{C}) + \rho_f\psi_f(\mathbf{C}, \{\zeta_n\}_{n=1}^{\mathrm{I}}), \tag{5.44}$$

with

$$\psi_f(\mathbf{C}, \{\zeta_n\}_{n=1}^{\mathrm{I}}) = \int_{\mathbb{S}_X^2} \wp(\boldsymbol{M}, \{\zeta_n\}_{n=1}^{\mathrm{I}})\Psi_f(\mathbf{C}, \mathbf{A}(\boldsymbol{M}))\mathrm{d}S. \tag{5.45}$$

According to (5.45), ψ_f results from the superposition of the continuous infinity of families of fibers, each with energy Ψ_f depending on the structure tensor $\mathbf{A} = \boldsymbol{M}\otimes\boldsymbol{M}$, and weighted by the probability density distribution $\wp$, whose dependence on the parameters $(\zeta_n)_{n=1}^{\mathrm{I}}$ is now written explicitly. In the case of a transversely isotropic material, $\wp$ can be taken as (102, 103)

$$\wp(\vartheta, \{\zeta_n\}_{n=1}^{\mathrm{I}}) = \frac{g(\vartheta, \{\zeta_n\}_{n=1}^{\mathrm{I}})}{\int_0^{2\pi} \left[\int_0^{\pi/2} g(\vartheta', \{\zeta_n\}_{n=1}^{\mathrm{I}}) \sin(\vartheta') \mathrm{d}\vartheta' \right] \mathrm{d}\varphi'}, \tag{5.46}$$

where ϑ and φ are the colatitude and longitude (with respect to the axis of transverse isotropy), respectively, and g is a non-normalized probability distribution (103). If, for example, the distribution g is assumed to be gaussian, i.e.

$$g(\vartheta, \Theta, \lambda) = \exp\left(- \frac{(\vartheta - \Theta)^2}{2\lambda^2} \right), \tag{5.47}$$

the set of parameters describing fiber reorientation comprises two elements: the mean angle $\zeta_1 = \Theta$ and the variance $\zeta_2 = \lambda$. Furthermore, if we assume that the variance is constant, substitution of (5.43) and (5.47) in (5.41) leads to the following model of fiber reorientation

$$\begin{aligned} \overset{c}{\mathrm{N}}{}^0_\Theta(\ldots)\mathrm{D}_S \Theta &= -\rho_f \frac{\partial \psi_f}{\partial \Theta} + \mathrm{R}^{\mathrm{ext}}_\Theta \\ &= -\rho_f \frac{\partial}{\partial \Theta} \int_{\mathbb{S}^2_X} \wp(\boldsymbol{M}, \Theta, \lambda) \Psi_f(\mathbf{C}, \mathbf{A}(\boldsymbol{M})) \mathrm{d}S + \mathrm{R}^{\mathrm{ext}}_\Theta . \end{aligned} \tag{5.48}$$

This means that the properties of the material depend on the evolution of Θ. Of course, a limitation of the proposed approach is that the probability distribution $\wp$ is regarded as given and, above all, it is presumed that its functional form does not vary. A further generalization of this model is still subject of our current investigation. Moreover, an exhaustive formulation of the theory of remodeling for statistical composites is for us "work in progress" at the moment.

We remark that (5.48) has been obtained under the strong assumption that the dissipation inequality is satisfied independently for each remodeling parameter. This does not mean, however, that there exists no coupling among different remodeling parameters. Indeed, each of these parameters has to be determined by solving an equation of the type $(5.33)_3$. The set formed by all these equations is coupled because each coefficient $\overset{c}{\mathrm{N}}{}^0_n$, the energy ψ_S and the external force $\mathrm{R}^{\mathrm{ext}}_n$ may depend, in general, on the whole list of remodeling parameters. An even more general approach could have been obtained by relaxing the hypothesis, leading to (5.41) and to (5.48), that each term of the sum $\sum_n \mathrm{N}_n \mathrm{D}_S \zeta_n$ is non-negative. Indeed, one may need the less restrictive assumption that each dissipative force N_n depends (linearly) on the whole set of generalized velocities $\{\mathrm{D}_S \zeta_m\}_{m=1}^{\mathrm{I}}$. This can be accounted for by admitting the existence of coupling coefficients $\overset{c}{\mathrm{N}}{}^{0}_{nm}$, such that (6.7) becomes $\overset{c}{\mathrm{N}}_{n}(\ldots,\{\mathrm{D}_S\zeta_m\}_{m=1}^{\mathrm{I}}) = \sum_m \overset{c}{\mathrm{N}}{}^{0}_{nm}(\ldots)\mathrm{D}_S\zeta_m$. Substituting this relation into the dissipation inequality (5.31) yields

$$\sum_{nm} \overset{c}{\mathrm{N}}{}^{0}_{nm}(\ldots)\mathrm{D}_S\zeta_m\mathrm{D}_S\zeta_n \geq 0, \tag{5.49}$$

which is respected by requiring that the coefficients $\overset{c}{\mathrm{N}}{}^{0}_{nm}(\ldots)$ form a symmetric, positive semi-definite matrix. Consequently, Equation (5.41) should be replaced by the more general one $\sum_m \overset{c}{\mathrm{N}}{}^{0}_{nm}(\ldots)\mathrm{D}_S\zeta_m = -(\rho_S \frac{\partial\psi_S}{\partial\zeta_n}) + \mathrm{R}_n^{\mathrm{ext}}$, which constitutes a system of differential equations coupled in the generalized velocities $\{\mathrm{D}_S\zeta_n\}_{n=1}^{\mathrm{I}}$ as well as in the unknown functions $\{\zeta_n\}_{n=1}^{\mathrm{I}}$. Of course, also in this case, information about the non-diagonal coefficients $\overset{c}{\mathrm{N}}{}^{0}_{nm}$ (with $n \neq m$) should be supplied. In our manuscript, we prefer however to follow a less general approach.

5.3.3 Mass transfer and growth

The scope of this section is to determine expressions for the transformed rates $\bar{\mathbf{V}}$ and $\bar{\mathbf{\Lambda}}$ that are in harmony with the non-standard dynamics and the dissipation inequality. Our results are reported in (5.53) and (5.60).

Let us consider mass transfer. We require the products $r_{aS}\,s_{aS}$ and $\overline{\mathbf{\Delta}'} : \overline{\mathbf{V}'}$ to be non-negative independently on one another. The inequalities $r_{aS}\,s_{aS} \geq 0$ and $\overline{\mathbf{\Delta}'} : \overline{\mathbf{V}'} \geq 0$ have to be studied consistently with the equation of motion $(5.33)_1$ for the "non-standard" degree of freedom $\mathbf{K}$, which, in view of (5.16), can be now rewritten as

$$\mathbf{\Delta} = \mathbf{F}_E^T\Big(\rho_S \frac{\partial\psi_S}{\partial\mathbf{F}_E}\Big) + \mathbf{G}^{-T}\mathbf{Y}^{\mathrm{ext}}\mathbf{K}^T\mathbf{G}^T. \tag{5.50}$$

Since $\mathbf{Y}^{\mathrm{ext}}$, an external force, is given from the outset and the first term on the right-hand side of (5.50) is provided by a constitutive law, the study of the dissipation inequality has to supply information about $\mathbf{\Delta}$. In order to extract this information, we classify $s_{aS} = s_{aS}^0 + \rho_{aS}\frac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}$, with $s_{aS}^0 = \rho_{aS}(\mu_{aF} - \mu_{aS})$, and $\overline{\mathbf{\Delta}'}$ as dissipative force-like fields, which should be related to their conjugate velocity-like quantities r_{aS} and $\overline{\mathbf{V}'}$. To this end, we follow here a much less general approach: we prescribe $s_{aS}r_{aS}$ and $\overline{\mathbf{\Delta}'} : \overline{\mathbf{V}'}$ to be quadratic forms of r_{aS} and $\overline{\mathbf{V}'}$, respectively, and determine s_{aS} and $\overline{\mathbf{\Delta}'}$ as constitutive functions of r_{aS} and $\overline{\mathbf{V}'}$. Furthermore, by requiring these functions to be invertible, we express r_{aS} and $\overline{\mathbf{V}'}$ as functions of s_{aS} and $\overline{\mathbf{\Delta}'}$, respectively. The first relation is $r_{aS} = R_{aS}\,s_{aS}$, with non-negative R_{aS}, for all a. Relations of this type have been proposed in (18, 130). As above, each R_{aS} is allowed to depend on all constitutive variables that need not vanish when dissipation is zero. By multiplying by ρ_{aS}, adding over all

a, and bearing in mind that $\sum_a \rho_{aS} r_{aS} = \rho_S r_S$ and $r_S = \mathrm{tr}(\mathbf{V})$ (cf. $\mathrm{tr}(\mathbf{\Lambda}) = \gamma_s, \quad \mathrm{tr}(\mathbf{V}) = r_s$), we obtain

$$\mathrm{tr}(\mathbf{V}) = \textstyle\sum_a \frac{\rho_{aS} R_{aS}}{\rho_S} s_{aS} = \sum_a \frac{\rho_{aS} R_{aS}}{\rho_S} [s^0_{aS} + \rho_{aS} \frac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}]. \tag{5.51}$$

Analogously, studying the product $\overline{\mathbf{\Delta}'} : \overline{\mathbf{V}'}$ in (5.35), we postulate that $\overline{\mathbf{V}'}$ is constitutively determined, and require it to be expressed through the relation

$$\overline{\mathbf{V}'} = \hat{\mathbb{T}} : \overline{\mathbf{\Delta}'}, \tag{5.52}$$

where $\hat{\mathbb{T}}$ is a positive-definite, full-symmetric fourth-order tensor, which is constructed in such a way to fulfill the condition $\mathrm{tr}(\mathbf{V}') = 0$ or, equivalently, $\mathrm{tr}[\mathbf{C}^{-1}(\hat{\mathbb{T}} : \overline{\mathbf{\Delta}'})] = 0$. Tensor $\hat{\mathbb{T}}$ may depend on all variables that are not necessarily zero for vanishing dissipation. We can now determine $\bar{\mathbf{V}} = \mathrm{sym}(\mathbf{C}\mathbf{V})$ by using the results (5.51) and (5.52), i.e.

$$\begin{aligned} \bar{\mathbf{V}} &= \tfrac{\mathrm{tr}(\mathbf{V})}{3}\mathbf{C} + \mathrm{sym}(\mathbf{C}\mathbf{V}') \\ &= \frac{1}{3}\Big\{\textstyle\sum_a \frac{\rho_{aS} R_{aS}}{\rho_S} [s^0_{aS} + \rho_{aS} \frac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}]\Big\}\mathbf{C} + \hat{\mathbb{T}} : (\mathbf{C}^{-1}\mathbf{\Delta}'). \end{aligned} \tag{5.53}$$

Finally, since $\mathbf{V} = \mathbf{G}(\mathrm{D}_S\mathbf{K})\mathbf{K}^{-1}\mathbf{G}^{-1}$, we obtain

$$\begin{aligned} &\mathrm{sym}[\mathbf{C}\mathbf{G}(\mathrm{D}_S\mathbf{K})\mathbf{K}^{-1}\mathbf{G}^{-1}] \\ &= \frac{1}{3}\Big\{\textstyle\sum_a \frac{\rho_{aS} R_{aS}}{\rho_S} [s^0_{aS} + \rho_{aS} \frac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S}]\Big\}\mathbf{C} + \hat{\mathbb{T}} : (\mathbf{C}^{-1}\mathbf{\Delta}'). \end{aligned} \tag{5.54}$$

We conclude that the evolution of $\mathbf{K}$ is coupled with $\mathbf{G}$, and should comply with (5.54). Another consideration concerns the splitting of $\mathbf{V}$ into a spherical and non-spherical part. Only the spherical one, proportional to r_S, determines the variation of mass of the solid phase in response to exchange interactions with the fluid phase. The non-spherical part of $\mathbf{V}$, on the other hand, is responsible for *remodeling* the internal structure of the solid. However, let us now set $\mathbf{\Delta}' = \mathbf{0}$. In Mixture Theory (cf., for example, (18)), it is said that the mass exchange between the phases of a multi-constituent mixture ceases when the Gibbesean condition holds true, i.e. when $\mu_{aF} = \mu_{aS}$, for all a. Our model is able to retrieve the Gibbsean result when the additional requirement $\mathrm{tr}(\mathbf{\Delta}) = 0$ is satisfied, i.e. when the spherical part of the dissipative contribution of the field $\mathbf{Y}^{\mathrm{ext}}\mathbf{K}^T$ is zero. However, when this is not the case, our model proposes the weaker condition $s^0_{aS} = 0$ or, equivalently

$$\mu_{aF} - \mu_{aS} + \tfrac{\mathrm{tr}(\mathbf{\Delta})}{3\rho_S} = 0, \quad \forall a, \tag{5.55}$$

which means that, in the non-dissipative situation, the spherical part of $\boldsymbol{\Delta}$ opens a "gap" among chemical potentials. As remarked in (2), if the external force $\mathbf{Y}^{\text{ext}}$ were zero (which implies that $\mathbf{Y}^{\text{int}} = 0$ by virtue of $(5.33)_1$), $\boldsymbol{\Delta}$ would equal the Mandel-like stress tensor $\mathbf{F}_E^T(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E})$, and (5.55) would become

$$\mu_{aF} - \mu_{aS} + \tfrac{1}{3\rho_S}\mathrm{tr}\Big[\mathbf{F}_E^T\Big(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\Big)\Big] = 0, \quad \forall a. \tag{5.56}$$

Since the Mandel stress needs not vanish when the dissipation is zero, our model would be unable to reproduce the Gibbsean result if the force $\mathbf{Y}^{\text{ext}}$ were zero from the outset.

Also for growth, we require the products $y_{aS}\gamma_{aS}$ and $\overline{\boldsymbol{\Pi}'} : \overline{\boldsymbol{\Lambda}'}$ to be non-negative independently on one another. Again, the inequalities $\gamma_{aS}y_{aS} \geq 0$ and $\overline{\boldsymbol{\Pi}'} : \overline{\boldsymbol{\Lambda}'} \geq 0$ have to be studied consistently with the equation of motion $(5.33)_2$ for the "non-standard" degree of freedom $\mathbf{G}$, which, in view of (5.15), can be now rewritten as

$$\boldsymbol{\Pi} = \mathbf{F}_E^T\Big(\rho_S \frac{\partial \psi_S}{\partial \mathbf{F}_E}\Big) + \mathbf{Z}^{\text{ext}}\mathbf{G}^T. \tag{5.57}$$

As for mass transfer, $\mathbf{Z}^{\text{ext}}$ is regarded as known from the outset, and the dissipation inequality is investigated for extracting information about $\boldsymbol{\Pi}$. In this case, the dissipative force-like fields are $\overline{\boldsymbol{\Pi}'}$ and $y_{aS} = y_{aS}^0 + \rho_{aS}\frac{\mathrm{tr}(\boldsymbol{\Pi})}{3\rho_S}$, with $y_{aS}^0 = \rho_{aS}(\mathrm{A}_{aS} + \psi_{aS} - \mu_{aS})$. Here, the term A_{aS} is regarded as given, while ψ_{aS} and μ_{aS} are determined constitutively. By following the same reasoning done for studying mass transfer, we express γ_{aS} and $\overline{\boldsymbol{\Lambda}'}$ as functions of y_{aS} and $\overline{\boldsymbol{\Pi}'}$, respectively. The first relation is $\gamma_{aS} = \Gamma_{aS}y_{aS}$, with non-negative Γ_{aS}, for all a. As above, each Γ_{aS} is allowed to depend on all constitutive variables that need not vanish when dissipation is zero. By multiplying by ρ_{aS}, adding over all a, and bearing in mind that $\sum_a \rho_{aS}\gamma_{aS} = \rho_S\gamma_S$ and $\gamma_S = \mathrm{tr}(\boldsymbol{\Lambda})$ (cf. $\mathrm{tr}(\boldsymbol{\Lambda}) = \gamma_s, \quad \mathrm{tr}(\mathbf{V}) = r_s$), we obtain

$$\mathrm{tr}(\boldsymbol{\Lambda}) = \textstyle\sum_a \frac{\rho_{aS}\Gamma_{aS}}{\rho_S} y_{aS} = \sum_a \frac{\rho_{aS}\Gamma_{aS}}{\rho_S}[y_{aS}^0 + \rho_{aS}\frac{\mathrm{tr}(\boldsymbol{\Pi})}{3\rho_S}]. \tag{5.58}$$

Analogously, studying the product $\overline{\boldsymbol{\Pi}'} : \overline{\boldsymbol{\Lambda}'}$ in (5.35), we postulate that $\bar{\boldsymbol{\Lambda}}$ is constitutively determined, and require it to be expressed through the relation

$$\overline{\boldsymbol{\Lambda}'} = \hat{\mathbb{G}} : \overline{\boldsymbol{\Pi}'}, \tag{5.59}$$

where $\hat{\mathbb{G}}$ is a positive-definite, full-symmetric fourth-order tensor such that $\mathrm{tr}(\boldsymbol{\Lambda}') = 0$ or, equivalently, $\mathrm{tr}[\mathbf{C}^{-1}(\hat{\mathbb{G}} : \overline{\boldsymbol{\Pi}'})] = 0$. On account of (5.58) and (5.59), tensor $\bar{\boldsymbol{\Lambda}} = \mathrm{sym}(\mathbf{C}\boldsymbol{\Lambda})$ reads

$$\begin{aligned} \bar{\boldsymbol{\Lambda}} &= \tfrac{\mathrm{tr}(\boldsymbol{\Lambda})}{3}\mathbf{C} + \mathrm{sym}(\mathbf{C}\boldsymbol{\Lambda}') \\ &= \frac{1}{3}\Big\{\textstyle\sum_a \frac{\rho_{aS}\Gamma_{aS}}{\rho_S}[y_{aS}^0 + \rho_{aS}\frac{\mathrm{tr}(\boldsymbol{\Pi})}{3\rho_S}]\Big\}\mathbf{C} + \hat{\mathbb{G}} : \overline{\boldsymbol{\Pi}'}. \end{aligned} \tag{5.60}$$

We remark that, since growth should be made possible by the availability of nutrients (which can be identified with some of the constituents of the phases), it has been proposed that growth occurs only when the concentration of nutrients exceeds a given threshold (85, 109). This is modeled by assuming that the coefficients Γ_{aS} and $\hat{\mathbb{G}}$ contain a function of the type

$$f(\omega_{aS}) = -\frac{\omega_{aS} - \omega_{a0}}{1 - \omega_{a0}} H(\omega_{aS} - \omega_{a0}), \tag{5.61}$$

where ω_{a0} is a threshold value, and $H(\,\cdot\,)$ is the Heaviside function.

Chapter 6

Growth and Remodeling of a Soft Tissue in the presence of Chemical Agents

In this Chapter we adapt the model for growth and remodeling in elastic arteries put forward by Olsson and Klarbring (126) to the case of a multi-constituent solid in the presence of chemical agents.

6.1 Equations to be solved

It is necessary to solve the following equations, which are written in material form:

1. Equations of motion

$$\mathrm{Div}(\mathbf{P}) = \mathbf{0}, \tag{6.1}$$

2. Mass balance of a chemical agent

$$\mathrm{Div}(J_g \varrho_n \mathbf{F}^{-1} \mathbf{D} \mathbf{F}^{-T} \mathrm{Grad}(\omega)) - a J_g \varrho_n \omega = 0, \quad r > 0, \tag{6.2}$$

3. Evolution equation of the growth tensor $\mathbf{F}_g$

$$\dot{\mathbf{F}}_g = \mathbf{L}_g \mathbf{F}_g. \tag{6.3}$$

In order to simplify the problem, we shall assume:

- cylindrical symmetry and $\mathbf{F} = \mathrm{Diag}\{\varphi'(R), R^{-1}\varphi(R), 1\}$,

- that the growth tensor is diagonal $\mathbf{F}_g = \mathrm{Diag}\{\gamma_1, \gamma_2, \gamma_3\}$.

Moreover, we shall assume that the material is elastically incompressible, so that the admissible deformations are those which satisfy the contraint

$$\det(\mathbf{F}) = \det(\mathbf{F}_g) \quad \Rightarrow \quad \varphi'(R)\frac{\varphi(R)}{R} = \gamma(R) \quad \Rightarrow \quad \varphi'(R) = \frac{\gamma(R)R}{\varphi(R)}, \tag{6.4}$$

where $\gamma := J_g = \det(\mathbf{F}_g)$. By integrating this constraint it is possible to find the following closed form for the deformation

$$r = \varphi(t, R) = \left[\int_{R_0}^{R} 2A\gamma(A)\mathrm{d}A + K(t) \right]^{1/2}. \tag{6.5}$$

6.2 Stress

The energy of the incompressible material, measured per unit volume of the intermediate configuration, is given by

$$W_n(\mathbf{C}_e) = \frac{\mu}{2}\{\mathrm{tr}(\mathbf{C}_e) - 3\}. \tag{6.6}$$

Therefore, the first Piola-Kirchhoff stress tensor is determined by the relation

$$\begin{aligned} \mathbf{P} &= J_g \mathbf{P}_n (\mathbf{F}_g)^{-T} = J_g \mathbf{F}_e \mathbf{S}_n (\mathbf{F}_g)^{-T} \\ &= -J_g p \mathbf{F}^{-T} + J_g \mathbf{F}(\mathbf{F}_g)^{-1} \mu \{\mathbf{G}^{-1} - \tfrac{1}{3}\mathrm{tr}(\mathbf{C}_e)\mathbf{B}_e\}(\mathbf{F}_g)^{-T}. \end{aligned} \tag{6.7}$$

In order to obtain this expression the following steps have been employed: decomposition of the deformation gradient tensor $\mathbf{F} = \mathbf{F}_e\mathbf{F}_g$, the fact that the metric tensor $\mathbf{G}$ remains unchanged when passing from the reference to the intermediate configuration (this saves a lot of work). The tensor $\mathbf{P}$ has to satisfy the following equation:

$$\frac{\partial P^{rR}}{\partial R} + \frac{P^{rR} - P^{\vartheta\Theta}}{R} = 0. \tag{6.8}$$

6.3 Relations and known parameters

In order to solve the problem, it is necessary to account for the following relations

$$\begin{aligned}
\mathbf{P} &= J_g \mathbf{P}_n (\mathbf{F}_g)^{-T} = J_g \mathbf{F}_e \mathbf{S}_n (\mathbf{F}_g)^{-T} && (6.9)\\
&= -J_g p \mathbf{g}^{-1} \mathbf{F}^{-T} + J_g \mathbf{F} (\mathbf{F}_g)^{-1} \mu \{\mathbf{G}^{-1} - \tfrac{1}{3} \mathrm{tr}(\mathbf{C}_e) \mathbf{B}_e\} (\mathbf{F}_g)^{-T}, \quad \mathbf{F}_e = \mathbf{F}(\mathbf{F}_g)^{-1}, \\
W_n &= \frac{\mu}{2} \{\mathrm{tr}[\mathbf{C}_e] - 3\}, && (6.10)\\
J_g &= \det(\mathbf{F}_g), && (6.11)\\
\mathbf{L}_g &= \frac{3\ell_g + 2m_g}{3} \frac{1}{3} \mathrm{tr}\Big[\mathbf{C}_e \mathbf{S}_n + \mathbf{Y}_n\Big] \mathbf{I} + 2m_g \mathrm{Dev}\Big(\mathbf{C}_e \mathbf{S}_n + \mathbf{Y}_n\Big). && (6.12)
\end{aligned}$$

Moreover, the following parameters are assumed to be given from the outset:

$$\mathscr{P} = \{\varrho_n, a, \mu, \ell_g, m_g\}. \tag{6.13}$$

The tensor $\mathbf{Y}_n$ is assumed to be given too (although it needs not be a constant). It might turn out to be necessary to play with the signs of the coefficients of this tensor in order to obtain physical results.

It is also necessary to impose boundary conditions for φ (actually for the pressure, in the case of elastically incompressible material) and for ω as well as initial conditions for $\{\gamma_1, \gamma_2, \gamma_3\}$.

6.4 Dissipation

The dissipation measured per unit volume of the intermediate configuration reads

$$D_n = \left[\frac{1}{2} \mathbf{S}_n - \frac{\partial W_n}{\partial \mathbf{C}_e}\right] : \dot{\mathbf{C}}_e + (\mathbf{C}_e \mathbf{S}_n + \mathbf{Y}_n) : \mathbf{L}_g \geq 0 \tag{6.14}$$

Under the assumption of Neo-Hookean material,

$$W_n = \frac{\mu}{2} \{\mathrm{tr}(\mathbf{C}_e) - 3\}, \tag{6.15}$$

we obtain, as consequence of the incompressibility constraint, the following expression for the second Piola-Kirchhoff stress tensor:

$$\mathbf{S}_n = -p \mathbf{B}_e + \mu \{\mathbf{G}^{-1} - \tfrac{1}{3} \mathrm{tr}(\mathbf{C}_e) \mathbf{B}_e\}, \tag{6.16}$$

where $\mathbf{B}_e = (\mathbf{C}_e)^{-1}$. Thus, the residual dissipation becomes

$$D_n = (\mathbf{C}_e \mathbf{S}_n + \mathbf{Y}_n) : \mathbf{L}_g \geq 0. \tag{6.17}$$

From (6.16) it follows that the first Piola-Kirchhoff stress tensor, when measured with respect to the intermediate (natural) configuration, is given by $\mathbf{P}_n = \mathbf{F}_e\mathbf{S}_n$, and that $\mathbf{P}$ becomes

$$\begin{aligned} \mathbf{P} &= J_g\mathbf{P}_n(\mathbf{F}_g)^{-T} = J_g\mathbf{F}_e\mathbf{S}_n(\mathbf{F}_g)^{-T} \qquad (6.18) \\ &= -J_g p\mathbf{g}^{-1}\mathbf{F}^{-T} + J_g\mathbf{F}(\mathbf{F}_g)^{-1}\mu\{\mathbf{G}^{-1} - \tfrac{1}{3}\mathrm{tr}(\mathbf{C}_e)\mathbf{B}_e\}(\mathbf{F}_g)^{-T}. \end{aligned}$$

The quantity $\mathrm{tr}(\mathbf{C}_e)$ is given by

$$\mathrm{tr}(\mathbf{C}_e) = \frac{\gamma_2^2\gamma_3^2R^2}{r^2} + \frac{r^2}{\gamma_2^2R^2} + \frac{1}{\gamma_3^2} = \frac{\gamma_2^4\gamma_3^4R^4 + \gamma_3^2r^4 + \gamma_2^2r^2R^2}{r^2R^2\gamma_2^2\gamma_3^2} \qquad (6.19)$$

Relevant components of $\mathbf{P}$:

$$\begin{aligned} P^{rR} &= -\frac{r}{R}p + \mu\frac{2\gamma_2^4\gamma_3^4R^5 - \gamma_3^2r^4R - \gamma_2^2r^2R^3}{3rR^4\gamma_2^2\gamma_3^2}, \qquad (6.20) \\ P^{\vartheta\Theta} &= -\gamma\frac{R}{r}p + \mu\gamma\frac{2\gamma_3^2r^4 - \gamma_2^4\gamma_3^4R^4 - \gamma_2^2r^2R^2}{3r^3R\gamma_2^2\gamma_3^2}. \qquad (6.21) \end{aligned}$$

Diffusion equation:

$$\frac{\partial}{\partial R}\left\{\frac{D(t,R)[\varphi(t,R)]^2}{\gamma(t,R)R}\frac{\partial\omega}{\partial R}(t,R)\right\} - aR\gamma(t,R)\omega(t,R) = 0. \qquad (6.22)$$

Pressure and deformed radius

$$\begin{aligned} p(R) &= -\frac{R}{\varphi(R)}\ell(R) + h(R), \qquad (6.23) \\ \varphi(R) &= \sqrt{\int_{R_{in}}^{R} 2A\gamma(A)\mathrm{d}A + K}, \qquad (6.24) \\ \gamma(R) &:= \gamma_1(R)\gamma_2(R)\gamma_3(R), \qquad (6.25) \\ \ell(R) &:= \mathrm{e}^{-\int_{R_{in}}^{R} q(A)\mathrm{d}A}\int_{R_{in}}^{R} Q(A)h(A)\mathrm{e}^{\int_{R_{in}}^{A} q(B)\mathrm{d}B}\mathrm{d}A, \qquad (6.26) \\ q(R) &:= \frac{[\varphi(R)]^2 - \gamma(R)R^2}{R[\varphi(R)]^2}, \qquad (6.27) \\ Q(R) &:= q(R)\frac{\varphi(R)}{R} = \frac{[\varphi(R)]^2 - \gamma(R)R^2}{R^2\varphi(R)}, \qquad (6.28) \end{aligned}$$

$$h(R) := \frac{[\gamma(R)]^2 R^2}{[\gamma_1(R)]^2[\varphi(R)]^2} S_d^{RR}(R) - \frac{R}{\varphi(R)}[P_{in}^{rR} + \eta(R)], \tag{6.29}$$

$$\eta(R) := \int_{R_{in}}^{R} \left\{ \frac{\gamma(A)\varphi(A)}{[\gamma_2(A)]^2 A^2} S_d^{\Theta\Theta}(A) - \frac{[\gamma(A)]^2}{[\gamma_1(A)]^2 \varphi(A)} S_d^{RR}(A) \right\} \mathrm{d}A, \tag{6.30}$$

$$P_{in}^{rR} := -\lambda_{in} \frac{\varphi(R_{in})}{R_{in}}, \tag{6.31}$$

$$S_d^{RR}(R) := \mu \left\{ 1 - C_e(R) \frac{[\gamma_1(R)]^2 [\varphi(R)]^2}{[\gamma(R)]^2 R^2} \right\}, \tag{6.32}$$

$$S_d^{\Theta\Theta}(R) := \mu \left\{ 1 - C_e(R) \frac{[\gamma_2(R)]^2 R^2}{[\varphi(R)]^2} \right\}, \tag{6.33}$$

$$C_e(R) := \frac{[\gamma_2(R)]^4 [\gamma_3(R)]^4 R^4 + [\gamma_3(R)]^2 [\varphi(R)]^4 + [\gamma_2(R)]^2 R^2 [\varphi(R)]^2}{3[\gamma_2(R)]^2 [\gamma_3(R)]^2 R^2 [\varphi(R)]^2}, \tag{6.34}$$

where $C_e \equiv \frac{1}{3}\mathrm{tr}(\mathbf{C}_e)$. The functional form of p and φ is specified by (6.23) and (6.24), respectively. However, these functions are defined up the unknown K, which has to be determined by solving the following auxiliary problem:

$$\lambda_{in} = \frac{R_{in}}{\varphi(R_{in})} \int_{R_{in}}^{R_{out}} Q(R) p(R) \mathrm{d}R + \frac{R_{in}}{\varphi(R_{in})} \eta(R_{out}). \tag{6.35}$$

Equation (6.1) determines K.

Parameters:
$\{R_{in} = 1\,\mathrm{mm}, R_{out} = 2\,\mathrm{mm}, \lambda_{in} = 10\mathrm{kPa} = 10 \cdot 10^{-3}\,\mathrm{N} \cdot \mathrm{mm}^{-2}, \mu = 36\,\mathrm{kPa} = 36 \cdot 10^{-3}\,\mathrm{N} \cdot \mathrm{mm}^{-2}\}$.

Remark: Every quantity featuring in these equations (except, of course, for the underformed radial coordinate R) does depend on time. The dependence has been written explicitly just for ease of notation.

Concentration

$$\frac{\partial}{\partial R}\left[R\Delta(R) \frac{\partial \omega}{\partial R}(R) \right] - aR\gamma(R)\omega(R) = 0, \tag{6.36}$$

$$\Delta(R) = \frac{[\varphi(R)]^2}{R^2} \frac{D(R)}{\gamma(R)}, \tag{6.37}$$

$$D(R) = D_0. \tag{6.38}$$

Boundary conditions: $\omega(R_{in}) = \omega_{in} = 0.001$; $\omega(R_{out}) = \omega_{out} = 0.002$.

Parameters: $\{D_0 = 10^{-9}\,\mathrm{m}^2\mathrm{s}^{-1}, a = 10^{-3}\,\mathrm{s}^{-1}\}$.

Remark: Every quantity featuring in these equations (except, of course, for the underformed radial coordinate R) does depend on time. The dependence has been written explicitly just for ease of notation.

Growth tensor

$$\begin{aligned} \dot{\gamma}_1(t,R) &= L_{gRR}(t,R)\gamma_1(t,R), && (6.39)\\ \dot{\gamma}_2(t,R) &= L_{g\Theta\Theta}(t,R)\gamma_2(t,R), && (6.40)\\ \dot{\gamma}_3(t,R) &= L_{gZZ}(t,R)\gamma_3(t,R), && (6.41) \end{aligned}$$

$$\begin{aligned} L_{gRR}(t,R) &= k_g\Omega(t,R) + 2m_g Z_{RR}(t,R), && (6.42)\\ L_{g\Theta\Theta}(t,R) &= k_g\Omega(t,R) + 2m_g Z_{\Theta\Theta}(t,R), && (6.43)\\ L_{gZZ}(t,R) &= k_g\Omega(t,R) + 2m_g Z_{ZZ}(t,R), && (6.44) \end{aligned}$$

$$\begin{aligned} \Omega(t,R) &= \frac{M^{RR}(t,R) + M^{\Theta\Theta}(t,R) + M^{ZZ}(t,R)}{3}, && (6.45)\\ Z_{RR}(t,R) &= \frac{2M^{RR}(t,R) - M^{\Theta\Theta}(t,R) - M^{ZZ}(t,R)}{3}, && (6.46)\\ Z_{\Theta\Theta}(t,R) &= \frac{-M^{RR}(t,R) + 2M^{\Theta\Theta}(t,R) - M^{ZZ}(t,R)}{3}, && (6.47)\\ Z_{ZZ}(t,R) &= \frac{-M^{RR}(t,R) - M^{\Theta\Theta}(t,R) + 2M^{ZZ}(t,R)}{3}, && (6.48) \end{aligned}$$

$$\begin{aligned} M^{RR}(t,R) &= -p(t,R) + \frac{[\gamma(t,R)]^2R^2}{[\gamma_1(t,R)]^2[\varphi(t,R)]^2}S_d^{RR}(t,R) + Y_n^{RR}(t,R), && (6.49)\\ M^{\Theta\Theta}(t,R) &= -p(t,R) + \frac{[\varphi(t,R)]^2}{[\gamma_2(t,R)]^2R^2}S_d^{\Theta\Theta}(t,R) + Y_n^{\Theta\Theta}(t,R), && (6.50)\\ M^{ZZ}(t,R) &= -p(t,R) + \frac{1}{[\gamma_3(t,R)]^2}S_d^{ZZ}(t,R) + Y_n^{ZZ}(t,R). && (6.51) \end{aligned}$$

Initial conditions:

$$\gamma_1(0,R) = \gamma_{10}(R) = 1.5, \quad \gamma_2(0,R) = \gamma_{20}(R) = 1.2, \quad \gamma_3(0,R) = \gamma_{30}(R) = 1. \qquad (6.52)$$

Parameters: $\{k_g = 0.0036\ \mathrm{s}^{-1}\mathrm{N}^{-1}\mathrm{mm}^2, m_g = 0.0024\ \mathrm{s}^{-1}\mathrm{N}^{-1}\mathrm{mm}^2\}$.

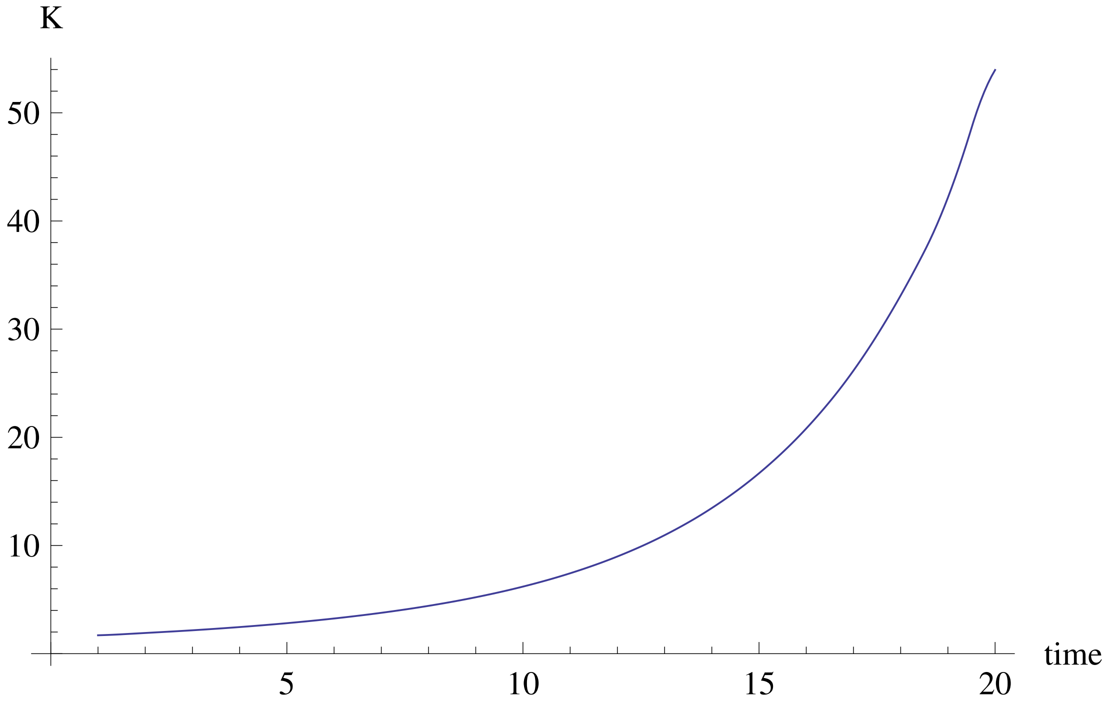

Figure 6.1: evolution of K in 20 time steps -

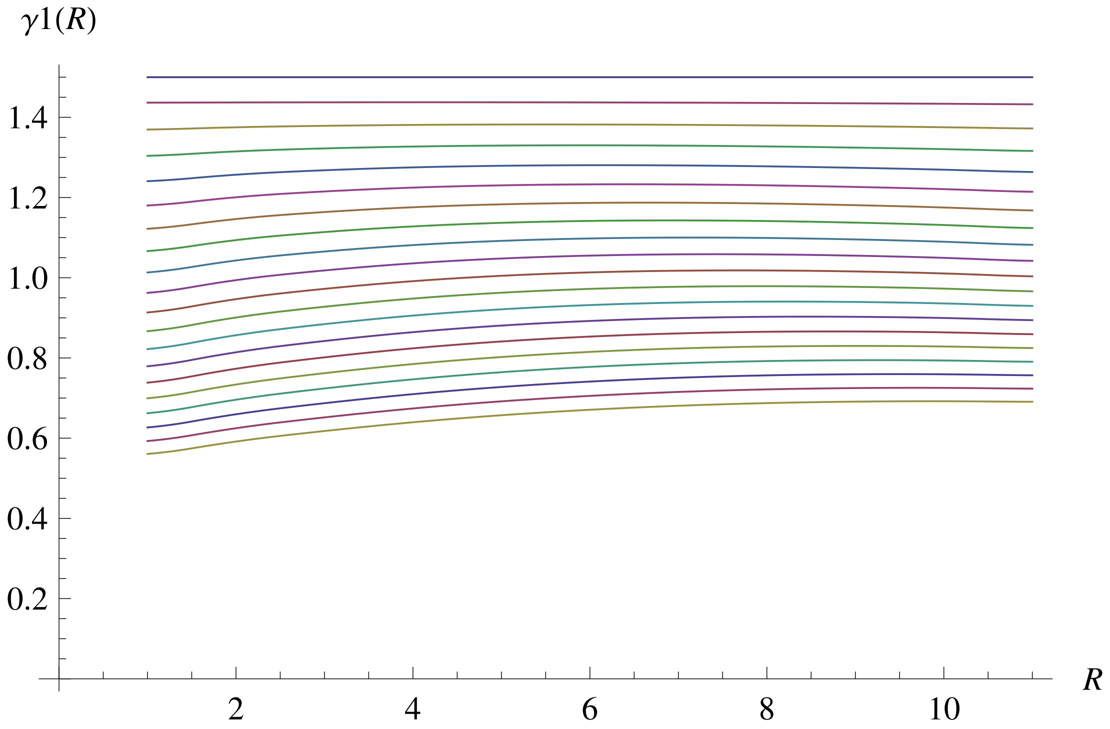

Figure 6.2: γ_1 as function of R -

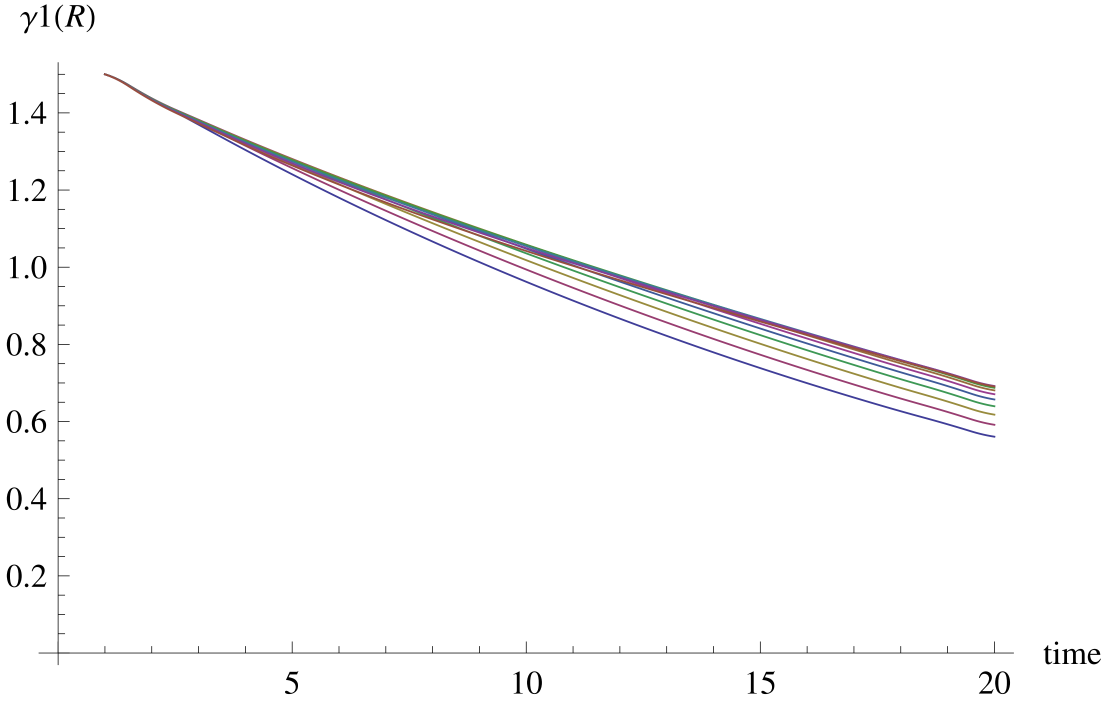

Figure 6.3: evolution of γ_1 in 20 steps of time -

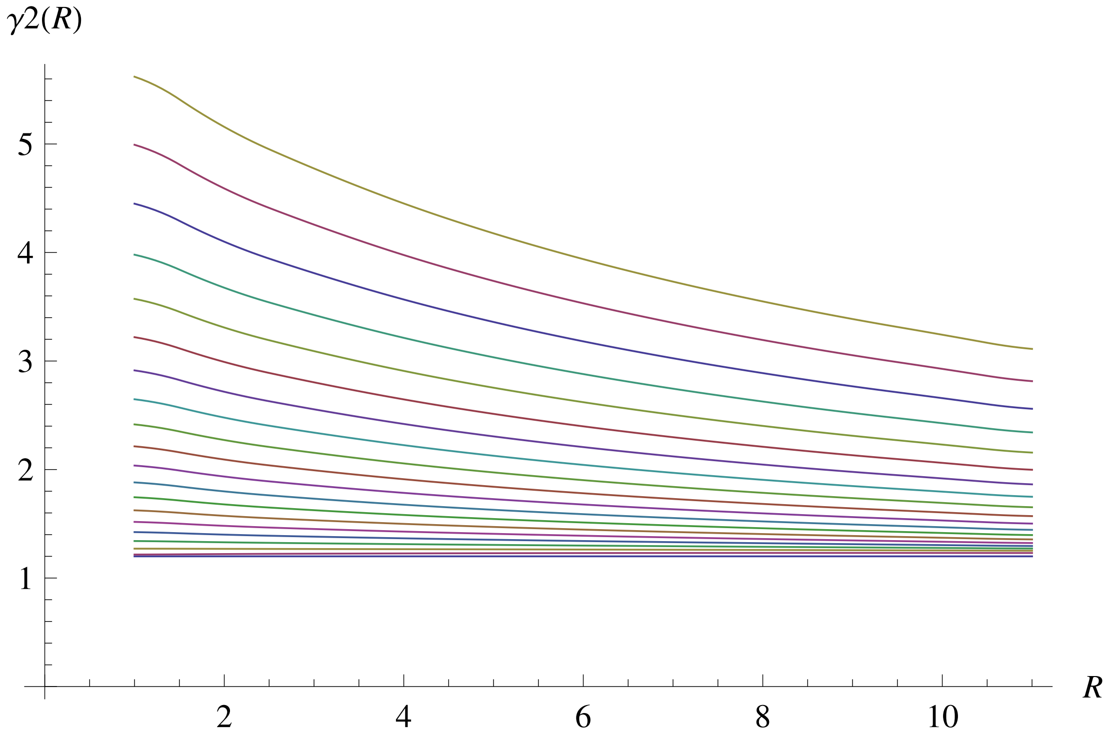

Figure 6.4: γ_2 as function of R -

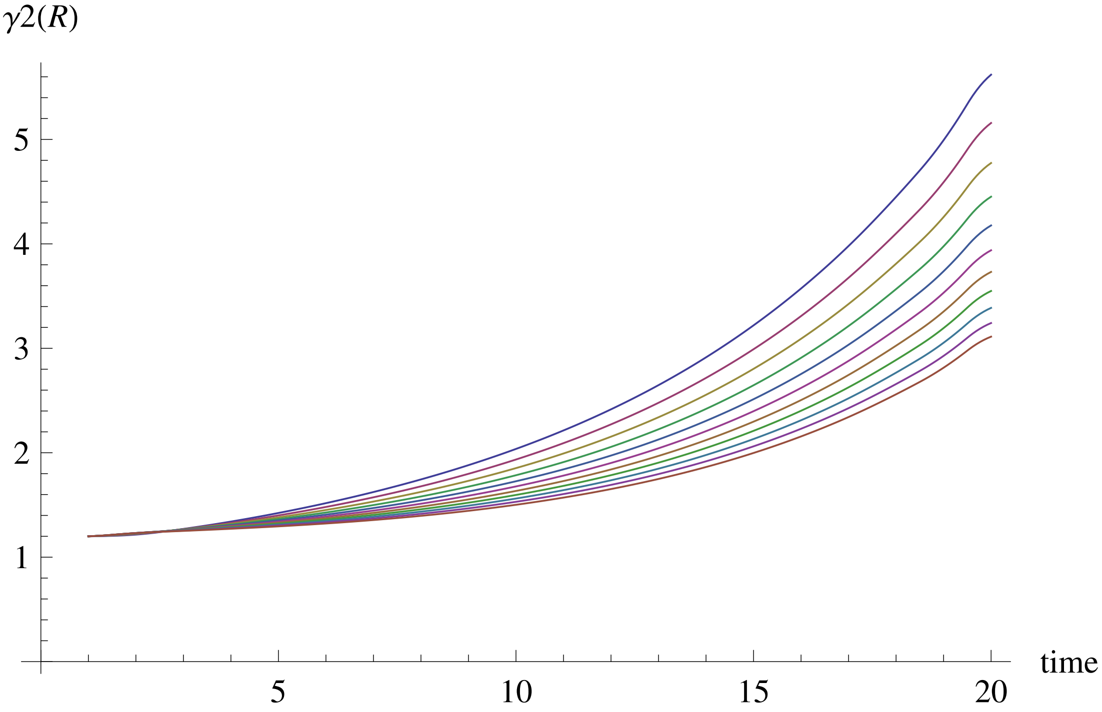

Figure 6.5: evolution of γ_2 in 20 steps of time -

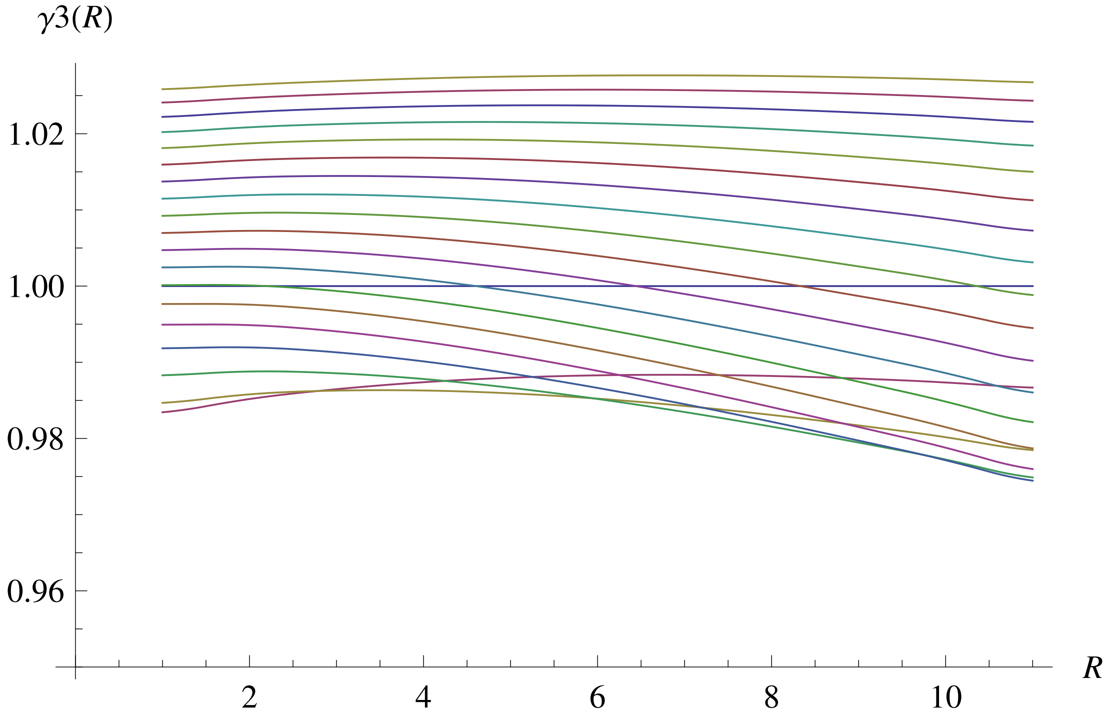

Figure 6.6: γ_3 **as function of R -**

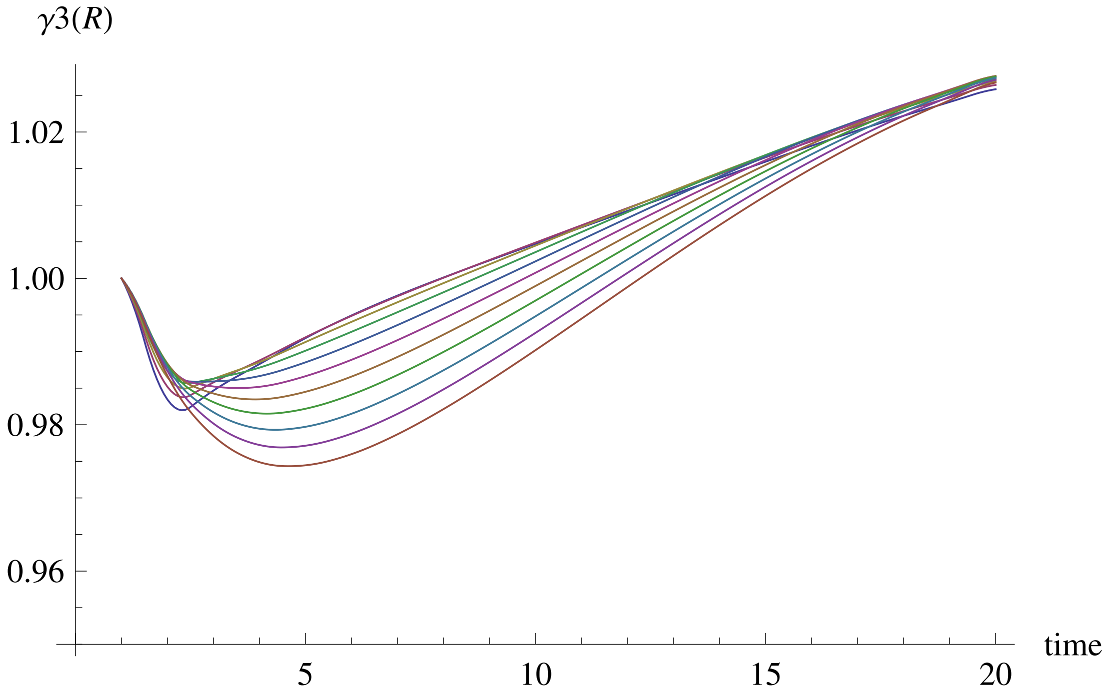

Figure 6.7: evolution of γ_3 **in 20 steps of time -**

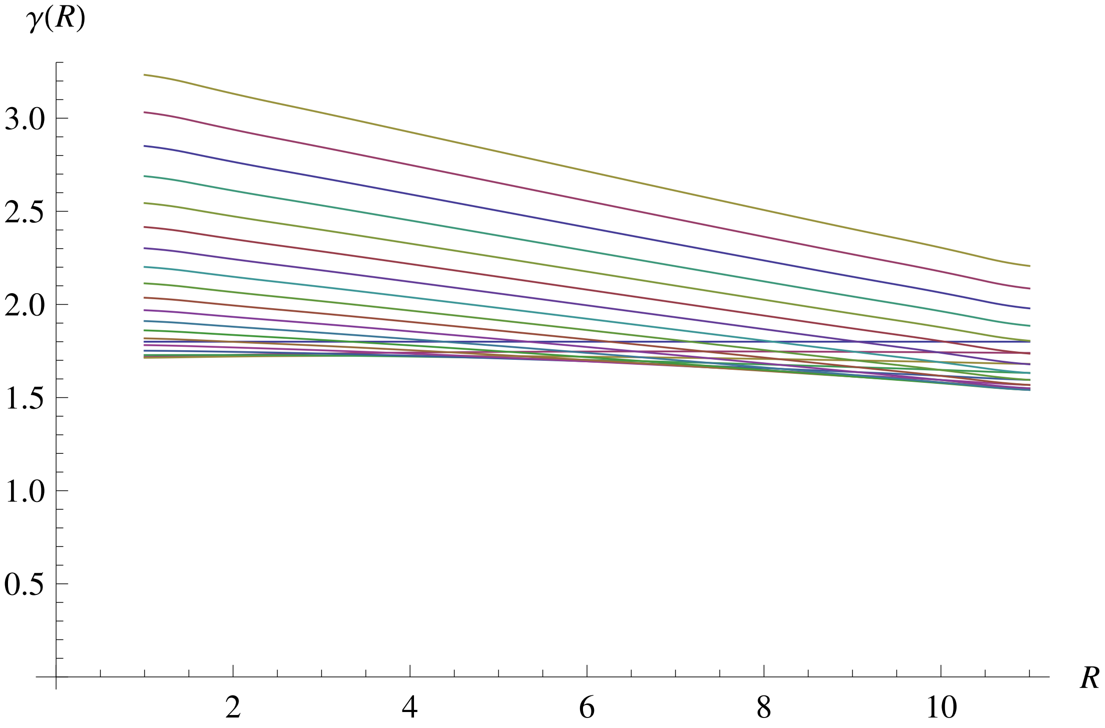

Figure 6.8: γ **as function of R -**

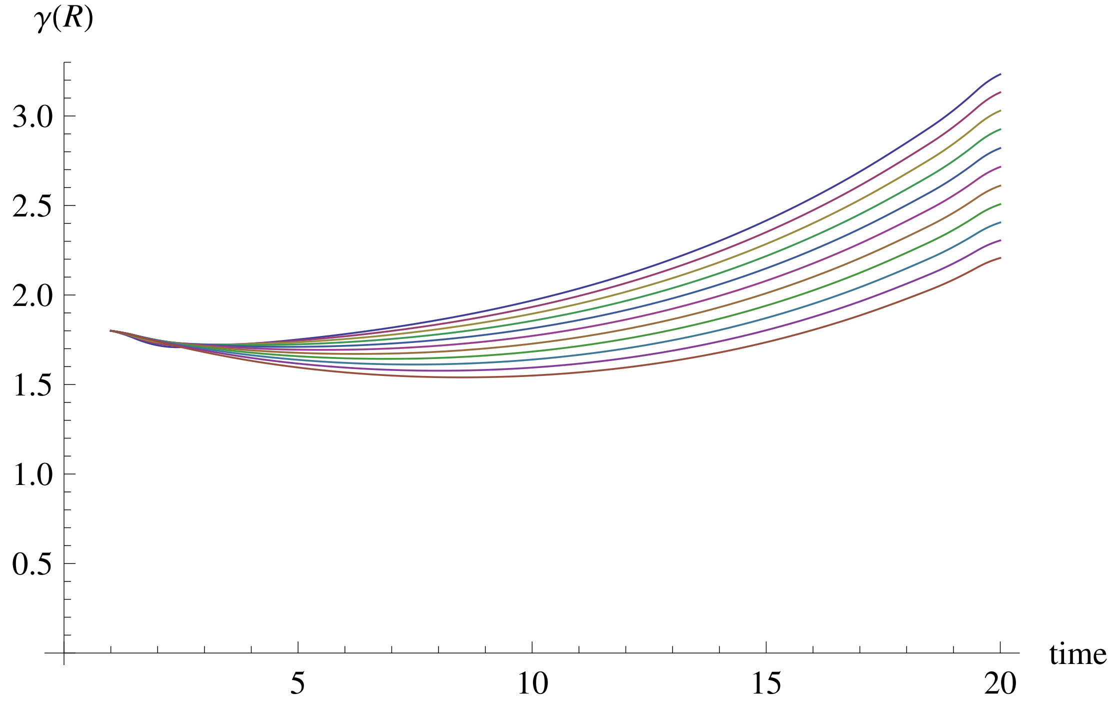

Figure 6.9: evolution of γ in 20 steps of time -

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